Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


# Raw Data of Thermochemical Calculations

EXPLO 5 (v. 6.04)

# Calculations Number 1-26 Were Conducted for <u>Promoter-free</u> [EMIM][$BH_3CN$] and Hydrogen Peroxide (conc. 95%) Bipropellant System

(The enthalpy of formation value for [EMIM][$BH_3CN$] fuel was adopted from Zhang, Q.; Yin, P.; Zhang, J.; Shreeve, J. M., *Chem. Eur. J.* **2014**, *20(23)*, 6909-6914)

# Calculation Number 1

**Combustion conditions (Number 1):**

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Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 50.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 35.00 %**
3. **Water ($H_2O$, liquid), 15.00 %**

C(1,057) H(3,812) N(0,453) O(1,318) B(0,151)

Molecular weight = 45,61
Oxygen balance = -102,7224 %
Enthalpy of formation = -3588,06 kJ/kg
Internal energy of formation = -3384,54 kJ/kg

Parameters in combustion chamber:

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- Heat of isobaric combustion = -2341,92 kJ/kg
- Total enthalpy of combustion prod. = -3588,06 kJ/kg
- Entropy of combustion products = 11,86 kJ/K kg
- Isobaric combustion temperature = 1335,88 K
- Mole number of gaseous products = 59,54 mol/kg expl.
- Total mole number of products = 61,079 mol/kg expl.
- Volume of gaseous products (at SATP) = 1475,95 L/kg expl.
- Mass of gaseous products = 892,9 g/kg expl.
- Mass of condensed products = 107,1 g/kg expl.
- Mean molecular mass of gaseous prod. = 14,997 g
- Mean molecular mass of all products = 16,372 g
- Density of products = 10,585 kg/m3
- Specific gas constant = 495,02 J/kg K
- Specific heat capacity at p=const. (Cp) = 2503,61 J/kgK
- Specific heat capacity at V=const. (Cv) = 2008,59 J/molK
- Specific heat ratio (Cp/Cv) = 1,2465

Composition of combustion products in chamber (43):

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| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 1,226764E+00 | 2,689947E+01 | 44,0408 | 5,4229 | |
| CO = | 7,639263E-01 | 1,675075E+01 | 27,4249 | 46,9189 | |
| CH4 = | 2,329844E-01 | 5,108691E+00 | | 8,3641 | 8,1959 |
| N2 = | 2,253466E-01 | 4,941216E+00 | 8,0899 | 13,8418 | |
| H2O = | 1,937289E-01 | 4,247930E+00 | | 6,9549 | 7,6528 |
| B2O3(l) = | 7,014285E-02 | 1,538035E+00 | | 2,5181 | 10,7061 |
| CO2 = | 5,932288E-02 | 1,300784E+00 | | 2,1297 | 5,7247 |
| B(OH)3 = | 1,009383E-02 | 2,213292E-01 | | 0,3624 | 1,3685 |
| NH3 = | 2,145855E-03 | 4,705256E-02 | | 0,0770 | 0,0801 |
| BHO2 = | 6,084305E-04 | 1,334117E-02 | | 0,0218 | 0,0584 |
| C2H6 = | 1,698105E-04 | 3,723466E-03 | | 0,0061 | 0,0112 |
| HCN = | 1,435788E-04 | 3,148278E-03 | | 0,0052 | 0,0085 |
| C2H4 = | 1,027545E-04 | 2,253117E-03 | | 0,0037 | 0,0063 |
| CH2O = | 3,142007E-05 | 6,889537E-04 | | 0,0011 | 0,0021 |
| HCNO = | 1,988001E-06 | 4,359127E-05 | | 0,0001 | 0,0002 |
| CH3OH = | 1,495420E-06 | 3,279034E-05 | | 0,0001 | 0,0001 |
| BHO = | 5,361530E-07 | 1,175633E-05 | | 0,0000 | 0,0000 |
| H = | 4,415149E-07 | 9,681177E-06 | 0,0000 | 0,0000 | |
| B2O3 = | 2,355544E-08 | 5,165045E-07 | | 0,0000 | 0,0000 |
| NH2 = | 1,249090E-09 | 2,738903E-08 | | 0,0000 | 0,0000 |
| BO = | 6,372871E-12 | 1,397391E-10 | 0,0000 | 0,0000 | |
| BO2 = | 3,696989E-12 | 8,106455E-11 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| NO = | 2,902710E-12 | 6,364825E-11 | 0,0000 | 0,0000 |
| B2O2 = | 2,782253E-12 | 6,100696E-11 | 0,0000 | 0,0000 |
| BH2 = | 2,129573E-13 | 4,669553E-12 | 0,0000 | 0,0000 |
| CNO = | 4,689697E-14 | 1,028318E-12 | 0,0000 | 0,0000 |
| H2O2 = | 3,450194E-16 | 7,565302E-15 | 0,0000 | 0,0000 |
| C(gr) = | 1,907629E-16 | 4,182893E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,776906E-16 | 3,896254E-15 | 0,0000 | 0,0000 |
| N2O3 = | 1,294385E-16 | 2,838222E-15 | 0,0000 | 0,0000 |
| N = 4,987440E-17 | 1,093605E-15 | 0,0000 | 0,0000 | |
| BN(s) = | 3,752310E-17 | 8,227758E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,429095E-17 | 3,133603E-16 | 0,0000 | 0,0000 |
| BH = 1,558281E-20 | 3,416870E-19 | 0,0000 | 0,0000 | |
| NO2 = | 1,444112E-21 | 3,166532E-20 | 0,0000 | 0,0000 |
| BN = 1,122598E-21 | 2,461541E-20 | 0,0000 | 0,0000 | |
| B(OH)3(s) = | 2,916873E-22 | 6,395880E-21 | 0,0000 | 0,0000 |
| B(s) = | 9,836782E-23 | 2,156929E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,363030E-23 | 7,374177E-22 | 0,0000 | 0,0000 |
| B = 2,148249E-23 | 4,710505E-22 | 0,0000 | 0,0000 | |
| B(l) = | 2,575594E-24 | 5,647552E-23 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(l) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

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- Total enthalpy of combustion prod. = -3963,62 kJ/kg
- Entropy of combustion products = 11,86 kJ/K kg
- Temperature at nozzle throat = 1243,12 K
- Pressure at nozzle throat = 3,864253 MPa
- Mole number of gaseous products = 58,392 mol/kg expl.
- Total mole number of products = 59,944 mol/kg expl.
- Volume of gaseous products (at SATP) = 1447,49 L/kg expl.
- Mass of gaseous products = 892,0 g/kg expl.
- Mass of condensed products = 108,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,276 g
- Mean molecular mass of all products = 16,682 g
- Density of products = 6,403 kg/m3
- Specific gas constant = 485,474 J/kg K
- Specific heat capacity at p=const. (Cp) = 2467,87 J/kgK
- Specific heat capacity at V=const. (Cv) = 1982,39 J/molK
- Specific heat ratio (Cp/Cv) = 1,2449

Characteristic parameters at the nozzle throat:

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- Flow velocity at nozzle throat = 866,7 m/s
- Sound velocity at throat) = 866,8 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,552
- Pressure ratio (pc/pt) = 1,811

Composition of combustion products at nozzle throat:

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| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = 1,165028E+00 | 2,554579E+01 | 42,6163 | 5,1500 | |
| CO = 7,201328E-01 | 1,579048E+01 | 26,3422 | 44,2291 | |
| CH4 = | 2,597575E-01 | 5,695749E+00 | 9,5018 | 9,1377 |
| N2 = 2,256436E-01 | 4,947729E+00 | 8,2540 | 13,8601 | |
| H2O = | 2,044340E-01 | 4,482662E+00 | 7,4781 | 8,0756 |
| CO2 = | 7,660939E-02 | 1,679828E+00 | 2,8023 | 7,3929 |
| B2O3(l) = | 7,074843E-02 | 1,551314E+00 | 2,5880 | 10,7985 |
| B(OH)3 = | 9,232357E-03 | 2,024396E-01 | 0,3377 | 1,2517 |
| NH3 = | 1,630200E-03 | 3,574570E-02 | 0,0596 | 0,0609 |
| BHO2 = | 2,662528E-04 | 5,838173E-03 | 0,0097 | 0,0256 |
| C2H6 = | 1,334131E-04 | 2,925374E-03 | 0,0049 | 0,0088 |
| HCN = | 6,831510E-05 | 1,497958E-03 | 0,0025 | 0,0040 |
| C2H4 = | 5,759747E-05 | 1,262950E-03 | 0,0021 | 0,0035 |

| | | | | |
|---|---|---|---|---|
| CH2O = | 1,723732E-05 | 3,779659E-04 | 0,0006 | 0,0011 |
| HCNO = | 9,741099E-07 | 2,135948E-05 | 0,0000 | 0,0001 |
| CH3OH = | 8,125099E-07 | 1,781605E-05 | 0,0000 | 0,0001 |
| H = | 1,275532E-07 | 2,796882E-06 | 0,0000 | 0,0000 |
| BHO = | 9,643689E-08 | 2,114589E-06 | 0,0000 | 0,0000 |
| B2O3 = | 3,040334E-09 | 6,666595E-08 | 0,0000 | 0,0000 |
| NH2 = | 2,580120E-10 | 5,657476E-09 | 0,0000 | 0,0000 |
| NO = | 4,345167E-13 | 9,527727E-12 | 0,0000 | 0,0000 |
| BO = | 4,135397E-13 | 9,067760E-12 | 0,0000 | 0,0000 |
| BO2 = | 3,249198E-13 | 7,124575E-12 | 0,0000 | 0,0000 |
| B2O2 = | 1,338321E-13 | 2,934560E-12 | 0,0000 | 0,0000 |
| BH2 = | 9,205859E-15 | 2,018585E-13 | 0,0000 | 0,0000 |
| CNO = | 5,268681E-15 | 1,155273E-13 | 0,0000 | 0,0000 |
| N2O3 = | 9,828122E-16 | 2,155030E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,226726E-16 | 4,882582E-15 | 0,0000 | 0,0000 |
| C(gr) = | 1,979589E-16 | 4,340680E-15 | 0,0000 | 0,0000 |
| H2O2 = | 3,674316E-17 | 8,056740E-16 | 0,0000 | 0,0000 |
| BN(s) = | 2,519946E-17 | 5,525532E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,562536E-17 | 3,426201E-16 | 0,0000 | 0,0000 |
| N = | 2,691257E-18 | 5,901168E-17 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,161224E-22 | 4,738956E-21 | 0,0000 | 0,0000 |
| BH = | 1,737522E-22 | 3,809895E-21 | 0,0000 | 0,0000 |
| NO2 = | 6,730809E-23 | 1,475877E-21 | 0,0000 | 0,0000 |
| B(s) = | 5,487940E-24 | 1,203351E-22 | 0,0000 | 0,0000 |
| BN = | 3,802495E-24 | 8,337800E-23 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,325816E-25 | 5,099858E-24 | 0,0000 | 0,0000 |
| B = | 1,696717E-25 | 3,720422E-24 | 0,0000 | 0,0000 |
| B(l) = | 1,684425E-27 | 3,693470E-26 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(l) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

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- Total enthalpy of combustion prod. = -5703,79 kJ/kg
- Entropy of combustion products = 11,86 kJ/K kg
- Temperature at nozzle exit = 878,38 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 51,737 mol/kg expl.
- Total mole number of products = 53,36 mol/kg expl.
- Volume of gaseous products (at SATP) = 1282,51 L/kg expl.
- Mass of gaseous products = 887,0 g/kg expl.
- Mass of condensed products = 113,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,145 g
- Mean molecular mass of all products = 18,741 g
- Density of products = 0,265 kg/m3
- Specific gas constant = 430,141 J/kg K
- Specific heat capacity at p=const. (Cp) = 2284,55 J/kgK
- Specific heat capacity at V=const. (Cv) = 1854,41 J/molK
- Specific heat ratio (Cp/Cv) = 1,232

Characteristic parameters at the nozzle exit:

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- Specific impulse = 209,76 s
- Vacuum-specific impulse (pa=0) = 228,13 s
- Exhaust (or nozzle exit) velocity = 2057,1 m/s
- Characteristic exhaust velocity (c*) = 1261,4 m/s
- Thrust coefficient (Cf) = 1,631
- Nozzle area expansion ratio (Ae/At) = 10,19
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 685,82 m/s
- Mach number at nozzle exit = 2,999

Composition of combustion products at the nozzle exit:

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| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

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| | | | | |
|---|---|---|---|---|
| H2 = 8,608548E-01 | 1,887612E+01 | 35,3752 | 3,8054 | |
| CH4 = 4,140416E-01 | 9,078766E+00 | 17,0143 | 14,5651 | |
| CO = 4,105151E-01 | 9,001440E+00 | 16,8693 | 25,2130 | |
| CO2 = 2,323616E-01 | 5,095035E+00 | 9,5485 | 22,4233 | |
| N2 = 2,263549E-01 | 4,963325E+00 | 9,3016 | 13,9038 | |
| H2O = 2,120811E-01 | 4,650342E+00 | 8,7151 | 8,3777 | |
| B2O3(l) = 7,399483E-02 | 1,622498E+00 | 3,0407 | 11,2940 | |
| B(OH)3 = 2,977118E-03 | 6,527982E-02 | 0,1223 | 0,4036 | |
| NH3 = 2,761729E-04 | 6,055692E-03 | 0,0113 | 0,0103 | |
| C2H6 = 2,328061E-05 | 5,104781E-04 | 0,0010 | 0,0015 | |
| B2O3(s) = 1,366593E-05 | 2,996554E-04 | 0,0006 | 0,0021 | |
| C2H4 = 1,474841E-06 | 3,233910E-05 | 0,0001 | 0,0001 | |
| BHO2 = 1,459797E-06 | 3,200923E-05 | 0,0001 | 0,0001 | |
| HCN = 7,735065E-07 | 1,696082E-05 | 0,0000 | 0,0000 | |
| CH2O = 3,474277E-07 | 7,618110E-06 | 0,0000 | 0,0000 | |
| CH3OH = 1,410741E-08 | 3,093357E-07 | 0,0000 | 0,0000 | |
| HCNO = 1,032104E-08 | 2,263112E-07 | 0,0000 | 0,0000 | |
| H = 8,413949E-11 | 1,844942E-09 | 0,0000 | 0,0000 | |
| BHO = 3,369521E-12 | 7,388411E-11 | 0,0000 | 0,0000 | |
| NH2 = 1,904210E-14 | 4,175395E-13 | 0,0000 | 0,0000 | |
| B2O3 = 1,201541E-14 | 2,634640E-13 | 0,0000 | 0,0000 | |
| B4C(l) = 5,048021E-16 | 1,106889E-14 | 0,0000 | 0,0000 | |
| C(gr) = 2,483853E-16 | 5,446389E-15 | 0,0000 | 0,0000 | |
| BHO2(s) = 2,321118E-17 | 5,089557E-16 | 0,0000 | 0,0000 | |
| NO = 4,206369E-18 | 9,223382E-17 | 0,0000 | 0,0000 | |
| BN(s) = 3,030458E-18 | 6,644941E-17 | 0,0000 | 0,0000 | |
| BO2 = 1,341545E-19 | 2,941629E-18 | 0,0000 | 0,0000 | |
| BO = 3,319451E-20 | 7,278620E-19 | 0,0000 | 0,0000 | |
| CNO = 8,992046E-21 | 1,971702E-19 | 0,0000 | 0,0000 | |
| B2O2 = 1,831505E-21 | 4,015975E-20 | 0,0000 | 0,0000 | |
| N2O3 = 1,090506E-21 | 2,391173E-20 | 0,0000 | 0,0000 | |
| BH2 = 6,511268E-23 | 1,427738E-21 | 0,0000 | 0,0000 | |
| H2O2 = 3,405309E-23 | 7,466884E-22 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 1,085331E-24 | 2,379824E-23 | 0,0000 | 0,0000 | |
| N = 7,645096E-26 | 1,676354E-24 | 0,0000 | 0,0000 | |
| B(l) = 2,914272E-26 | 6,390178E-25 | 0,0000 | 0,0000 | |
| B(s) = 1,441389E-27 | 3,160560E-26 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 6,207183E-28 | 1,361060E-26 | 0,0000 | 0,0000 | |
| NO2 = 4,757297E-31 | 1,043141E-29 | 0,0000 | 0,0000 | |
| BN = 8,732995E-36 | 1,914900E-34 | 0,0000 | 0,0000 | |
| BH = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |
| B4C(s) = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |
| B = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |

Excluded products (12):

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C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

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DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 2

**Combustion conditions (Number 2):**

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Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 33.33 %**
2. **Hydrogen peroxide ($H_2O_2$), 46.67 %**
3. **Water ($H_2O$, liquid), 20.00 %**

C(0,572) H(2,980) N(0,245) O(1,426) B(0,082)

Molecular weight = 37,0
Oxygen balance = -57,49692 %
Enthalpy of formation = -5266,82 kJ/kg
Internal energy of formation = -5061,11 kJ/kg

Parameters in combustion chamber:

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- Heat of isobaric combustion = -2700,74 kJ/kg
- Total enthalpy of combustion prod. = -5266,33 kJ/kg
- Entropy of combustion products = 12,12 kJ/K kg
- Isobaric combustion temperature = 1545,21 K
- Mole number of gaseous products = 58,428 mol/kg expl.
- Total mole number of products = 58,84 mol/kg expl.
- Volume of gaseous products (at SATP) = 1448,36 L/kg expl.
- Mass of gaseous products = 971,3 g/kg expl.
- Mass of condensed products = 28,7 g/kg expl.
- Mean molecular mass of gaseous prod. = 16,624 g
- Mean molecular mass of all products = 16,995 g
- Density of products = 9,326 kg/m3
- Specific gas constant = 485,767 J/kg K
- Specific heat capacity at p=const. (Cp) = 2406,88 J/kgK
- Specific heat capacity at V=const. (Cv) = 1921,11 J/molK
- Specific heat ratio (Cp/Cv) = 1,2529

Composition of combustion products in chamber (43):

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| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 8,560138E-01 | 2,313782E+01 | 39,3232 | 4,6646 | |
| H2O = | 5,601361E-01 | 1,514033E+01 | | 25,7313 | 27,2758 |
| CO = | 4,660226E-01 | 1,259646E+01 | 21,4079 | 35,2827 | |
| N2 = | 1,221794E-01 | 3,302475E+00 | 5,6126 | 9,2512 | |
| CO2 = | 1,038708E-01 | 2,807601E+00 | | 4,7716 | 12,3563 |
| B(OH)3 = | 4,400820E-02 | 1,189530E+00 | | 2,0216 | 7,3549 |
| B2O3(l) = | 1,526376E-02 | 4,125754E-01 | | 0,7012 | 2,8719 |
| BHO2 = | 7,105406E-03 | 1,920572E-01 | | 0,3264 | 0,8412 |
| CH4 = | 1,640811E-03 | 4,435067E-02 | | 0,0754 | 0,0712 |
| NH3 = | 5,825112E-04 | 1,574512E-02 | | 0,0268 | 0,0268 |
| HCN = | 1,569996E-05 | 4,243656E-04 | | 0,0007 | 0,0011 |
| CH2O = | 1,443093E-05 | 3,900641E-04 | | 0,0007 | 0,0012 |
| BHO = | 6,241558E-06 | 1,687076E-04 | | 0,0003 | 0,0005 |
| H = | 5,088052E-06 | 1,375287E-04 | 0,0002 | 0,0000 | |
| B2O3 = | 2,075581E-06 | 5,610240E-05 | | 0,0001 | 0,0004 |
| HCNO = | 1,041583E-06 | 2,815371E-05 | | 0,0000 | 0,0001 |
| CH3OH = | 1,974740E-07 | 5,337668E-06 | | 0,0000 | 0,0000 |
| C2H4 = | 1,223464E-07 | 3,306990E-06 | | 0,0000 | 0,0000 |
| C2H6 = | 3,087557E-08 | 8,345582E-07 | | 0,0000 | 0,0000 |
| NH2 = | 6,790511E-09 | 1,835457E-07 | | 0,0000 | 0,0000 |
| BO2 = | 1,514391E-09 | 4,093359E-08 | | 0,0000 | 0,0000 |
| BO = | 8,858314E-10 | 2,394378E-08 | 0,0000 | 0,0000 | |

| | | | | |
|---|---|---|---|---|
| NO = | 5,122714E-10 | 1,384656E-08 | 0,0000 | 0,0000 |
| B2O2 = | 2,907386E-10 | 7,858585E-09 | 0,0000 | 0,0000 |
| BH2 = | 3,468881E-12 | 9,376291E-11 | 0,0000 | 0,0000 |
| CNO = | 6,746463E-13 | 1,823551E-11 | 0,0000 | 0,0000 |
| H2O2 = | 3,260487E-13 | 8,813009E-12 | 0,0000 | 0,0000 |
| N = | 1,115760E-14 | 3,015869E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,780011E-15 | 4,811322E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 3,171123E-16 | 8,571460E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,199342E-16 | 3,241789E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,460261E-17 | 3,947046E-16 | 0,0000 | 0,0000 |
| NO2 = | 1,072132E-17 | 2,897943E-16 | 0,0000 | 0,0000 |
| C(gr) = | 7,384320E-18 | 1,995962E-16 | 0,0000 | 0,0000 |
| BH = | 5,038411E-18 | 1,361869E-16 | 0,0000 | 0,0000 |
| BN(s) = | 3,104943E-18 | 8,392578E-17 | 0,0000 | 0,0000 |
| BN = | 4,581287E-19 | 1,238309E-17 | 0,0000 | 0,0000 |
| B = | 4,689103E-20 | 1,267452E-18 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 5,916605E-22 | 1,599242E-20 | 0,0000 | 0,0000 |
| B(s) = | 2,104338E-22 | 5,687969E-21 | 0,0000 | 0,0000 |
| N2O3 = | 6,892283E-23 | 1,862966E-21 | 0,0000 | 0,0000 |
| B(l) = | 1,168909E-23 | 3,159529E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,481869E-24 | 4,005452E-23 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5689,59 kJ/kg
- Entropy of combustion products = 12,12 kJ/K kg
- Temperature at nozzle throat = 1388,34 K
- Pressure at nozzle throat = 3,861323 MPa
- Mole number of gaseous products = 58,328 mol/kg expl.
- Total mole number of products = 58,888 mol/kg expl.
- Volume of gaseous products (at SATP) = 1445,9 L/kg expl.
- Mass of gaseous products = 961,1 g/kg expl.
- Mass of condensed products = 38,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 16,477 g
- Mean molecular mass of all products = 16,982 g
- Density of products = 5,735 kg/m3
- Specific gas constant = 484,943 J/kg K
- Specific heat capacity at p=const. (Cp) = 2363,74 J/kgK
- Specific heat capacity at V=const. (Cv) = 1878,8 J/molK
- Specific heat ratio (Cp/Cv) = 1,2581

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 920,1 m/s
- Sound velocity at throat) = 920,3 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,552
- Pressure ratio (pc/pt) = 1,813

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = | 8,705544E-01 | 2,353085E+01 | 39,9587 | 4,7438 |
| H2O = | 5,528103E-01 | 1,494231E+01 | 25,3742 | 26,9190 |
| CO = | 4,431035E-01 | 1,197697E+01 | 20,3386 | 33,5475 |
| CO2 = | 1,246837E-01 | 3,370168E+00 | 5,7230 | 14,8321 |
| N2 = | 1,222036E-01 | 3,303129E+00 | 5,6092 | 9,2531 |
| B(OH)3 = | 3,806934E-02 | 1,029004E+00 | 1,7474 | 6,3623 |
| B2O3(l) = | 2,069759E-02 | 5,594502E-01 | 0,9500 | 3,8943 |
| CH4 = | 3,763191E-03 | 1,017180E-01 | 0,1727 | 0,1632 |
| BHO2 = | 2,187225E-03 | 5,912011E-02 | 0,1004 | 0,2589 |
| NH3 = | 5,416672E-04 | 1,464112E-02 | 0,0249 | 0,0249 |
| HCN = | 8,819869E-06 | 2,383987E-04 | 0,0004 | 0,0006 |
| CH2O = | 8,601676E-06 | 2,325010E-04 | 0,0004 | 0,0007 |
| H = | 9,566561E-07 | 2,585816E-05 | 0,0000 | 0,0000 |
| BHO = | 7,121214E-07 | 1,924845E-05 | 0,0000 | 0,0001 |

| | | | | |
|---|---|---|---|---|
| HCNO = | 5,108440E-07 | 1,380798E-05 | 0,0000 | 0,0001 |
| C2H4 = | 1,620164E-07 | 4,379260E-06 | 0,0000 | 0,0000 |
| CH3OH = | 1,476541E-07 | 3,991051E-06 | 0,0000 | 0,0000 |
| B2O3 = | 1,268646E-07 | 3,429117E-06 | 0,0000 | 0,0000 |
| C2H6 = | 8,099822E-08 | 2,189360E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,017294E-09 | 2,749719E-08 | 0,0000 | 0,0000 |
| BO2 = | 5,005794E-11 | 1,353053E-09 | 0,0000 | 0,0000 |
| NO = | 3,296428E-11 | 8,910155E-10 | 0,0000 | 0,0000 |
| BO = 2,365718E-11 | | 6,394472E-10 | 0,0000 | 0,0000 |
| B2O2 = | 5,814781E-12 | 1,571720E-10 | 0,0000 | 0,0000 |
| BH2 = | 8,214385E-14 | 2,220326E-12 | 0,0000 | 0,0000 |
| CNO = | 4,242168E-14 | 1,146646E-12 | 0,0000 | 0,0000 |
| H2O2 = | 1,335395E-14 | 3,609536E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 2,717396E-15 | 7,345049E-14 | 0,0000 | 0,0000 |
| N = 2,236980E-16 | | 6,046498E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,584500E-16 | 4,282861E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,691531E-17 | 4,572164E-16 | 0,0000 | 0,0000 |
| C(gr) = | 1,097343E-17 | 2,966089E-16 | 0,0000 | 0,0000 |
| BN(s) = | 2,666785E-18 | 7,208248E-17 | 0,0000 | 0,0000 |
| NO2 = | 1,256788E-19 | 3,397065E-18 | 0,0000 | 0,0000 |
| BH = 1,890693E-20 | | 5,110492E-19 | 0,0000 | 0,0000 |
| BN = 1,250771E-21 | | 3,380800E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 5,962644E-22 | 1,611687E-20 | 0,0000 | 0,0000 |
| B = 8,986212E-23 | | 2,428949E-21 | 0,0000 | 0,0000 |
| B(s) = | 1,668186E-23 | 4,509063E-22 | 0,0000 | 0,0000 |
| N2O3 = | 1,434260E-23 | 3,876767E-22 | 0,0000 | 0,0000 |
| B(l) = | 4,759630E-24 | 1,286515E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,862382E-26 | 1,043991E-24 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7548,64 kJ/kg
- Entropy of combustion products = 12,12 kJ/K kg
- Temperature at nozzle exit = 873,96 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 53,871 mol/kg expl.
- Total mole number of products = 54,808 mol/kg expl.
- Volume of gaseous products (at SATP) = 1335,42 L/kg expl.
- Mass of gaseous products = 934,8 g/kg expl.
- Mass of condensed products = 65,2 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,352 g
- Mean molecular mass of all products = 18,246 g
- Density of products = 0,255 kg/m3
- Specific gas constant = 447,886 J/kg K
- Specific heat capacity at p=const. (Cp) = 2182,87 J/kgK
- Specific heat capacity at V=const. (Cv) = 1734,98 J/molK
- Specific heat ratio (Cp/Cv) = 1,2582

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 217,86 s
- Vacuum-specific impulse (pa=0) = 236,18 s
- Exhaust (or nozzle exit) velocity = 2136,5 m/s
- Characteristic exhaust velocity (c*) = 1326,6 m/s
- Thrust coefficient (Cf) = 1,611
- Nozzle area expansion ratio (Ae/At) = 9,67
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 701,76 m/s
- Mach number at nozzle exit = 3,044

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 7,731137E-01 | 2,089706E+01 | 38,1274 | 4,2128 |

| | | | | |
|---|---|---|---|---|
| H2O = | 5,134621E-01 | 1,387874E+01 | 25,3223 | 25,0030 |
| CO2 = | 2,922751E-01 | 7,900118E+00 | 14,4141 | 34,7684 |
| CO = | 1,870132E-01 | 5,054916E+00 | 9,2229 | 14,1588 |
| N2 = | 1,223728E-01 | 3,307704E+00 | 6,0350 | 9,2659 |
| CH4 = | 9,227784E-02 | 2,494245E+00 | 4,5508 | 4,0015 |
| B2O3(l) = | 3,465930E-02 | 9,368315E-01 | 1,7093 | 6,5212 |
| B(OH)3 = | 1,230748E-02 | 3,326678E-01 | 0,6070 | 2,0569 |
| NH3 = | 2,123800E-04 | 5,740575E-03 | 0,0105 | 0,0098 |
| B2O3(s) = | 1,239506E-05 | 3,350352E-04 | 0,0006 | 0,0023 |
| BHO2 = | 1,847303E-06 | 4,993209E-05 | 0,0001 | 0,0002 |
| C2H6 = | 1,224328E-06 | 3,309326E-05 | 0,0001 | 0,0001 |
| CH2O = | 1,696492E-07 | 4,585572E-06 | 0,0000 | 0,0000 |
| HCN = | 1,079649E-07 | 2,918262E-06 | 0,0000 | 0,0000 |
| C2H4 = | 6,609039E-08 | 1,786405E-06 | 0,0000 | 0,0000 |
| CH3OH = | 7,801782E-09 | 2,108801E-07 | 0,0000 | 0,0000 |
| HCNO = | 3,858989E-09 | 1,043074E-07 | 0,0000 | 0,0000 |
| H = | 6,286777E-11 | 1,699299E-09 | 0,0000 | 0,0000 |
| BHO = | 1,457755E-12 | 3,940272E-11 | 0,0000 | 0,0000 |
| NH2 = | 1,202858E-14 | 3,251292E-13 | 0,0000 | 0,0000 |
| B2O3 = | 7,684003E-15 | 2,076965E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 3,726048E-16 | 1,007141E-14 | 0,0000 | 0,0000 |
| C(gr) = | 4,504146E-17 | 1,217459E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,152332E-17 | 1,122364E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 1,558820E-17 | 4,213448E-16 | 0,0000 | 0,0000 |
| NO = | 6,062163E-18 | 1,638586E-16 | 0,0000 | 0,0000 |
| BN(s) = | 5,468823E-19 | 1,478208E-17 | 0,0000 | 0,0000 |
| BO2 = | 1,353837E-19 | 3,659385E-18 | 0,0000 | 0,0000 |
| BO = | 1,213444E-20 | 3,279905E-19 | 0,0000 | 0,0000 |
| CNO = | 2,715371E-21 | 7,339575E-20 | 0,0000 | 0,0000 |
| B2O2 = | 3,950691E-22 | 1,067861E-20 | 0,0000 | 0,0000 |
| N2O3 = | 2,483617E-22 | 6,713149E-21 | 0,0000 | 0,0000 |
| H2O2 = | 1,740189E-22 | 4,703684E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,630645E-23 | 1,792245E-21 | 0,0000 | 0,0000 |
| BH2 = | 1,156241E-23 | 3,125287E-22 | 0,0000 | 0,0000 |
| N = | 3,717202E-26 | 1,004750E-24 | 0,0000 | 0,0000 |
| B = | 1,346812E-28 | 3,640398E-27 | 0,0000 | 0,0000 |
| B(s) = | 2,732839E-30 | 7,386791E-29 | 0,0000 | 0,0000 |
| NO2 = | 1,623522E-30 | 4,388336E-29 | 0,0000 | 0,0000 |
| B(l) = | 3,850422E-32 | 1,040759E-30 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,284716E-35 | 1,969039E-33 | 0,0000 | 0,0000 |
| BH = | 5,387541E-35 | 1,456238E-33 | 0,0000 | 0,0000 |
| BN = | 2,950686E-37 | 7,975624E-36 | 0,0000 | 0,0000 |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 3

**Combustion conditions (Number 3):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 28.57 %**
2. **Hydrogen peroxide ($H_2O_2$), 50.00 %**
3. **Water ($H_2O$, liquid), 21.43 %**

C(0,465) H(2,797) N(0,199) O(1,450) B(0,066)

Molecular weight = 35,1
Oxygen balance = -44,58418 %
Enthalpy of formation = -5746,41 kJ/kg
Internal energy of formation = -5540,08 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3016,7 kJ/kg
- Total enthalpy of combustion prod. = -5745,68 kJ/kg
- Entropy of combustion products = 12,1 kJ/K kg
- Isobaric combustion temperature = 1714,06 K
- Mole number of gaseous products = 55,581 mol/kg expl.
- Total mole number of products = 55,581 mol/kg expl.
- Volume of gaseous products (at SATP) = 1377,79 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,991 g
- Mean molecular mass of all products = 17,992 g
- Density of products = 8,838 kg/m3
- Specific gas constant = 462,099 J/kg K
- Specific heat capacity at p=const. (Cp) = 2407,04 J/kgK
- Specific heat capacity at V=const. (Cv) = 1944,94 J/molK
- Specific heat ratio (Cp/Cv) = 1,2376

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|---|
| H2O = | 6,982976E-01 | | 1,989263E+01 | | 35,7903 | 35,8372 |
| H2 = | 6,217821E-01 | | 1,771291E+01 | 31,8686 | 3,5709 | |
| CO = | 3,556854E-01 | | 1,013253E+01 | 18,2302 | 28,3812 | |
| CO2 = | 1,090897E-01 | | 3,107673E+00 | | 5,5912 | 13,6769 |
| N2 = | 9,949506E-02 | | 2,834348E+00 | 5,0995 | 7,9399 | |
| B(OH)3 = | 4,467091E-02 | | 1,272555E+00 | | 2,2895 | 7,8682 |
| BHO2 = | 2,164625E-02 | | 6,166438E-01 | | 1,1094 | 2,7008 |
| NH3 = | 2,342806E-04 | | 6,674027E-03 | | 0,0120 | 0,0114 |
| CH4 = | 8,248866E-05 | | 2,349881E-03 | | 0,0042 | 0,0038 |
| BHO = | 2,694053E-05 | | 7,674637E-04 | | 0,0014 | 0,0021 |
| H = | 2,318931E-05 | | 6,606013E-04 | 0,0012 | 0,0001 | |
| B2O3 = | 2,298787E-05 | | 6,548630E-04 | | 0,0012 | 0,0046 |
| B2O3(l) = | 1,008703E-05 | | 2,873525E-04 | | 0,0005 | 0,0020 |
| CH2O = | 8,083995E-06 | | 2,302914E-04 | | 0,0004 | 0,0007 |
| HCN = | 5,813236E-06 | | 1,656035E-04 | | 0,0003 | 0,0004 |
| HCNO = | 7,288050E-07 | | 2,076171E-05 | | 0,0000 | 0,0001 |
| BO2 = | 4,642964E-08 | | 1,322656E-06 | | 0,0000 | 0,0000 |
| CH3OH = | 4,447944E-08 | | 1,267100E-06 | | 0,0000 | 0,0000 |
| BO = | 1,932857E-08 | | 5,506192E-07 | 0,0000 | 0,0000 | |
| NH2 = | 1,916721E-08 | | 5,460226E-07 | | 0,0000 | 0,0000 |
| NO = | 1,044259E-08 | | 2,974814E-07 | | 0,0000 | 0,0000 |
| B2O2 = | 5,072213E-09 | | 1,444938E-07 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| C2H4 = | 2,873676E-09 | 8,186333E-08 | 0,0000 | 0,0000 |
| C2H6 = | 1,954824E-10 | 5,568770E-09 | 0,0000 | 0,0000 |
| BH2 = | 2,452409E-11 | 6,986256E-10 | 0,0000 | 0,0000 |
| H2O2 = | 1,096600E-11 | 3,123919E-10 | 0,0000 | 0,0000 |
| CNO = | 4,060403E-12 | 1,156700E-10 | 0,0000 | 0,0000 |
| N = 3,754715E-13 | 1,069618E-11 | 0,0000 | 0,0000 | |
| NO2 = | 1,619890E-15 | 4,614632E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 7,771750E-16 | 2,213963E-14 | 0,0000 | 0,0000 |
| BH = 2,537822E-16 | 7,229576E-15 | 0,0000 | 0,0000 | |
| B2O3(s) = | 6,156842E-17 | 1,753919E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 5,586667E-17 | 1,591492E-15 | 0,0000 | 0,0000 |
| BN = 3,194516E-17 | 9,100320E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = | 9,487102E-18 | 2,702622E-16 | 0,0000 | 0,0000 |
| B = 6,691771E-18 | 1,906307E-16 | 0,0000 | 0,0000 | |
| C(gr) = | 1,510398E-18 | 4,302721E-17 | 0,0000 | 0,0000 |
| BN(s) = | 9,620940E-19 | 2,740748E-17 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,218106E-22 | 1,771372E-20 | 0,0000 | 0,0000 |
| B(s) = | 3,310472E-23 | 9,430649E-22 | 0,0000 | 0,0000 |
| B(l) = | 3,051212E-23 | 8,692087E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,423631E-26 | 6,904277E-25 | 0,0000 | 0,0000 |
| N2O3 = | 1,061733E-28 | 3,024593E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -6190,28 kJ/kg
- Entropy of combustion products = 12,1 kJ/K kg
- Temperature at nozzle throat = 1554,68 K
- Pressure at nozzle throat = 3,878442 MPa
- Mole number of gaseous products = 55,399 mol/kg expl.
- Total mole number of products = 55,529 mol/kg expl.
- Volume of gaseous products (at SATP) = 1373,28 L/kg expl.
- Mass of gaseous products = 990,9 g/kg expl.
- Mass of condensed products = 9,1 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,887 g
- Mean molecular mass of all products = 18,009 g
- Density of products = 5,416 kg/m3
- Specific gas constant = 460,586 J/kg K
- Specific heat capacity at p=const. (Cp) = 2363,83 J/kgK
- Specific heat capacity at V=const. (Cv) = 1903,24 J/molK
- Specific heat ratio (Cp/Cv) = 1,242

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 943,0 m/s
- Sound velocity at throat) = 943,1 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,554
- Pressure ratio (pc/pt) = 1,805

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 6,865695E-01 | 1,955853E+01 | 35,2221 | 35,2353 |
| H2 = 6,362592E-01 | 1,812532E+01 | 32,6411 | 3,6541 | |
| CO = 3,410808E-01 | 9,716480E+00 | 17,4980 | 27,2159 | |
| CO2 = | 1,236458E-01 | 3,522337E+00 | 6,3432 | 15,5018 |
| N2 = 9,951261E-02 | 2,834848E+00 | 5,1052 | 7,9413 | |
| B(OH)3 = | 4,641708E-02 | 1,322298E+00 | 2,3813 | 8,1758 |
| BHO2 = | 1,083512E-02 | 3,086637E-01 | 0,5559 | 1,3519 |
| B2O3(l) = | 4,571975E-03 | 1,302433E-01 | 0,2345 | 0,9066 |
| NH3 = | 2,020425E-04 | 5,755650E-03 | 0,0104 | 0,0098 |
| CH4 = | 1,371104E-04 | 3,905908E-03 | 0,0070 | 0,0063 |
| H = 6,214029E-06 | 1,770211E-04 | 0,0003 | 0,0000 | |
| BHO = | 6,095768E-06 | 1,736521E-04 | 0,0003 | 0,0005 |
| CH2O = | 4,807157E-06 | 1,369431E-04 | 0,0002 | 0,0004 |
| B2O3 = | 4,034517E-06 | 1,149326E-04 | 0,0002 | 0,0008 |

| | | | | |
|---|---|---|---|---|
| HCN = | 3,334248E-06 | 9,498381E-05 | 0,0002 | 0,0003 |
| HCNO = | 3,668703E-07 | 1,045115E-05 | 0,0000 | 0,0000 |
| CH3OH = | 2,885003E-08 | 8,218600E-07 | 0,0000 | 0,0000 |
| BO2 = | 3,906294E-09 | 1,112799E-07 | 0,0000 | 0,0000 |
| NH2 = | 3,897856E-09 | 1,110395E-07 | 0,0000 | 0,0000 |
| C2H4 = | 2,784593E-09 | 7,932559E-08 | 0,0000 | 0,0000 |
| BO = 1,403203E-09 | | 3,997349E-08 | 0,0000 | 0,0000 |
| NO = | 1,141393E-09 | 3,251522E-08 | 0,0000 | 0,0000 |
| B2O2 = | 3,643570E-10 | 1,037956E-08 | 0,0000 | 0,0000 |
| C2H6 = | 3,008095E-10 | 8,569258E-09 | 0,0000 | 0,0000 |
| BH2 = | 1,491062E-12 | 4,247636E-11 | 0,0000 | 0,0000 |
| H2O2 = | 7,804195E-13 | 2,223206E-11 | 0,0000 | 0,0000 |
| CNO = | 3,981345E-13 | 1,134179E-11 | 0,0000 | 0,0000 |
| N = 1,607102E-14 | | 4,578202E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 6,683584E-16 | 1,903974E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,182049E-16 | 3,367341E-15 | 0,0000 | 0,0000 |
| NO2 = | 4,308786E-17 | 1,227458E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,235973E-17 | 3,520955E-16 | 0,0000 | 0,0000 |
| BH = 3,587314E-18 | | 1,021930E-16 | 0,0000 | 0,0000 |
| C(gr) = | 1,902206E-18 | 5,418877E-17 | 0,0000 | 0,0000 |
| BN(s) = | 1,030141E-18 | 2,934595E-17 | 0,0000 | 0,0000 |
| BN = 3,471147E-19 | | 9,888368E-18 | 0,0000 | 0,0000 |
| B = 5,240976E-20 | | 1,493014E-18 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,062494E-22 | 1,157296E-20 | 0,0000 | 0,0000 |
| B(s) = | 1,129214E-22 | 3,216829E-21 | 0,0000 | 0,0000 |
| B(l) = | 8,310292E-23 | 2,367380E-21 | 0,0000 | 0,0000 |
| N2O3 = | 2,609632E-23 | 7,434143E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,327451E-27 | 6,630286E-26 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8131,13 kJ/kg
- Entropy of combustion products = 12,1 kJ/K kg
- Temperature at nozzle exit = 881,51 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 53,616 mol/kg expl.
- Total mole number of products = 54,331 mol/kg expl.
- Volume of gaseous products (at SATP) = 1329,09 L/kg expl.
- Mass of gaseous products = 950,3 g/kg expl.
- Mass of condensed products = 49,8 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,723 g
- Mean molecular mass of all products = 18,406 g
- Density of products = 0,254 kg/m3
- Specific gas constant = 445,765 J/kg K
- Specific heat capacity at p=const. (Cp) = 2145,24 J/kgK
- Specific heat capacity at V=const. (Cv) = 1699,48 J/molK
- Specific heat ratio (Cp/Cv) = 1,2623

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 222,73 s
- Vacuum-specific impulse (pa=0) = 240,72 s
- Exhaust (or nozzle exit) velocity = 2184,2 m/s
- Characteristic exhaust velocity (c*) = 1370,5 m/s
- Thrust coefficient (Cf) = 1,594
- Nozzle area expansion ratio (Ae/At) = 9,19
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 698,6 m/s
- Mach number at nozzle exit = 3,127

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 6,900333E-01 | 1,965720E+01 | 36,1804 | 3,9629 |

| | | | | |
|---|---|---|---|---|
| H2O = | 6,112825E-01 | 1,741380E+01 | 32,0513 | 31,3715 |
| CO2 = | 2,857901E-01 | 8,141396E+00 | 14,9848 | 35,8303 |
| CO = | 1,427942E-01 | 4,067825E+00 | 7,4871 | 11,3940 |
| N2 = | 9,953521E-02 | 2,835492E+00 | 5,2189 | 7,9431 |
| CH4 = | 3,628726E-02 | 1,033727E+00 | 1,9026 | 1,6584 |
| B2O3(l) = | 2,508384E-02 | 7,145714E-01 | 1,3152 | 4,9741 |
| B(OH)3 = | 1,621926E-02 | 4,620434E-01 | 0,8504 | 2,8568 |
| NH3 = | 1,604917E-04 | 4,571980E-03 | 0,0084 | 0,0078 |
| B2O3(s) = | 1,048642E-05 | 2,987302E-04 | 0,0005 | 0,0021 |
| BHO2 = | 2,413006E-06 | 6,874009E-05 | 0,0001 | 0,0003 |
| C2H6 = | 2,311379E-07 | 6,584502E-06 | 0,0000 | 0,0000 |
| CH2O = | 1,207465E-07 | 3,439744E-06 | 0,0000 | 0,0000 |
| HCN = | 5,563942E-08 | 1,585018E-06 | 0,0000 | 0,0000 |
| C2H4 = | 1,561960E-08 | 4,449606E-07 | 0,0000 | 0,0000 |
| CH3OH = | 4,712730E-09 | 1,342531E-07 | 0,0000 | 0,0000 |
| HCNO = | 2,681563E-09 | 7,639054E-08 | 0,0000 | 0,0000 |
| H = | 7,493693E-11 | 2,134753E-09 | 0,0000 | 0,0000 |
| BHO = | 1,640383E-12 | 4,673013E-11 | 0,0000 | 0,0000 |
| NH2 = | 1,240625E-14 | 3,534209E-13 | 0,0000 | 0,0000 |
| B2O3 = | 1,166339E-14 | 3,322589E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 8,157730E-16 | 2,323919E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 5,189905E-17 | 1,478465E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,386270E-17 | 1,249531E-15 | 0,0000 | 0,0000 |
| C(gr) = | 2,334895E-17 | 6,651490E-16 | 0,0000 | 0,0000 |
| NO = | 1,056257E-17 | 3,008994E-16 | 0,0000 | 0,0000 |
| BN(s) = | 3,289872E-19 | 9,371966E-18 | 0,0000 | 0,0000 |
| BO2 = | 2,538427E-19 | 7,231299E-18 | 0,0000 | 0,0000 |
| BO = | 1,776102E-20 | 5,059638E-19 | 0,0000 | 0,0000 |
| CNO = | 2,650595E-21 | 7,550835E-20 | 0,0000 | 0,0000 |
| N2O3 = | 9,143778E-22 | 2,604818E-20 | 0,0000 | 0,0000 |
| B2O2 = | 5,262401E-22 | 1,499117E-20 | 0,0000 | 0,0000 |
| H2O2 = | 4,191898E-22 | 1,194160E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,677158E-22 | 7,626506E-21 | 0,0000 | 0,0000 |
| BH2 = | 1,134370E-23 | 3,231517E-22 | 0,0000 | 0,0000 |
| N = | 5,706962E-26 | 1,625761E-24 | 0,0000 | 0,0000 |
| B(s) = | 1,320625E-29 | 3,762106E-28 | 0,0000 | 0,0000 |
| NO2 = | 4,704960E-30 | 1,340317E-28 | 0,0000 | 0,0000 |
| B(l) = | 1,072608E-30 | 3,055574E-29 | 0,0000 | 0,0000 |
| B = | 4,843689E-33 | 1,379838E-31 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,042873E-33 | 2,970867E-32 | 0,0000 | 0,0000 |
| BH = | 3,604511E-34 | 1,026829E-32 | 0,0000 | 0,0000 |
| BN = | 9,629553E-35 | 2,743202E-33 | 0,0000 | 0,0000 |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 4

**Combustion conditions (Number 4):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 22.23 %**
2. **Hydrogen peroxide ($H_2O_2$), 54.44 %**
3. **Water ($H_2O$, liquid), 23.33 %**

C(0,339) H(2,581) N(0,145) O(1,478) B(0,048)

Molecular weight = 32,86
Oxygen balance = -27,38305 %
Enthalpy of formation = -6384,72 kJ/kg
Internal energy of formation = -6177,55 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3503,97 kJ/kg
- Total enthalpy of combustion prod. = -6385,46 kJ/kg
- Entropy of combustion products = 11,97 kJ/K kg
- Isobaric combustion temperature = 1960,16 K
- Mole number of gaseous products = 51,957 mol/kg expl.
- Total mole number of products = 51,957 mol/kg expl.
- Volume of gaseous products (at SATP) = 1287,96 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,247 g
- Mean molecular mass of all products = 19,247 g
- Density of products = 8,267 kg/m3
- Specific gas constant = 431,969 J/kg K
- Specific heat capacity at p=const. (Cp) = 2426,57 J/kgK
- Specific heat capacity at V=const. (Cv) = 1994,6 J/molK
- Specific heat ratio (Cp/Cv) = 1,2166

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 9,026192E-01 | 2,746447E+01 | | 52,8602 | 49,4781 |
| H2 = | 3,452541E-01 | 1,050523E+01 | 20,2192 | 2,1179 | |
| CO = | 2,170411E-01 | 6,604022E+00 | 12,7106 | 18,4979 | |
| CO2 = | 1,216007E-01 | 3,700007E+00 | | 7,1213 | 16,2837 |
| N2 = | 7,253744E-02 | 2,207135E+00 | 4,2480 | 6,1828 | |
| BHO2 = | 3,011862E-02 | 9,164350E-01 | | 1,7638 | 4,0138 |
| B(OH)3 = | 1,810428E-02 | 5,508683E-01 | | 1,0602 | 3,4060 |
| H = | 1,185856E-04 | 3,608265E-03 | 0,0069 | 0,0004 | |
| NH3 = | 5,784087E-05 | 1,759954E-03 | | 0,0034 | 0,0030 |
| B2O3 = | 5,458085E-05 | 1,660760E-03 | | 0,0032 | 0,0116 |
| BHO = | 4,455476E-05 | 1,355691E-03 | | 0,0026 | 0,0038 |
| CH2O = | 2,835214E-06 | 8,626852E-05 | | 0,0002 | 0,0003 |
| CH4 = | 1,177496E-06 | 3,582828E-05 | | 0,0001 | 0,0001 |
| HCN = | 1,083602E-06 | 3,297132E-05 | | 0,0001 | 0,0001 |
| BO2 = | 1,021222E-06 | 3,107326E-05 | | 0,0001 | 0,0001 |
| NO = | 4,004250E-07 | 1,218394E-05 | | 0,0000 | 0,0000 |
| HCNO = | 3,550959E-07 | 1,080469E-05 | | 0,0000 | 0,0000 |
| BO = | 2,261644E-07 | 6,881624E-06 | 0,0000 | 0,0000 | |
| NH2 = | 4,895417E-08 | 1,489554E-06 | | 0,0000 | 0,0000 |
| B2O2 = | 1,610711E-08 | 4,900994E-07 | | 0,0000 | 0,0000 |
| CH3OH = | 4,513173E-09 | 1,373247E-07 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| H2O2 = | 7,890170E-10 | 2,400783E-08 | 0,0000 | 0,0000 |
| BH2 = | 5,138416E-11 | 1,563493E-09 | 0,0000 | 0,0000 |
| CNO = | 2,603335E-11 | 7,921305E-10 | 0,0000 | 0,0000 |
| N = | 2,045243E-11 | 6,223169E-10 | 0,0000 | 0,0000 |
| C2H4 = | 1,163909E-11 | 3,541487E-10 | 0,0000 | 0,0000 |
| NO2 = | 7,819289E-13 | 2,379216E-11 | 0,0000 | 0,0000 |
| C2H6 = | 1,441386E-13 | 4,385782E-12 | 0,0000 | 0,0000 |
| N2H4 = | 9,397904E-14 | 2,859549E-12 | 0,0000 | 0,0000 |
| BH = | 5,589048E-15 | 1,700609E-13 | 0,0000 | 0,0000 |
| BN = | 1,097364E-15 | 3,339006E-14 | 0,0000 | 0,0000 |
| B = | 5,417255E-16 | 1,648336E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 9,847481E-17 | 2,996344E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 7,066794E-17 | 2,150250E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 9,913639E-18 | 3,016475E-16 | 0,0000 | 0,0000 |
| B2O3(s) = | 4,723116E-18 | 1,437127E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 2,360913E-18 | 7,183674E-17 | 0,0000 | 0,0000 |
| C(gr) = | 1,668712E-19 | 5,077476E-18 | 0,0000 | 0,0000 |
| BN(s) = | 6,802859E-20 | 2,069942E-18 | 0,0000 | 0,0000 |
| B(s) = | 3,223273E-22 | 9,807620E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,133310E-22 | 6,491135E-21 | 0,0000 | 0,0000 |
| B(l) = | 2,004962E-22 | 6,100603E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,984656E-22 | 6,038818E-21 | 0,0000 | 0,0000 |
| N2O3 = | 1,050841E-23 | 3,197449E-22 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -6854,16 kJ/kg
- Entropy of combustion products = 11,97 kJ/K kg
- Temperature at nozzle throat = 1783,23 K
- Pressure at nozzle throat = 3,915686 MPa
- Mole number of gaseous products = 51,766 mol/kg expl.
- Total mole number of products = 51,766 mol/kg expl.
- Volume of gaseous products (at SATP) = 1283,23 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,318 g
- Mean molecular mass of all products = 19,318 g
- Density of products = 5,102 kg/m3
- Specific gas constant = 430,383 J/kg K
- Specific heat capacity at p=const. (Cp) = 2377,77 J/kgK
- Specific heat capacity at V=const. (Cv) = 1947,39 J/molK
- Specific heat ratio (Cp/Cv) = 1,221

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 968,2 m/s
- Sound velocity at throat ) = 968,0 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,559
- Pressure ratio (pc/pt) = 1,788

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 8,867578E-01 | 2,698184E+01 | 52,1227 | 48,6086 |
| H2 = | 3,549011E-01 | 1,079876E+01 | 20,8607 | 2,1770 |
| CO = | 2,074777E-01 | 6,313033E+00 | 12,1953 | 17,6828 |
| CO2 = | 1,311658E-01 | 3,991050E+00 | 7,7098 | 17,5646 |
| N2 = | 7,254314E-02 | 2,207308E+00 | 4,2640 | 6,1833 |
| B(OH)3 = | 2,435020E-02 | 7,409163E-01 | 1,4313 | 4,5811 |
| BHO2 = | 2,395831E-02 | 7,289920E-01 | 1,4082 | 3,1928 |
| NH3 = | 4,750814E-05 | 1,445555E-03 | 0,0028 | 0,0025 |
| H = | 4,046714E-05 | 1,231315E-03 | 0,0024 | 0,0001 |
| B2O3 = | 2,555796E-05 | 7,776653E-04 | 0,0015 | 0,0054 |
| BHO = | 1,836546E-05 | 5,588156E-04 | 0,0011 | 0,0016 |

| | | | | |
|---|---|---|---|---|
| CH2O = | 1,673034E-06 | 5,090629E-05 | 0,0001 | 0,0002 |
| CH4 = | 1,560828E-06 | 4,749213E-05 | 0,0001 | 0,0001 |
| HCN = | 6,260509E-07 | 1,904918E-05 | 0,0000 | 0,0001 |
| BO2 = | 1,857446E-07 | 5,651749E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,808800E-07 | 5,503731E-06 | 0,0000 | 0,0000 |
| NO = | 6,308950E-08 | 1,919657E-06 | 0,0000 | 0,0000 |
| BO = | 3,720362E-08 | 1,132014E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,233766E-08 | 3,754045E-07 | 0,0000 | 0,0000 |
| B2O2 = | 3,604004E-09 | 1,096609E-07 | 0,0000 | 0,0000 |
| CH3OH = | 2,639684E-09 | 8,031905E-08 | 0,0000 | 0,0000 |
| H2O2 = | 8,257899E-11 | 2,512674E-09 | 0,0000 | 0,0000 |
| C2H4 = | 8,985556E-12 | 2,734082E-10 | 0,0000 | 0,0000 |
| BH2 = | 6,817951E-12 | 2,074533E-10 | 0,0000 | 0,0000 |
| CNO = | 3,442848E-12 | 1,047573E-10 | 0,0000 | 0,0000 |
| N = | 1,475790E-12 | 4,490463E-11 | 0,0000 | 0,0000 |
| C2H6 = | 1,519591E-13 | 4,623738E-12 | 0,0000 | 0,0000 |
| NO2 = | 3,665867E-14 | 1,115433E-12 | 0,0000 | 0,0000 |
| N2H4 = | 1,760033E-14 | 5,355345E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 4,574291E-16 | 1,391843E-14 | 0,0000 | 0,0000 |
| BH = | 2,251008E-16 | 6,849261E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 2,034100E-16 | 6,189264E-15 | 0,0000 | 0,0000 |
| BN = | 3,522635E-17 | 1,071851E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,402870E-17 | 4,268587E-16 | 0,0000 | 0,0000 |
| B = | 1,366901E-17 | 4,159142E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 3,764497E-18 | 1,145443E-16 | 0,0000 | 0,0000 |
| C(gr) = | 1,862785E-19 | 5,667994E-18 | 0,0000 | 0,0000 |
| BN(s) = | 9,616206E-20 | 2,925973E-18 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,968516E-22 | 5,989706E-21 | 0,0000 | 0,0000 |
| B(s) = | 1,342220E-22 | 4,084042E-21 | 0,0000 | 0,0000 |
| B(l) = | 6,110886E-23 | 1,859391E-21 | 0,0000 | 0,0000 |
| B4C(s) = | 4,159364E-26 | 1,265591E-24 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,915058E-28 | 1,191255E-26 | 0,0000 | 0,0000 |
| N2O3 = | 1,703548E-29 | 5,183476E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8950,53 kJ/kg
- Entropy of combustion products = 11,97 kJ/K kg
- Temperature at nozzle exit = 954,73 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 51,396 mol/kg expl.
- Total mole number of products = 51,798 mol/kg expl.
- Volume of gaseous products (at SATP) = 1274,05 L/kg expl.
- Mass of gaseous products = 972,0 g/kg expl.
- Mass of condensed products = 28,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 18,913 g
- Mean molecular mass of all products = 19,306 g
- Density of products = 0,245 kg/m3
- Specific gas constant = 427,304 J/kg K
- Specific heat capacity at p=const. (Cp) = 2099,91 J/kgK
- Specific heat capacity at V=const. (Cv) = 1672,61 J/molK
- Specific heat ratio (Cp/Cv) = 1,2555

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 230,96 s
- Vacuum-specific impulse (pa=0) = 248,97 s
- Exhaust (or nozzle exit) velocity = 2265,0 m/s
- Characteristic exhaust velocity (c*) = 1417,1 m/s
- Thrust coefficient (Cf) = 1,598
- Nozzle area expansion ratio (Ae/At) = 8,9
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 705,78 m/s
- Mach number at nozzle exit = 3,209

Composition of combustion products at the nozzle exit:

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 7,884438E-01 | 2,399039E+01 | | 46,3156 | 43,2194 |
| H2 = | 4,674757E-01 | 1,422413E+01 | 27,4610 | 2,8676 | |
| CO2 = | 2,457251E-01 | 7,476807E+00 | | 14,4347 | 32,9054 |
| CO = | 9,224588E-02 | 2,806813E+00 | 5,4188 | 7,8619 | |
| N2 = | 7,254320E-02 | 2,207310E+00 | 4,2614 | 6,1833 | |
| B(OH)3 = | 2,194388E-02 | 6,676980E-01 | | 1,2891 | 4,1284 |
| B2O3(l) = | 1,320860E-02 | 4,019051E-01 | | 0,7759 | 2,7976 |
| CH4 = | 6,764514E-04 | 2,058274E-02 | | 0,0397 | 0,0330 |
| NH3 = | 4,823852E-05 | 1,467779E-03 | | 0,0028 | 0,0025 |
| BHO2 = | 1,640809E-05 | 4,992576E-04 | | 0,0010 | 0,0022 |
| B2O3(s) = | 3,605730E-07 | 1,097134E-05 | | 0,0000 | 0,0001 |
| CH2O = | 5,197121E-08 | 1,581355E-06 | | 0,0000 | 0,0000 |
| HCN = | 1,446123E-08 | 4,400194E-07 | | 0,0000 | 0,0000 |
| HCNO = | 1,464620E-09 | 4,456475E-08 | | 0,0000 | 0,0000 |
| H = | 5,953137E-10 | 1,811392E-08 | 0,0000 | 0,0000 | |
| CH3OH = | 5,877159E-10 | 1,788274E-08 | | 0,0000 | 0,0000 |
| C2H6 = | 2,550723E-10 | 7,761218E-09 | | 0,0000 | 0,0000 |
| C2H4 = | 1,018988E-10 | 3,100527E-09 | | 0,0000 | 0,0000 |
| BHO = | 2,009696E-11 | 6,115006E-10 | | 0,0000 | 0,0000 |
| B2O3 = | 6,978530E-13 | 2,123394E-11 | | 0,0000 | 0,0000 |
| NH2 = | 5,297697E-14 | 1,611958E-12 | | 0,0000 | 0,0000 |
| NO = | 5,648095E-16 | 1,718575E-14 | | 0,0000 | 0,0000 |
| B4C(l) = | 2,259786E-16 | 6,875970E-15 | | 0,0000 | 0,0000 |
| BO2 = | 3,845746E-17 | 1,170165E-15 | | 0,0000 | 0,0000 |
| B4C(s) = | 3,248011E-17 | 9,882893E-16 | | 0,0000 | 0,0000 |
| BHO2(s) = | 2,957217E-17 | 8,998079E-16 | | 0,0000 | 0,0000 |
| C(gr) = | 2,595722E-18 | 7,898138E-17 | | 0,0000 | 0,0000 |
| BO = | 2,013169E-18 | 6,125575E-17 | 0,0000 | 0,0000 | |
| BN(s) = | 1,104562E-19 | 3,360910E-18 | | 0,0000 | 0,0000 |
| N2H4 = | 1,089577E-19 | 3,315313E-18 | | 0,0000 | 0,0000 |
| B2O2 = | 6,677814E-20 | 2,031893E-18 | | 0,0000 | 0,0000 |
| H2O2 = | 4,183884E-20 | 1,273052E-18 | | 0,0000 | 0,0000 |
| CNO = | 2,658185E-20 | 8,088198E-19 | | 0,0000 | 0,0000 |
| N2O3 = | 3,380905E-22 | 1,028726E-20 | | 0,0000 | 0,0000 |
| B(OH)3(s) = | 3,266120E-22 | 9,937994E-21 | | 0,0000 | 0,0000 |
| BH2 = | 3,105418E-22 | 9,449018E-21 | | 0,0000 | 0,0000 |
| N = | 6,721217E-24 | 2,045100E-22 | 0,0000 | 0,0000 | |
| B(l) = | 5,389657E-25 | 1,639939E-23 | | 0,0000 | 0,0000 |
| NO2 = | 3,407698E-27 | 1,036878E-25 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,206033E-28 | 9,755165E-27 | | 0,0000 | 0,0000 |
| B(s) = | 1,041093E-29 | 3,167789E-28 | | 0,0000 | 0,0000 |
| BH = | 3,821139E-32 | 1,162678E-30 | 0,0000 | 0,0000 | |
| B = | 9,511626E-34 | 2,894152E-32 | 0,0000 | 0,0000 | |
| BN = | 5,118836E-34 | 1,557535E-32 | 0,0000 | 0,0000 | |

Excluded products (11):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 5

**Combustion conditions (Number 5):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 20.41 %**
2. **Hydrogen peroxide ($H_2O_2$), 55.71 %**
3. **Water ($H_2O$, liquid), 23.88 %**

C(0,305) H(2,523) N(0,131) O(1,485) B(0,044)

Molecular weight = 32,27
Oxygen balance = -22,44737 %
Enthalpy of formation = -6568,43 kJ/kg
Internal energy of formation = -6361,02 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3656,23 kJ/kg
- Total enthalpy of combustion prod. = -6567,99 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Isobaric combustion temperature = 2036,72 K
- Mole number of gaseous products = 50,854 mol/kg expl.
- Total mole number of products = 50,854 mol/kg expl.
- Volume of gaseous products (at SATP) = 1260,62 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,664 g
- Mean molecular mass of all products = 19,664 g
- Density of products = 8,129 kg/m3
- Specific gas constant = 422,8 J/kg K
- Specific heat capacity at p=const. (Cp) = 2434,0 J/kgK
- Specific heat capacity at V=const. (Cv) = 2011,2 J/molK
- Specific heat ratio (Cp/Cv) = 1,2102

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 9,532890E-01 | 2,953831E+01 | | 58,0845 | 53,2142 |
| H2 = | 2,733631E-01 | 8,470342E+00 | 16,6562 | 1,7076 | |
| CO = | 1,792824E-01 | 5,555189E+00 | 10,9238 | 15,5601 | |
| CO2 = | 1,260355E-01 | 3,905296E+00 | | 7,6794 | 17,1872 |
| N2 = | 6,540722E-02 | 2,026687E+00 | 3,9853 | 5,6774 | |
| BHO2 = | 3,032771E-02 | 9,397248E-01 | | 1,8479 | 4,1158 |
| B(OH)3 = | 1,312453E-02 | 4,066724E-01 | | 0,7997 | 2,5145 |
| H = | 1,745674E-04 | 5,409090E-03 | 0,0106 | 0,0005 | |
| OH = | 6,011045E-05 | 1,862563E-03 | | 0,0037 | 0,0032 |
| B2O3 = | 5,916380E-05 | 1,833231E-03 | | 0,0036 | 0,0128 |
| BHO = | 4,387798E-05 | 1,359589E-03 | | 0,0027 | 0,0038 |
| NH3 = | 3,544028E-05 | 1,098141E-03 | | 0,0022 | 0,0019 |
| BO2 = | 2,200800E-06 | 6,819328E-05 | | 0,0001 | 0,0003 |
| CH2O = | 1,883451E-06 | 5,836000E-05 | | 0,0001 | 0,0002 |
| NO = | 1,099664E-06 | 3,407385E-05 | | 0,0001 | 0,0001 |
| HCN = | 5,873653E-07 | 1,819992E-05 | | 0,0000 | 0,0000 |
| BO = | 3,852087E-07 | 1,193596E-05 | 0,0000 | 0,0000 | |
| CH4 = | 2,936951E-07 | 9,100344E-06 | | 0,0000 | 0,0000 |
| HCNO = | 2,648758E-07 | 8,207356E-06 | | 0,0000 | 0,0000 |
| NH2 = | 5,733572E-08 | 1,776586E-06 | | 0,0000 | 0,0000 |
| O2 = | 4,729567E-08 | 1,465489E-06 | 0,0000 | 0,0000 | |
| O = | 2,606387E-08 | 8,076070E-07 | 0,0000 | 0,0000 | |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 1,759913E-08 | 5,453211E-07 | 0,0000 | 0,0000 |
| H2O2 = | 2,556334E-09 | 7,920977E-08 | 0,0000 | 0,0000 |
| N = | 5,758137E-11 | 1,784198E-09 | 0,0000 | 0,0000 |
| BH2 = | 4,848556E-11 | 1,502358E-09 | 0,0000 | 0,0000 |
| CNO = | 3,959090E-11 | 1,226751E-09 | 0,0000 | 0,0000 |
| NO2 = | 4,461078E-12 | 1,382296E-10 | 0,0000 | 0,0000 |
| N2H4 = | 7,182963E-14 | 2,225690E-12 | 0,0000 | 0,0000 |
| BH = | 1,012045E-14 | 3,135892E-13 | 0,0000 | 0,0000 |
| BN = | 2,299054E-15 | 7,123776E-14 | 0,0000 | 0,0000 |
| B = | 1,432476E-15 | 4,438626E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 5,860217E-16 | 1,815828E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 3,394062E-16 | 1,051673E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 3,269518E-17 | 1,013083E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,156368E-18 | 6,681653E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,536425E-18 | 4,760718E-17 | 0,0000 | 0,0000 |
| C(gr) = | 8,297669E-20 | 2,571090E-18 | 0,0000 | 0,0000 |
| BN(s) = | 2,848188E-20 | 8,825304E-19 | 0,0000 | 0,0000 |
| B(s) = | 2,409996E-22 | 7,467538E-21 | 0,0000 | 0,0000 |
| B(l) = | 1,724394E-22 | 5,343154E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,575270E-22 | 4,881080E-21 | 0,0000 | 0,0000 |
| N2O3 = | 1,546662E-22 | 4,792439E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,323652E-28 | 7,199996E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7043,04 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Temperature at nozzle throat = 1854,28 K
- Pressure at nozzle throat = 3,925182 MPa
- Mole number of gaseous products = 50,704 mol/kg expl.
- Total mole number of products = 50,704 mol/kg expl.
- Volume of gaseous products (at SATP) = 1256,91 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,722 g
- Mean molecular mass of all products = 19,722 g
- Density of products = 5,021 kg/m3
- Specific gas constant = 421,556 J/kg K
- Specific heat capacity at p=const. (Cp) = 2384,61 J/kgK
- Specific heat capacity at V=const. (Cv) = 1963,05 J/molK
- Specific heat ratio (Cp/Cv) = 1,2147

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 974,7 m/s
- Sound velocity at throat ) = 974,4 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,561
- Pressure ratio (pc/pt) = 1,783

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 9,401820E-01 | 2,913218E+01 | 57,4550 | 52,4825 |
| H2 = | 2,817738E-01 | 8,730953E+00 | 17,2193 | 1,7602 |
| CO = | 1,709397E-01 | 5,296684E+00 | 10,4462 | 14,8360 |
| CO2 = | 1,343795E-01 | 4,163842E+00 | 8,2120 | 18,3251 |
| N2 = | 6,541123E-02 | 2,026812E+00 | 3,9973 | 5,6777 |
| BHO2 = | 2,564666E-02 | 7,946794E-01 | 1,5673 | 3,4805 |
| B(OH)3 = | 1,788703E-02 | 5,542419E-01 | 1,0931 | 3,4269 |
| H = | 6,336004E-05 | 1,963254E-03 | 0,0039 | 0,0002 |
| B2O3 = | 3,161759E-05 | 9,796927E-04 | 0,0019 | 0,0068 |
| NH3 = | 2,879035E-05 | 8,920886E-04 | 0,0018 | 0,0015 |
| BHO = | 1,984383E-05 | 6,148747E-04 | 0,0012 | 0,0017 |
| OH = | 1,458589E-05 | 4,519538E-04 | 0,0009 | 0,0008 |

| | | | | |
|---|---|---|---|---|
| CH2O = | 1,107769E-06 | 3,432498E-05 | 0,0001 | 0,0001 |
| BO2 = | 4,594709E-07 | 1,423702E-05 | 0,0000 | 0,0001 |
| CH4 = | 3,666028E-07 | 1,135944E-05 | 0,0000 | 0,0000 |
| HCN = | 3,383610E-07 | 1,048435E-05 | 0,0000 | 0,0000 |
| NO = | 1,903740E-07 | 5,898868E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,350492E-07 | 4,184593E-06 | 0,0000 | 0,0000 |
| BO = | 7,339608E-08 | 2,274228E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,525967E-08 | 4,728312E-07 | 0,0000 | 0,0000 |
| B2O2 = | 4,659041E-09 | 1,443636E-07 | 0,0000 | 0,0000 |
| O2 = | 4,135571E-09 | 1,281435E-07 | 0,0000 | 0,0000 |
| O = | 2,335643E-09 | 7,237151E-08 | 0,0000 | 0,0000 |
| H2O2 = | 2,966133E-10 | 9,190767E-09 | 0,0000 | 0,0000 |
| BH2 = | 7,367195E-12 | 2,282776E-10 | 0,0000 | 0,0000 |
| CNO = | 5,629137E-12 | 1,744227E-10 | 0,0000 | 0,0000 |
| N = | 4,735802E-12 | 1,467421E-10 | 0,0000 | 0,0000 |
| NO2 = | 2,423091E-13 | 7,508113E-12 | 0,0000 | 0,0000 |
| N2H4 = | 1,385126E-14 | 4,291908E-13 | 0,0000 | 0,0000 |
| BH = | 4,987716E-16 | 1,545478E-14 | 0,0000 | 0,0000 |
| BN = | 9,105411E-17 | 2,821374E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 9,004773E-17 | 2,790190E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 7,200354E-17 | 2,231079E-15 | 0,0000 | 0,0000 |
| B = | 4,562646E-17 | 1,413767E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 6,399740E-18 | 1,983003E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 2,437760E-18 | 7,553565E-17 | 0,0000 | 0,0000 |
| C(gr) = | 8,940748E-20 | 2,770352E-18 | 0,0000 | 0,0000 |
| BN(s) = | 4,058219E-20 | 1,257467E-18 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,384322E-22 | 4,289418E-21 | 0,0000 | 0,0000 |
| B(s) = | 1,114105E-22 | 3,452131E-21 | 0,0000 | 0,0000 |
| B(l) = | 5,753683E-23 | 1,782818E-21 | 0,0000 | 0,0000 |
| N2O3 = | 6,403466E-25 | 1,984158E-23 | 0,0000 | 0,0000 |
| B4C(s) = | 4,996705E-27 | 1,548263E-25 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,531727E-29 | 7,844730E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9186,3 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Temperature at nozzle exit = 1001,75 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 50,218 mol/kg expl.
- Total mole number of products = 50,534 mol/kg expl.
- Volume of gaseous products (at SATP) = 1244,86 L/kg expl.
- Mass of gaseous products = 978,0 g/kg expl.
- Mass of condensed products = 22,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,476 g
- Mean molecular mass of all products = 19,789 g
- Density of products = 0,239 kg/m3
- Specific gas constant = 417,514 J/kg K
- Specific heat capacity at p=const. (Cp) = 2093,72 J/kgK
- Specific heat capacity at V=const. (Cv) = 1676,21 J/molK
- Specific heat ratio (Cp/Cv) = 1,2491

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 233,35 s
- Vacuum-specific impulse (pa=0) = 251,63 s
- Exhaust (or nozzle exit) velocity = 2288,4 m/s
- Characteristic exhaust velocity (c*) = 1430,2 m/s
- Thrust coefficient (Cf) = 1,6
- Nozzle area expansion ratio (Ae/At) = 8,95
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 712,78 m/s
- Mach number at nozzle exit = 3,21

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 8,517034E-01 | 2,639061E+01 | | 52,2238 | 47,5435 |
| H2 = | 3,749771E-01 | 1,161892E+01 | 22,9924 | 2,3424 | |
| CO2 = | 2,277651E-01 | 7,057458E+00 | | 13,9658 | 31,0599 |
| CO = | 7,747775E-02 | 2,400701E+00 | 4,7507 | 6,7244 | |
| N2 = | 6,541355E-02 | 2,026884E+00 | 4,0110 | 5,6779 | |
| B(OH)3 = | 2,320312E-02 | 7,189645E-01 | | 1,4227 | 4,4454 |
| B2O3(l) = | 1,018351E-02 | 3,155430E-01 | | 0,6244 | 2,1965 |
| CH4 = | 7,822661E-05 | 2,423905E-03 | | 0,0048 | 0,0039 |
| BHO2 = | 4,703979E-05 | 1,457560E-03 | | 0,0029 | 0,0064 |
| NH3 = | 2,481708E-05 | 7,689741E-04 | | 0,0015 | 0,0013 |
| CH2O = | 3,395790E-08 | 1,052209E-06 | | 0,0000 | 0,0000 |
| HCN = | 7,882210E-09 | 2,442357E-07 | | 0,0000 | 0,0000 |
| H = | 1,942829E-09 | 6,019990E-08 | 0,0000 | 0,0000 | |
| HCNO = | 1,139112E-09 | 3,529616E-08 | | 0,0000 | 0,0000 |
| BHO = | 8,574805E-11 | 2,656962E-09 | | 0,0000 | 0,0000 |
| OH = | 9,327539E-12 | 2,890202E-10 | | 0,0000 | 0,0000 |
| B2O3 = | 7,106280E-12 | 2,201929E-10 | | 0,0000 | 0,0000 |
| NH2 = | 1,234384E-13 | 3,824822E-12 | | 0,0000 | 0,0000 |
| NO = | 5,265527E-15 | 1,631559E-13 | | 0,0000 | 0,0000 |
| BO2 = | 6,451930E-16 | 1,999175E-14 | | 0,0000 | 0,0000 |
| B2O3(s) = | 5,296768E-16 | 1,641240E-14 | | 0,0000 | 0,0000 |
| B4C(l) = | 5,004287E-16 | 1,550613E-14 | | 0,0000 | 0,0000 |
| B4C(s) = | 9,180057E-17 | 2,844503E-15 | | 0,0000 | 0,0000 |
| BO = | 3,049136E-17 | 9,447956E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = | 2,271982E-17 | 7,039892E-16 | | 0,0000 | 0,0000 |
| B2O2 = | 1,108628E-18 | 3,435159E-17 | | 0,0000 | 0,0000 |
| C(gr) = | 8,530795E-19 | 2,643325E-17 | | 0,0000 | 0,0000 |
| H2O2 = | 4,954916E-19 | 1,535315E-17 | | 0,0000 | 0,0000 |
| N2H4 = | 1,154520E-19 | 3,577358E-18 | | 0,0000 | 0,0000 |
| CNO = | 1,082735E-19 | 3,354928E-18 | | 0,0000 | 0,0000 |
| O2 = | 7,894847E-20 | 2,446272E-18 | 0,0000 | 0,0000 | |
| BN(s) = | 6,719902E-20 | 2,082207E-18 | | 0,0000 | 0,0000 |
| O = | 5,334861E-20 | 1,653043E-18 | 0,0000 | 0,0000 | |
| BH2 = | 2,202685E-21 | 6,825172E-20 | | 0,0000 | 0,0000 |
| N2O3 = | 3,898792E-22 | 1,208068E-20 | | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,215218E-22 | 3,765437E-21 | | 0,0000 | 0,0000 |
| N = | 1,044896E-22 | 3,237682E-21 | 0,0000 | 0,0000 | |
| B = | 1,064709E-23 | 3,299075E-22 | 0,0000 | 0,0000 | |
| B(l) = | 6,715595E-24 | 2,080873E-22 | | 0,0000 | 0,0000 |
| B(s) = | 5,336624E-25 | 1,653590E-23 | | 0,0000 | 0,0000 |
| NO2 = | 1,300318E-25 | 4,029124E-24 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,472833E-26 | 4,563673E-25 | | 0,0000 | 0,0000 |
| BH = | 1,190641E-30 | 3,689282E-29 | 0,0000 | 0,0000 | |
| BN = | 8,400859E-35 | 2,603064E-33 | 0,0000 | 0,0000 | |

Excluded products (11):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 6

**Combustion conditions (Number 6):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

Reactant information:

---

1. **[EMIM][$BH_3CN$], 18.18 %**
2. **Hydrogen peroxide ($H_2O_2$), 57.27 %**
3. **Water ($H_2O$, liquid), 24.55 %**

C(0,266) H(2,456) N(0,114) O(1,494) B(0,038)

Molecular weight = 31,58
Oxygen balance = -16,39793 %
Enthalpy of formation = -6793,12 kJ/kg
Internal energy of formation = -6585,42 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3853,07 kJ/kg
- Total enthalpy of combustion prod. = -6793,13 kJ/kg
- Entropy of combustion products = 11,82 kJ/K kg
- Isobaric combustion temperature = 2133,79 K
- Mole number of gaseous products = 49,459 mol/kg expl.
- Total mole number of products = 49,459 mol/kg expl.
- Volume of gaseous products (at SATP) = 1226,05 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,219 g
- Mean molecular mass of all products = 20,219 g
- Density of products = 7,978 kg/m3
- Specific gas constant = 411,206 J/kg K
- Specific heat capacity at p=const. (Cp) = 2443,96 J/kgK
- Specific heat capacity at V=const. (Cv) = 2032,76 J/molK
- Specific heat ratio (Cp/Cv) = 1,2023

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|---|
| H2O = | 1,009952E+00 | | 3,198373E+01 | | 64,6666 | 57,6196 |
| H2 = | 1,903245E-01 | 6,027305E+00 | | 12,1864 | 1,2151 | |
| CO = | 1,332099E-01 | 4,218566E+00 | | 8,5293 | 11,8162 | |
| CO2 = | 1,328858E-01 | | 4,208303E+00 | | 8,5086 | 18,5207 |
| N2 = | 5,700997E-02 | 1,805424E+00 | | 3,6503 | 5,0575 | |
| BHO2 = | 2,923175E-02 | | 9,257276E-01 | | 1,8717 | 4,0545 |
| B(OH)3 = | 8,618436E-03 | | 2,729335E-01 | | 0,5518 | 1,6875 |
| H = | 2,615749E-04 | 8,283701E-03 | | 0,0167 | 0,0008 | |
| OH = | 1,615851E-04 | | 5,117169E-03 | | 0,0103 | 0,0087 |
| B2O3 = | 5,978668E-05 | | 1,893358E-03 | | 0,0038 | 0,0132 |
| BHO = | 3,786907E-05 | | 1,199259E-03 | | 0,0024 | 0,0033 |
| NH3 = | 1,742712E-05 | | 5,518917E-04 | | 0,0011 | 0,0009 |
| BO2 = | 5,375933E-06 | | 1,702481E-04 | | 0,0003 | 0,0007 |
| NO = | 3,842550E-06 | | 1,216880E-04 | | 0,0002 | 0,0004 |
| CH2O = | 9,968049E-07 | | 3,156738E-05 | | 0,0001 | 0,0001 |
| BO = | 6,563903E-07 | 2,078694E-05 | | 0,0000 | 0,0001 | |
| O2 = | 4,034833E-07 | 1,277774E-05 | | 0,0000 | 0,0000 | |
| HCN = | 2,338252E-07 | | 7,404907E-06 | | 0,0000 | 0,0000 |
| HCNO = | 1,664675E-07 | | 5,271785E-06 | | 0,0000 | 0,0000 |
| O = | 1,474817E-07 | 4,670534E-06 | | 0,0000 | 0,0000 | |
| NH2 = | 6,256718E-08 | | 1,981413E-06 | | 0,0000 | 0,0000 |
| CH4 = | 4,187014E-08 | | 1,325967E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 1,648662E-08 | 5,221075E-07 | 0,0000 | 0,0000 |
| H2O2 = | 1,088035E-08 | 3,445650E-07 | 0,0000 | 0,0000 |
| N = | 1,904234E-10 | 6,030434E-09 | 0,0000 | 0,0000 |
| CNO = | 5,957543E-11 | 1,886668E-09 | 0,0000 | 0,0000 |
| NO2 = | 3,978361E-11 | 1,259890E-09 | 0,0000 | 0,0000 |
| BH2 = | 3,503159E-11 | 1,109400E-09 | 0,0000 | 0,0000 |
| N2H4 = | 4,357125E-14 | 1,379839E-12 | 0,0000 | 0,0000 |
| BH = | 1,630113E-14 | 5,162333E-13 | 0,0000 | 0,0000 |
| BN = | 4,552675E-15 | 1,441767E-13 | 0,0000 | 0,0000 |
| B = | 3,745946E-15 | 1,186287E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,083195E-15 | 3,430324E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 7,057961E-16 | 2,235155E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,265426E-17 | 4,007422E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 8,986308E-19 | 2,845835E-17 | 0,0000 | 0,0000 |
| B2O3(s) = | 8,092556E-19 | 2,562796E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,152720E-20 | 9,984213E-19 | 0,0000 | 0,0000 |
| BN(s) = | 8,698286E-21 | 2,754622E-19 | 0,0000 | 0,0000 |
| N2O3 = | 4,659234E-21 | 1,475513E-19 | 0,0000 | 0,0000 |
| B(s) = | 1,544910E-22 | 4,892509E-21 | 0,0000 | 0,0000 |
| B(l) = | 1,228675E-22 | 3,891038E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,046222E-22 | 3,313236E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 4,184797E-29 | 1,325265E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7274,5 kJ/kg
- Entropy of combustion products = 11,82 kJ/K kg
- Temperature at nozzle throat = 1945,56 K
- Pressure at nozzle throat = 3,939058 MPa
- Mole number of gaseous products = 49,357 mol/kg expl.
- Total mole number of products = 49,357 mol/kg expl.
- Volume of gaseous products (at SATP) = 1223,51 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,261 g
- Mean molecular mass of all products = 20,261 g
- Density of products = 4,934 kg/m3
- Specific gas constant = 410,355 J/kg K
- Specific heat capacity at p=const. (Cp) = 2394,41 J/kgK
- Specific heat capacity at V=const. (Cv) = 1984,06 J/molK
- Specific heat ratio (Cp/Cv) = 1,2068

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 981,2 m/s
- Sound velocity at throat ) = 981,6 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,563
- Pressure ratio (pc/pt) = 1,777

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,000327E+00 | 3,167890E+01 | 64,1831 | 57,0705 |
| H2 = | 1,969754E-01 | 6,237927E+00 | 12,6384 | 1,2576 |
| CO2 = | 1,394975E-01 | 4,417685E+00 | 8,9505 | 19,4422 |
| CO = | 1,265990E-01 | 4,009209E+00 | 8,1229 | 11,2298 |
| N2 = | 5,701337E-02 | 1,805532E+00 | 3,6581 | 5,0578 |
| BHO2 = | 2,620384E-02 | 8,298380E-01 | 1,6813 | 3,6345 |
| B(OH)3 = | 1,171692E-02 | 3,710579E-01 | 0,7518 | 2,2943 |
| H = | 1,027065E-04 | 3,252568E-03 | 0,0066 | 0,0003 |
| OH = | 4,342661E-05 | 1,375258E-03 | 0,0028 | 0,0023 |
| B2O3 = | 3,638117E-05 | 1,152139E-03 | 0,0023 | 0,0080 |
| BHO = | 1,891710E-05 | 5,990772E-04 | 0,0012 | 0,0017 |
| NH3 = | 1,397856E-05 | 4,426809E-04 | 0,0009 | 0,0008 |

| | | | | |
|---|---|---|---|---|
| BO2 = | 1,311114E-06 | 4,152108E-05 | 0,0001 | 0,0002 |
| NO = | 7,490237E-07 | 2,372050E-05 | 0,0000 | 0,0001 |
| CH2O = | 5,845723E-07 | 1,851257E-05 | 0,0000 | 0,0001 |
| BO = | 1,478813E-07 | 4,683189E-06 | 0,0000 | 0,0000 |
| HCN = | 1,344807E-07 | 4,258810E-06 | 0,0000 | 0,0000 |
| HCNO = | 8,506651E-08 | 2,693934E-06 | 0,0000 | 0,0000 |
| CH4 = | 4,858738E-08 | 1,538693E-06 | 0,0000 | 0,0000 |
| O2 = | 4,195631E-08 | 1,328696E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,785753E-08 | 5,655223E-07 | 0,0000 | 0,0000 |
| O = | 1,572876E-08 | 4,981072E-07 | 0,0000 | 0,0000 |
| B2O2 = | 5,207708E-09 | 1,649206E-07 | 0,0000 | 0,0000 |
| H2O2 = | 1,437100E-09 | 4,551090E-08 | 0,0000 | 0,0000 |
| N = | 1,849250E-11 | 5,856310E-10 | 0,0000 | 0,0000 |
| CNO = | 9,292902E-12 | 2,942929E-10 | 0,0000 | 0,0000 |
| BH2 = | 6,218559E-12 | 1,969328E-10 | 0,0000 | 0,0000 |
| NO2 = | 2,599070E-12 | 8,230881E-11 | 0,0000 | 0,0000 |
| N2H4 = | 8,742578E-15 | 2,768649E-13 | 0,0000 | 0,0000 |
| BH = | 1,020189E-15 | 3,230793E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 4,424039E-16 | 1,401029E-14 | 0,0000 | 0,0000 |
| BN = | 2,313110E-16 | 7,325288E-15 | 0,0000 | 0,0000 |
| B = | 1,575531E-16 | 4,989482E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 3,329380E-17 | 1,054367E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,322925E-18 | 7,356371E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,392434E-18 | 4,409638E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,253944E-20 | 1,030477E-18 | 0,0000 | 0,0000 |
| BN(s) = | 1,231479E-20 | 3,899917E-19 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 8,832927E-23 | 2,797261E-21 | 0,0000 | 0,0000 |
| B(s) = | 7,499846E-23 | 2,375094E-21 | 0,0000 | 0,0000 |
| B(l) = | 4,530969E-23 | 1,434893E-21 | 0,0000 | 0,0000 |
| N2O3 = | 3,964919E-23 | 1,255633E-21 | 0,0000 | 0,0000 |
| B4C(s) = | 7,710895E-26 | 2,441930E-24 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 4,845012E-31 | 1,534346E-29 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9473,14 kJ/kg
- Entropy of combustion products = 11,82 kJ/K kg
- Temperature at nozzle exit = 1063,93 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 48,74 mol/kg expl.
- Total mole number of products = 48,954 mol/kg expl.
- Volume of gaseous products (at SATP) = 1208,22 L/kg expl.
- Mass of gaseous products = 985,2 g/kg expl.
- Mass of condensed products = 14,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,212 g
- Mean molecular mass of all products = 20,428 g
- Density of products = 0,232 kg/m3
- Specific gas constant = 405,226 J/kg K
- Specific heat capacity at p=const. (Cp) = 2089,47 J/kgK
- Specific heat capacity at V=const. (Cv) = 1684,24 J/molK
- Specific heat ratio (Cp/Cv) = 1,2406

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 236,08 s
- Vacuum-specific impulse (pa=0) = 254,7 s
- Exhaust (or nozzle exit) velocity = 2315,2 m/s
- Characteristic exhaust velocity (c*) = 1445,9 m/s
- Thrust coefficient (Cf) = 1,601
- Nozzle area expansion ratio (Ae/At) = 9,01
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 721,32 m/s
- Mach number at nozzle exit = 3,21

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 9,259459E-01 | 2,932338E+01 | | 59,9004 | 52,8269 |
| H2 = | 2,654662E-01 | 8,406935E+00 | 17,1733 | 1,6948 | |
| CO2 = | 2,079470E-01 | 6,585384E+00 | | 13,4523 | 28,9823 |
| CO = | 5,814571E-02 | 1,841391E+00 | 3,7615 | 5,1577 | |
| N2 = | 5,701590E-02 | 1,805612E+00 | 3,6884 | 5,0581 | |
| B(OH)3 = | 2,437418E-02 | 7,718953E-01 | | 1,5768 | 4,7726 |
| B2O3(l) = | 6,738760E-03 | 2,134069E-01 | | 0,4359 | 1,4855 |
| BHO2 = | 1,620025E-04 | 5,130387E-03 | | 0,0105 | 0,0225 |
| NH3 = | 9,876811E-06 | 3,127844E-04 | | 0,0006 | 0,0005 |
| CH4 = | 4,379389E-06 | 1,386890E-04 | | 0,0003 | 0,0002 |
| CH2O = | 1,742315E-08 | 5,517662E-07 | | 0,0000 | 0,0000 |
| H = | 7,588373E-09 | 2,403129E-07 | 0,0000 | 0,0000 | |
| HCN = | 3,128530E-09 | 9,907605E-08 | | 0,0000 | 0,0000 |
| HCNO = | 7,451567E-10 | 2,359804E-08 | | 0,0000 | 0,0000 |
| BHO = | 4,382557E-10 | 1,387893E-08 | | 0,0000 | 0,0000 |
| B2O3 = | 1,097835E-10 | 3,476687E-09 | | 0,0000 | 0,0000 |
| OH = | 8,743278E-11 | 2,768871E-09 | | 0,0000 | 0,0000 |
| NH2 = | 3,073659E-13 | 9,733838E-12 | | 0,0000 | 0,0000 |
| NO = | 7,983230E-14 | 2,528174E-12 | | 0,0000 | 0,0000 |
| BO2 = | 1,888345E-14 | 5,980117E-13 | | 0,0000 | 0,0000 |
| BO = | 7,293651E-16 | 2,309795E-14 | 0,0000 | 0,0000 | |
| B2O3(s) = | 4,056554E-16 | 1,284652E-14 | | 0,0000 | 0,0000 |
| B4C(l) = | 8,376605E-17 | 2,652751E-15 | | 0,0000 | 0,0000 |
| B2O2 = | 2,829144E-17 | 8,959492E-16 | | 0,0000 | 0,0000 |
| B4C(s) = | 1,905200E-17 | 6,033495E-16 | | 0,0000 | 0,0000 |
| BHO2(s) = | 1,661321E-17 | 5,261167E-16 | | 0,0000 | 0,0000 |
| H2O2 = | 9,993533E-18 | 3,164808E-16 | | 0,0000 | 0,0000 |
| O2 = | 5,762559E-18 | 1,824920E-16 | 0,0000 | 0,0000 | |
| O = | 2,611661E-18 | 8,270756E-17 | 0,0000 | 0,0000 | |
| CNO = | 5,273002E-19 | 1,669884E-17 | | 0,0000 | 0,0000 |
| C(gr) = | 1,957201E-19 | 6,198175E-18 | | 0,0000 | 0,0000 |
| N2H4 = | 1,036776E-19 | 3,283320E-18 | | 0,0000 | 0,0000 |
| BN(s) = | 3,277048E-20 | 1,037794E-18 | | 0,0000 | 0,0000 |
| BH2 = | 1,828022E-20 | 5,789083E-19 | | 0,0000 | 0,0000 |
| N = | 2,691637E-21 | 8,524029E-20 | 0,0000 | 0,0000 | |
| B(OH)3(s) = | 1,310280E-23 | 4,149470E-22 | | 0,0000 | 0,0000 |
| NO2 = | 1,134314E-23 | 3,592209E-22 | | 0,0000 | 0,0000 |
| N2O3 = | 6,968356E-24 | 2,206778E-22 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,799198E-25 | 5,697801E-24 | | 0,0000 | 0,0000 |
| B(l) = | 1,164376E-29 | 3,687411E-28 | | 0,0000 | 0,0000 |
| B(s) = | 6,081657E-30 | 1,925974E-28 | | 0,0000 | 0,0000 |
| BN = | 4,129022E-31 | 1,307602E-29 | 0,0000 | 0,0000 | |
| BH = | 2,693463E-31 | 8,529812E-30 | 0,0000 | 0,0000 | |
| B = | 1,721773E-32 | 5,452607E-31 | 0,0000 | 0,0000 | |

Excluded products(11):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity : Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 7

**Combustion conditions (Number 7):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 16.95 %**
2. **Hydrogen peroxide ($H_2O_2$), 58.14 %**
3. **Water ($H_2O$, liquid), 24.91 %**

C(0,245) H(2,420) N(0,105) O(1,498) B(0,035)

Molecular weight = 31,21
Oxygen balance = -13,05675 %
Enthalpy of formation = -6916,06 kJ/kg
Internal energy of formation = -6708,21 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3966,78 kJ/kg
- Total enthalpy of combustion prod. = -6916,64 kJ/kg
- Entropy of combustion products = 11,76 kJ/K kg
- Isobaric combustion temperature = 2189,16 K
- Mole number of gaseous products = 48,671 mol/kg expl.
- Total mole number of products = 48,671 mol/kg expl.
- Volume of gaseous products (at SATP) = 1206,52 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,546 g
- Mean molecular mass of all products = 20,546 g
- Density of products = 7,902 kg/m3
- Specific gas constant = 404,655 J/kg K
- Specific heat capacity at p=const. (Cp) = 2449,85 J/kgK
- Specific heat capacity at V=const. (Cv) = 2045,2 J/molK
- Specific heat ratio (Cp/Cv) = 1,1979

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 1,038550E+00 | 3,327798E+01 | 68,3726 | 59,9513 |
| H2 = | 1,470905E-01 | 4,713180E+00 | 9,6837 | 0,9502 |
| CO2 = | 1,376469E-01 | 4,410581E+00 | 9,0619 | 19,4110 |
| CO = | 1,075492E-01 | 3,446169E+00 | 7,0805 | 9,6527 |
| N2 = | 5,253270E-02 | 1,683291E+00 | 3,4585 | 4,7154 |
| BHO2 = | 2,811299E-02 | 9,008168E-01 | 1,8508 | 3,9454 |
| B(OH)3 = | 6,757147E-03 | 2,165174E-01 | 0,4449 | 1,3387 |
| H = | 3,136325E-04 | 1,004964E-02 | 0,0206 | 0,0010 |
| OH = | 2,812255E-04 | 9,011231E-03 | 0,0185 | 0,0153 |
| B2O3 = | 5,798966E-05 | 1,858147E-03 | 0,0038 | 0,0129 |
| BHO = | 3,224829E-05 | 1,033323E-03 | 0,0021 | 0,0029 |
| NH3 = | 1,081069E-05 | 3,464041E-04 | 0,0007 | 0,0006 |
| BO2 = | 8,745904E-06 | 2,802426E-04 | 0,0006 | 0,0012 |
| NO = | 7,909041E-06 | 2,534272E-04 | 0,0005 | 0,0008 |
| O2 = | 1,425552E-06 | 4,567857E-05 | 0,0001 | 0,0001 |
| BO = | 8,276892E-07 | 2,652142E-05 | 0,0001 | 0,0001 |
| CH2O = | 6,308955E-07 | 2,021561E-05 | 0,0000 | 0,0001 |
| O = | 3,935475E-07 | 1,261034E-05 | 0,0000 | 0,0000 |
| HCN = | 1,228783E-07 | 3,937356E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,187412E-07 | 3,804792E-06 | 0,0000 | 0,0000 |
| NH2 = | 6,115658E-08 | 1,959623E-06 | 0,0000 | 0,0000 |
| H2O2 = | 2,493067E-08 | 7,988465E-07 | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 1,442145E-08 | 4,621027E-07 | 0,0000 | 0,0000 |
| N = 3,574959E-10 | 1,145515E-08 | 0,0000 | 0,0000 | |
| NO2 = | 1,434047E-10 | 4,595079E-09 | 0,0000 | 0,0000 |
| CNO = | 6,974215E-11 | 2,234729E-09 | 0,0000 | 0,0000 |
| BH2 = | 2,469241E-11 | 7,912121E-10 | 0,0000 | 0,0000 |
| N2H4 = | 2,918879E-14 | 9,352883E-13 | 0,0000 | 0,0000 |
| BH = 1,814581E-14 | 5,814414E-13 | 0,0000 | 0,0000 | |
| BN = 5,817603E-15 | 1,864119E-13 | 0,0000 | 0,0000 | |
| B = 5,568778E-15 | 1,784388E-13 | 0,0000 | 0,0000 | |
| B4C(l) = | 5,052628E-17 | 1,619000E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 3,516556E-17 | 1,126800E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 7,446527E-18 | 2,386070E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 6,655945E-19 | 2,132746E-17 | 0,0000 | 0,0000 |
| B2O3(s) = | 4,674764E-19 | 1,497922E-17 | 0,0000 | 0,0000 |
| N2O3 = | 3,403264E-20 | 1,090498E-18 | 0,0000 | 0,0000 |
| C(gr) = | 1,677851E-20 | 5,376293E-19 | 0,0000 | 0,0000 |
| BN(s) = | 4,131804E-21 | 1,323943E-19 | 0,0000 | 0,0000 |
| B(s) = | 1,075002E-22 | 3,444600E-21 | 0,0000 | 0,0000 |
| B(l) = | 9,185729E-23 | 2,943358E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 8,329287E-23 | 2,668931E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,638668E-30 | 2,447637E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7401,86 kJ/kg
- Entropy of combustion products = 11,76 kJ/K kg
- Temperature at nozzle throat = 1998,09 K
- Pressure at nozzle throat = 3,944898 MPa
- Mole number of gaseous products = 48,59 mol/kg expl.
- Total mole number of products = 48,59 mol/kg expl.
- Volume of gaseous products (at SATP) = 1204,51 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,58 g
- Mean molecular mass of all products = 20,58 g
- Density of products = 4,887 kg/m3
- Specific gas constant = 403,981 J/kg K
- Specific heat capacity at p=const. (Cp) = 2400,46 J/kgK
- Specific heat capacity at V=const. (Cv) = 1996,48 J/molK
- Specific heat ratio (Cp/Cv) = 1,2023

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 985,1 m/s
- Sound velocity at throat ) = 985,2 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,564
- Pressure ratio (pc/pt) = 1,774

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,030868E+00 | 3,303182E+01 | 67,9801 | 59,5078 |
| H2 = 1,526149E-01 | 4,890197E+00 | 10,0641 | 0,9859 | |
| CO2 = | 1,431731E-01 | 4,587655E+00 | 9,4415 | 20,1903 |
| CO = 1,020235E-01 | 3,269112E+00 | 6,7279 | 9,1568 | |
| N2 = 5,253703E-02 | 1,683430E+00 | 3,4645 | 4,7158 | |
| BHO2 = | 2,584132E-02 | 8,280264E-01 | 1,7041 | 3,6266 |
| B(OH)3 = | 9,092582E-03 | 2,913511E-01 | 0,5996 | 1,8014 |
| H = 1,288806E-04 | 4,129685E-03 | 0,0085 | 0,0004 | |
| OH = | 8,012795E-05 | 2,567518E-03 | 0,0053 | 0,0044 |
| B2O3 = | 3,740105E-05 | 1,198432E-03 | 0,0025 | 0,0083 |
| BHO = | 1,692108E-05 | 5,421976E-04 | 0,0011 | 0,0015 |
| NH3 = | 8,607562E-06 | 2,758098E-04 | 0,0006 | 0,0005 |
| BO2 = | 2,312923E-06 | 7,411237E-05 | 0,0002 | 0,0003 |

| | | | | |
|---|---|---|---|---|
| NO = | 1,649926E-06 | 5,286813E-05 | 0,0001 | 0,0002 |
| CH2O = | 3,692949E-07 | 1,183322E-05 | 0,0000 | 0,0000 |
| BO = | 2,036530E-07 | 6,525597E-06 | 0,0000 | 0,0000 |
| O2 = | 1,636470E-07 | 5,243696E-06 | 0,0000 | 0,0000 |
| HCN = | 7,063434E-08 | 2,263317E-06 | 0,0000 | 0,0000 |
| HCNO = | 6,074573E-08 | 1,946459E-06 | 0,0000 | 0,0000 |
| O = | 4,637906E-08 | 1,486112E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,816662E-08 | 5,821080E-07 | 0,0000 | 0,0000 |
| B2O2 = | 4,960910E-09 | 1,589611E-07 | 0,0000 | 0,0000 |
| H2O2 = | 3,544522E-09 | 1,135762E-07 | 0,0000 | 0,0000 |
| N = | 3,819745E-11 | 1,223950E-09 | 0,0000 | 0,0000 |
| CNO = | 1,147168E-11 | 3,675840E-10 | 0,0000 | 0,0000 |
| NO2 = | 1,040943E-11 | 3,335465E-10 | 0,0000 | 0,0000 |
| BH2 = | 4,755030E-12 | 1,523641E-10 | 0,0000 | 0,0000 |
| N2H4 = | 5,990514E-15 | 1,919524E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,554915E-15 | 4,982372E-14 | 0,0000 | 0,0000 |
| BH = | 1,292407E-15 | 4,141225E-14 | 0,0000 | 0,0000 |
| BN = | 3,383214E-16 | 1,084074E-14 | 0,0000 | 0,0000 |
| B = | 2,726406E-16 | 8,736147E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,898242E-17 | 6,082485E-16 | 0,0000 | 0,0000 |
| B4C(s) = | 4,548458E-18 | 1,457450E-16 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,296934E-18 | 4,155731E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,009336E-18 | 3,234187E-17 | 0,0000 | 0,0000 |
| C(gr) = | 1,689977E-20 | 5,415146E-19 | 0,0000 | 0,0000 |
| BN(s) = | 5,784800E-21 | 1,853608E-19 | 0,0000 | 0,0000 |
| N2O3 = | 3,423433E-22 | 1,096961E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,801336E-23 | 2,179334E-21 | 0,0000 | 0,0000 |
| B(s) = | 5,422640E-23 | 1,737562E-21 | 0,0000 | 0,0000 |
| B(l) = | 3,063691E-23 | 9,816900E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9629,94 kJ/kg
- Entropy of combustion products = 11,76 kJ/K kg
- Temperature at nozzle exit = 1099,75 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 47,924 mol/kg expl.
- Total mole number of products = 48,081 mol/kg expl.
- Volume of gaseous products (at SATP) = 1187,98 L/kg expl.
- Mass of gaseous products = 989,1 g/kg expl.
- Mass of condensed products = 11,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,638 g
- Mean molecular mass of all products = 20,799 g
- Density of products = 0,228 kg/m3
- Specific gas constant = 398,436 J/kg K
- Specific heat capacity at p=const. (Cp) = 2088,45 J/kgK
- Specific heat capacity at V=const. (Cv) = 1690,01 J/molK
- Specific heat ratio (Cp/Cv) = 1,2358

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 237,54 s
- Vacuum-specific impulse (pa=0) = 256,35 s
- Exhaust (or nozzle exit) velocity = 2329,5 m/s
- Characteristic exhaust velocity (c*) = 1454,0 m/s
- Thrust coefficient (Cf) = 1,602
- Nozzle area expansion ratio (Ae/At) = 9,06
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 725,84 m/s
- Mach number at nozzle exit = 3,209

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | |
|---|---|---|---|---|
| H2O = | 9,649538E-01 | 3,091975E+01 | 64,3076 | 55,7029 |
| H2 = | 2,077214E-01 | 6,655961E+00 | 13,8432 | 1,3418 |
| CO2 = | 1,982362E-01 | 6,352028E+00 | 13,2111 | 27,9553 |
| N2 = | 5,253948E-02 | 1,683508E+00 | 3,5014 | 4,7160 |
| CO = | 4,696085E-02 | 1,504754E+00 | 3,1296 | 4,2148 |
| B(OH)3 = | 2,488734E-02 | 7,974582E-01 | 1,6586 | 4,9307 |
| B2O3(l) = | 4,916136E-03 | 1,575264E-01 | 0,3276 | 1,0965 |
| BHO2 = | 3,085348E-04 | 9,886297E-03 | 0,0206 | 0,0433 |
| NH3 = | 5,508689E-06 | 1,765134E-04 | 0,0004 | 0,0003 |
| H = | 1,502691E-08 | 4,815032E-07 | 0,0000 | 0,0000 |
| CH2O = | 1,082325E-08 | 3,468066E-07 | 0,0000 | 0,0000 |
| HCN = | 1,640977E-09 | 5,258137E-08 | 0,0000 | 0,0000 |
| BHO = | 9,651405E-10 | 3,092573E-08 | 0,0000 | 0,0000 |
| HCNO = | 5,407703E-10 | 1,732775E-08 | 0,0000 | 0,0000 |
| B2O3 = | 4,590609E-10 | 1,470956E-08 | 0,0000 | 0,0000 |
| OH = | 2,914164E-10 | 9,337775E-09 | 0,0000 | 0,0000 |
| NH2 = | 4,630846E-13 | 1,483849E-11 | 0,0000 | 0,0000 |
| NO = | 3,520211E-13 | 1,127972E-11 | 0,0000 | 0,0000 |
| BO2 = | 1,142027E-13 | 3,659366E-12 | 0,0000 | 0,0000 |
| B4C(l) = | 4,008110E-15 | 1,284308E-13 | 0,0000 | 0,0000 |
| BO = | 3,723400E-15 | 1,193079E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 5,492476E-16 | 1,759939E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 3,506454E-16 | 1,123564E-14 | 0,0000 | 0,0000 |
| B2O2 = | 1,446236E-16 | 4,634136E-15 | 0,0000 | 0,0000 |
| O2 = | 6,196205E-17 | 1,985433E-15 | 0,0000 | 0,0000 |
| H2O2 = | 5,135776E-17 | 1,645643E-15 | 0,0000 | 0,0000 |
| O = | 2,140520E-17 | 6,858811E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,411646E-17 | 4,523298E-16 | 0,0000 | 0,0000 |
| CNO = | 1,132605E-18 | 3,629174E-17 | 0,0000 | 0,0000 |
| N2H4 = | 8,565042E-20 | 2,744473E-18 | 0,0000 | 0,0000 |
| C(gr) = | 7,995773E-20 | 2,562064E-18 | 0,0000 | 0,0000 |
| BH2 = | 4,727529E-20 | 1,514829E-18 | 0,0000 | 0,0000 |
| BN(s) = | 2,035996E-20 | 6,523886E-19 | 0,0000 | 0,0000 |
| N = | 1,473950E-20 | 4,722936E-19 | 0,0000 | 0,0000 |
| B(s) = | 3,827226E-22 | 1,226347E-20 | 0,0000 | 0,0000 |
| N2O3 = | 1,379214E-22 | 4,419378E-21 | 0,0000 | 0,0000 |
| NO2 = | 1,333419E-22 | 4,272638E-21 | 0,0000 | 0,0000 |
| B = | 1,058781E-22 | 3,392622E-21 | 0,0000 | 0,0000 |
| B(l) = | 9,459581E-23 | 3,031108E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,378865E-23 | 2,043962E-21 | 0,0000 | 0,0000 |
| BH = | 4,593466E-28 | 1,471872E-26 | 0,0000 | 0,0000 |
| BN = | 1,850205E-29 | 5,928560E-28 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 6,840948E-35 | 2,192026E-33 | 0,0000 | 0,0000 |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; CH4; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 8

**Combustion conditions (Number 8):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 50.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 47.50 %**
3. **Water ($H_2O$, liquid), 2.50 %**

C(1,242) H(4,129) N(0,532) O(1,571) B(0,177)

Molecular weight = 53,58
Oxygen balance = -96,84287 %
Enthalpy of formation = -2293,11 kJ/kg
Internal energy of formation = -2101,21 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -2883,85 kJ/kg
- Total enthalpy of combustion prod. = -2292,61 kJ/kg
- Entropy of combustion products = 12,46 kJ/K kg
- Isobaric combustion temperature = 1567,09 K
- Mole number of gaseous products = 64,175 mol/kg expl.
- Total mole number of products = 65,762 mol/kg expl.
- Volume of gaseous products (at SATP) = 1590,83 L/kg expl.
- Mass of gaseous products = 889,5 g/kg expl.
- Mass of condensed products = 110,5 g/kg expl.
- Mean molecular mass of gaseous prod. = 13,861 g
- Mean molecular mass of all products = 15,206 g
- Density of products = 8,372 kg/m3
- Specific gas constant = 533,55 J/kg K
- Specific heat capacity at p=const. (Cp) = 2476,54 J/kgK
- Specific heat capacity at V=const. (Cv) = 1942,99 J/molK
- Specific heat ratio (Cp/Cv) = 1,2746

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 1,820717E+00 | 3,398091E+01 | 51,6724 | 6,8506 |
| CO = | 1,153461E+00 | 2,152760E+01 | 32,7355 | 60,2988 |
| N2 = | 2,650067E-01 | 4,945947E+00 | 7,5210 | 13,8551 |
| H2O = | 1,022323E-01 | 1,908011E+00 | 2,9014 | 3,4373 |
| B2O3(l) = | 8,504468E-02 | 1,587230E+00 | 2,4136 | 11,0485 |
| CH4 = | 6,607920E-02 | 1,233268E+00 | 1,8753 | 1,9785 |
| CO2 = | 2,136859E-02 | 3,988123E-01 | 0,6064 | 1,7552 |
| BHO2 = | 4,584276E-03 | 8,555854E-02 | 0,1301 | 0,3747 |
| B(OH)3 = | 2,662100E-03 | 4,968405E-02 | 0,0756 | 0,3072 |
| NH3 = | 1,573647E-03 | 2,936972E-02 | 0,0447 | 0,0500 |
| HCN = | 6,094177E-04 | 1,137385E-02 | 0,0173 | 0,0307 |
| C2H4 = | 8,863675E-05 | 1,654270E-03 | 0,0025 | 0,0046 |
| BHO = | 5,323638E-05 | 9,935760E-04 | 0,0015 | 0,0028 |
| CH2O = | 4,712824E-05 | 8,795769E-04 | 0,0013 | 0,0026 |
| C2H6 = | 2,561251E-05 | 4,780185E-04 | 0,0007 | 0,0014 |
| H = | 1,195107E-05 | 2,230486E-04 | 0,0003 | 0,0000 |
| B2O3 = | 5,006906E-06 | 9,344628E-05 | 0,0001 | 0,0007 |
| HCNO = | 3,515896E-06 | 6,561885E-05 | 0,0001 | 0,0003 |
| CH3OH = | 7,812306E-07 | 1,458048E-05 | 0,0000 | 0,0000 |
| NH2 = | 2,059354E-08 | 3,843471E-07 | 0,0000 | 0,0000 |
| B2O2 = | 9,414077E-09 | 1,756994E-07 | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| BO = 8,097401E-09 | 1,511257E-07 | 0,0000 | 0,0000 | |
| BO2 = 1,153823E-09 | 2,153436E-08 | 0,0000 | 0,0000 | |
| BH2 = 4,688501E-10 | 8,750373E-09 | 0,0000 | 0,0000 | |
| NO = 1,184622E-10 | 2,210916E-09 | 0,0000 | 0,0000 | |
| CNO = 2,630526E-12 | 4,909476E-11 | 0,0000 | 0,0000 | |
| N = 3,485327E-14 | 6,504832E-13 | 0,0000 | 0,0000 | |
| H2O2 = 7,542515E-15 | 1,407696E-13 | 0,0000 | 0,0000 | |
| B4C(s) = 8,687263E-16 | 1,621345E-14 | 0,0000 | 0,0000 | |
| BH = 7,661481E-16 | 1,429899E-14 | 0,0000 | 0,0000 | |
| B4C(l) = 7,371963E-16 | 1,375865E-14 | 0,0000 | 0,0000 | |
| BN(s) = 1,654419E-16 | 3,087722E-15 | 0,0000 | 0,0000 | |
| C(gr) = 1,330528E-16 | 2,483227E-15 | 0,0000 | 0,0000 | |
| B2O3(s) = 1,160819E-16 | 2,166492E-15 | 0,0000 | 0,0000 | |
| BN = 7,307114E-17 | 1,363762E-15 | 0,0000 | 0,0000 | |
| B = 7,037124E-18 | 1,313372E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = 4,638441E-18 | 8,656944E-17 | 0,0000 | 0,0000 | |
| NO2 = 2,616587E-19 | 4,883461E-18 | 0,0000 | 0,0000 | |
| N2O3 = 9,306108E-20 | 1,736843E-18 | 0,0000 | 0,0000 | |
| B(s) = 1,083494E-20 | 2,022177E-19 | 0,0000 | 0,0000 | |
| B(l) = 3,096007E-21 | 5,778227E-20 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 2,765046E-23 | 5,160538E-22 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 2,377622E-24 | 4,437470E-23 | 0,0000 | 0,0000 | |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -2769,14 kJ/kg
- Entropy of combustion products = 12,46 kJ/K kg
- Temperature at nozzle throat = 1422,34 K
- Pressure at nozzle throat = 3,832146 MPa
- Mole number of gaseous products = 63,224 mol/kg expl.
- Total mole number of products = 64,836 mol/kg expl.
- Volume of gaseous products (at SATP) = 1567,27 L/kg expl.
- Mass of gaseous products = 887,8 g/kg expl.
- Mass of condensed products = 112,2 g/kg expl.
- Mean molecular mass of gaseous prod. = 14,042 g
- Mean molecular mass of all products = 15,423 g
- Density of products = 5,126 kg/m3
- Specific gas constant = 525,647 J/kg K
- Specific heat capacity at p=const. (Cp) = 2439,82 J/kgK
- Specific heat capacity at V=const. (Cv) = 1914,18 J/molK
- Specific heat ratio (Cp/Cv) = 1,2746

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 976,2 m/s
- Sound velocity at throat ) = 976,2 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,547
- Pressure ratio (pc/pt) = 1,827

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = 1,756547E+00 | 3,278328E+01 | 50,5633 | 6,6091 | |
| CO = 1,118885E+00 | 2,088229E+01 | 32,2078 | 58,4913 | |
| N2 = 2,653179E-01 | 4,951754E+00 | 7,6373 | 13,8713 | |
| H2O = 1,180445E-01 | 2,203121E+00 | 3,3980 | 3,9690 | |
| CH4 = 9,114993E-02 | 1,701175E+00 | 2,6238 | 2,7292 | |
| B2O3(l) = 8,635999E-02 | 1,611778E+00 | 2,4859 | 11,2194 | |
| CO2 = 3,128974E-02 | 5,839753E-01 | 0,9007 | 2,5701 | |
| B(OH)3 = 2,872269E-03 | 5,360653E-02 | 0,0827 | 0,3314 | |
| BHO2 = 1,800155E-03 | 3,359715E-02 | 0,0518 | 0,1471 | |
| NH3 = 1,286980E-03 | 2,401953E-02 | 0,0370 | 0,0409 | |
| HCN = 2,765870E-04 | 5,162075E-03 | 0,0080 | 0,0140 | |
| C2H4 = 5,828634E-05 | 1,087826E-03 | 0,0017 | 0,0031 | |

| | | | | |
|---|---|---|---|---|
| C2H6 = | 2,761539E-05 | 5,153992E-04 | 0,0008 | 0,0015 |
| CH2O = | 2,699559E-05 | 5,038315E-04 | 0,0008 | 0,0015 |
| BHO = | 7,049193E-06 | 1,315625E-04 | 0,0002 | 0,0004 |
| H = | 2,721282E-06 | 5,078859E-05 | 0,0001 | 0,0000 |
| HCNO = | 1,737335E-06 | 3,242471E-05 | 0,0001 | 0,0001 |
| CH3OH = | 4,889661E-07 | 9,125807E-06 | 0,0000 | 0,0000 |
| B2O3 = | 4,474644E-07 | 8,351242E-06 | 0,0000 | 0,0001 |
| NH2 = | 3,522557E-09 | 6,574316E-08 | 0,0000 | 0,0000 |
| BO = | 3,126054E-10 | 5,834305E-09 | 0,0000 | 0,0000 |
| B2O2 = | 2,541019E-10 | 4,742425E-09 | 0,0000 | 0,0000 |
| BO2 = | 6,602123E-11 | 1,232186E-09 | 0,0000 | 0,0000 |
| NO = | 1,313402E-11 | 2,451264E-10 | 0,0000 | 0,0000 |
| BH2 = | 1,183259E-11 | 2,208373E-10 | 0,0000 | 0,0000 |
| CNO = | 2,217946E-13 | 4,139458E-12 | 0,0000 | 0,0000 |
| N = | 1,116595E-15 | 2,083955E-14 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,725107E-16 | 1,441774E-14 | 0,0000 | 0,0000 |
| H2O2 = | 6,338197E-16 | 1,182928E-14 | 0,0000 | 0,0000 |
| C(gr) = | 1,482680E-16 | 2,767197E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,481284E-16 | 2,764592E-15 | 0,0000 | 0,0000 |
| BN(s) = | 9,715111E-17 | 1,813178E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,525315E-18 | 1,031216E-16 | 0,0000 | 0,0000 |
| BH = | 3,977944E-18 | 7,424227E-17 | 0,0000 | 0,0000 |
| BN = | 2,941844E-19 | 5,490503E-18 | 0,0000 | 0,0000 |
| B = | 1,932962E-20 | 3,607579E-19 | 0,0000 | 0,0000 |
| NO2 = | 7,856240E-21 | 1,466248E-19 | 0,0000 | 0,0000 |
| B(s) = | 1,287616E-21 | 2,403140E-20 | 0,0000 | 0,0000 |
| B(l) = | 2,488197E-22 | 4,643842E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,544814E-23 | 4,749507E-22 | 0,0000 | 0,0000 |
| N2O3 = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(l) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -4631,8 kJ/kg
- Entropy of combustion products = 12,46 kJ/K kg
- Temperature at nozzle exit = 616,47 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 63,224 mol/kg expl.
- Total mole number of products = 64,836 mol/kg expl.
- Volume of gaseous products (at SATP) = 1567,27 L/kg expl.
- Mass of gaseous products = 887,8 g/kg expl.
- Mass of condensed products = 112,2 g/kg expl.
- Mean molecular mass of gaseous prod. = 14,042 g
- Mean molecular mass of all products = 15,423 g
- Density of products = 0,309 kg/m3
- Specific gas constant = 525,647 J/kg K
- Specific heat capacity at p=const. (Cp) = 2165,81 J/kgK
- Specific heat capacity at V=const. (Cv) = 1640,16 J/molK
- Specific heat ratio (Cp/Cv) = 1,3205

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 220,56 s
- Vacuum-specific impulse (pa=0) = 235,54 s
- Exhaust (or nozzle exit) velocity = 2163,0 m/s
- Characteristic exhaust velocity (c*) = 1398,9 m/s
- Thrust coefficient (Cf) = 1,546
- Nozzle area expansion ratio (Ae/At) = 7,5
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 642,67 m/s
- Mach number at nozzle exit = 3,366

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | |
|---|---|---|---|---|
| H2 = | 1,756547E+00 | 3,278328E+01 | 50,5633 | 6,6091 |
| CO = | 1,118885E+00 | 2,088229E+01 | 32,2078 | 58,4913 |
| N2 = | 2,653179E-01 | 4,951754E+00 | 7,6373 | 13,8713 |
| H2O = | 1,180445E-01 | 2,203121E+00 | 3,3980 | 3,9690 |
| CH4 = | 9,114993E-02 | 1,701175E+00 | 2,6238 | 2,7292 |
| B2O3(l) = | 8,635999E-02 | 1,611778E+00 | 2,4859 | 11,2194 |
| CO2 = | 3,128974E-02 | 5,839753E-01 | 0,9007 | 2,5701 |
| B(OH)3 = | 2,872269E-03 | 5,360653E-02 | 0,0827 | 0,3314 |
| BHO2 = | 1,800155E-03 | 3,359715E-02 | 0,0518 | 0,1471 |
| NH3 = | 1,286980E-03 | 2,401953E-02 | 0,0370 | 0,0409 |
| HCN = | 2,765870E-04 | 5,162075E-03 | 0,0080 | 0,0140 |
| C2H4 = | 5,828634E-05 | 1,087826E-03 | 0,0017 | 0,0031 |
| C2H6 = | 2,761539E-05 | 5,153992E-04 | 0,0008 | 0,0015 |
| CH2O = | 2,699559E-05 | 5,038315E-04 | 0,0008 | 0,0015 |
| BHO = | 7,049193E-06 | 1,315625E-04 | 0,0002 | 0,0004 |
| H = | 2,721282E-06 | 5,078859E-05 | 0,0001 | 0,0000 |
| HCNO = | 1,737335E-06 | 3,242471E-05 | 0,0001 | 0,0001 |
| CH3OH = | 4,889661E-07 | 9,125807E-06 | 0,0000 | 0,0000 |
| B2O3 = | 4,474644E-07 | 8,351242E-06 | 0,0000 | 0,0001 |
| NH2 = | 3,522557E-09 | 6,574316E-08 | 0,0000 | 0,0000 |
| BO = | 3,126054E-10 | 5,834305E-09 | 0,0000 | 0,0000 |
| B2O2 = | 2,541019E-10 | 4,742425E-09 | 0,0000 | 0,0000 |
| BO2 = | 6,602123E-11 | 1,232186E-09 | 0,0000 | 0,0000 |
| NO = | 1,313402E-11 | 2,451264E-10 | 0,0000 | 0,0000 |
| BH2 = | 1,183259E-11 | 2,208373E-10 | 0,0000 | 0,0000 |
| CNO = | 2,217946E-13 | 4,139458E-12 | 0,0000 | 0,0000 |
| N = | 1,116595E-15 | 2,083955E-14 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,725107E-16 | 1,441774E-14 | 0,0000 | 0,0000 |
| H2O2 = | 6,338197E-16 | 1,182928E-14 | 0,0000 | 0,0000 |
| C(gr) = | 1,482680E-16 | 2,767197E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,481284E-16 | 2,764592E-15 | 0,0000 | 0,0000 |
| BN(s) = | 9,715111E-17 | 1,813178E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,525315E-18 | 1,031216E-16 | 0,0000 | 0,0000 |
| BH = | 3,977944E-18 | 7,424227E-17 | 0,0000 | 0,0000 |
| BN = | 2,941844E-19 | 5,490503E-18 | 0,0000 | 0,0000 |
| B = | 1,932962E-20 | 3,607579E-19 | 0,0000 | 0,0000 |
| NO2 = | 7,856240E-21 | 1,466248E-19 | 0,0000 | 0,0000 |
| B(s) = | 1,287616E-21 | 2,403140E-20 | 0,0000 | 0,0000 |
| B(l) = | 2,488197E-22 | 4,643842E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,544814E-23 | 4,749507E-22 | 0,0000 | 0,0000 |
| N2O3 = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(l) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Excluded products(12):

- ---

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 9

**Combustion conditions (Number 9):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 40.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 57.00 %**
3. **Water ($H_2O$, liquid), 3.00 %**

C(0,880) H(3,508) N(0,377) O(1,670) B(0,126)

Molecular weight = 47,46
Oxygen balance = -68,53736 %
Enthalpy of formation = -3041,23 kJ/kg
Internal energy of formation = -2850,35 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3474,46 kJ/kg
- Total enthalpy of combustion prod. = -3041,51 kJ/kg
- Entropy of combustion products = 12,64 kJ/K kg
- Isobaric combustion temperature = 1897,61 K
- Mole number of gaseous products = 60,087 mol/kg expl.
- Total mole number of products = 60,344 mol/kg expl.
- Volume of gaseous products (at SATP) = 1489,49 L/kg expl.
- Mass of gaseous products = 982,0 g/kg expl.
- Mass of condensed products = 17,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 16,344 g
- Mean molecular mass of all products = 16,571 g
- Density of products = 7,384 kg/m3
- Specific gas constant = 499,56 J/kg K
- Specific heat capacity at p=const. (Cp) = 2417,87 J/kgK
- Specific heat capacity at V=const. (Cv) = 1918,31 J/molK
- Specific heat ratio (Cp/Cv) = 1,2604

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 1,220357E+00 | 2,571514E+01 | 42,6141 | 5,1842 | |
| CO = | 8,102332E-01 | 1,707308E+01 | 28,2928 | 47,8217 | |
| H2O = | 4,617497E-01 | 9,729902E+00 | | 16,1240 | 17,5287 |
| N2 = | 1,883157E-01 | 3,968153E+00 | 6,5759 | 11,1160 | |
| BHO2 = | 7,837998E-02 | 1,651608E+00 | | 2,7370 | 7,2337 |
| CO2 = | 6,937490E-02 | 1,461855E+00 | | 2,4225 | 6,4336 |
| B(OH)3 = | 2,092774E-02 | 4,409854E-01 | | 0,7308 | 2,7266 |
| B2O3(l) = | 1,222689E-02 | 2,576427E-01 | | 0,4270 | 1,7934 |
| B2O3 = | 6,497488E-04 | 1,369138E-02 | | 0,0227 | 0,0953 |
| BHO = | 6,344033E-04 | 1,336803E-02 | | 0,0222 | 0,0372 |
| NH3 = | 4,149608E-04 | 8,743976E-03 | | 0,0145 | 0,0149 |
| CH4 = | 2,152092E-04 | 4,534848E-03 | | 0,0075 | 0,0073 |
| H = | 1,821914E-04 | 3,839102E-03 | 0,0064 | 0,0004 | |
| HCN = | 5,093100E-05 | 1,073209E-03 | | 0,0018 | 0,0029 |
| CH2O = | 2,289633E-05 | 4,824672E-04 | | 0,0008 | 0,0014 |
| HCNO = | 2,350822E-06 | 4,953609E-05 | | 0,0001 | 0,0002 |
| BO = | 1,489597E-06 | 3,138850E-05 | 0,0001 | 0,0001 | |
| B2O2 = | 1,021481E-06 | 2,152445E-05 | | 0,0000 | 0,0001 |
| BO2 = | 1,020731E-06 | 2,150864E-05 | | 0,0000 | 0,0001 |
| NH2 = | 1,488368E-07 | 3,136261E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| CH3OH = | 9,225007E-08 | 1,943876E-06 | 0,0000 | 0,0000 |
| NO = | 6,020294E-08 | 1,268585E-06 | 0,0000 | 0,0000 |
| C2H4 = | 3,324098E-08 | 7,004477E-07 | 0,0000 | 0,0000 |
| BH2 = | 5,447236E-09 | 1,147831E-07 | 0,0000 | 0,0000 |
| C2H6 = | 1,159284E-09 | 2,442822E-08 | 0,0000 | 0,0000 |
| CNO = | 6,906044E-11 | 1,455229E-09 | 0,0000 | 0,0000 |
| H2O2 = | 2,816004E-11 | 5,933830E-10 | 0,0000 | 0,0000 |
| N = | 1,614372E-11 | 3,401774E-10 | 0,0000 | 0,0000 |
| BH = | 2,502229E-13 | 5,272650E-12 | 0,0000 | 0,0000 |
| BN = | 3,922319E-14 | 8,265036E-13 | 0,0000 | 0,0000 |
| B = | 1,302283E-14 | 2,744146E-13 | 0,0000 | 0,0000 |
| NO2 = | 1,153912E-14 | 2,431502E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,872034E-15 | 3,944714E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 8,035240E-17 | 1,693171E-15 | 0,0000 | 0,0000 |
| BN(s) = | 6,235044E-18 | 1,313837E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,616702E-18 | 1,183541E-16 | 0,0000 | 0,0000 |
| B4C(s) = | 4,483659E-18 | 9,447882E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,246655E-18 | 6,841291E-17 | 0,0000 | 0,0000 |
| B(s) = | 1,429386E-20 | 3,011976E-19 | 0,0000 | 0,0000 |
| B(l) = | 7,983137E-21 | 1,682192E-19 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,813325E-25 | 3,821004E-24 | 0,0000 | 0,0000 |
| N2O3 = | 1,446558E-26 | 3,048159E-25 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,781518E-27 | 3,753981E-26 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -3583,51 kJ/kg
- Entropy of combustion products = 12,64 kJ/K kg
- Temperature at nozzle throat = 1732,16 K
- Pressure at nozzle throat = 3,841721 MPa
- Mole number of gaseous products = 59,693 mol/kg expl.
- Total mole number of products = 60,396 mol/kg expl.
- Volume of gaseous products (at SATP) = 1479,72 L/kg expl.
- Mass of gaseous products = 951,0 g/kg expl.
- Mass of condensed products = 48,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,932 g
- Mean molecular mass of all products = 16,557 g
- Density of products = 4,469 kg/m3
- Specific gas constant = 496,284 J/kg K
- Specific heat capacity at p=const. (Cp) = 2392,62 J/kgK
- Specific heat capacity at V=const. (Cv) = 1896,33 J/molK
- Specific heat ratio (Cp/Cv) = 1,2617

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1041,2 m/s
- Sound velocity at throat) = 1041,5 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,549
- Pressure ratio (pc/pt) = 1,822

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = | 1,233264E+00 | 2,598711E+01 | 43,0281 | 5,2390 |
| CO = | 7,979009E-01 | 1,681322E+01 | 27,8384 | 47,0938 |
| H2O = | 4,720519E-01 | 9,946988E+00 | 16,4697 | 17,9198 |
| N2 = | 1,883720E-01 | 3,969339E+00 | 6,5722 | 11,1193 |
| CO2 = | 8,169780E-02 | 1,721521E+00 | 2,8504 | 7,5764 |
| BHO2 = | 4,009629E-02 | 8,449014E-01 | 1,3989 | 3,7005 |
| B2O3(l) = | 3,337075E-02 | 7,031822E-01 | 1,1643 | 4,8948 |
| B(OH)3 = | 1,845987E-02 | 3,889829E-01 | 0,6441 | 2,4051 |
| NH3 = | 3,266431E-04 | 6,882962E-03 | 0,0114 | 0,0117 |
| CH4 = | 2,582404E-04 | 5,441592E-03 | 0,0090 | 0,0087 |
| BHO = | 1,593972E-04 | 3,358788E-03 | 0,0056 | 0,0093 |

| | | | | |
|---|---|---|---|---|
| B2O3 = | 1,212232E-04 | 2,554393E-03 | 0,0042 | 0,0178 |
| H = | 6,269399E-05 | 1,321076E-03 | 0,0022 | 0,0001 |
| HCN = | 2,796836E-05 | 5,893440E-04 | 0,0010 | 0,0016 |
| CH2O = | 1,347977E-05 | 2,840433E-04 | 0,0005 | 0,0009 |
| HCNO = | 1,206398E-06 | 2,542098E-05 | 0,0000 | 0,0001 |
| BO = | 1,525985E-07 | 3,215528E-06 | 0,0000 | 0,0000 |
| BO2 = | 1,226424E-07 | 2,584298E-06 | 0,0000 | 0,0000 |
| B2O2 = | 8,629303E-08 | 1,818350E-06 | 0,0000 | 0,0000 |
| CH3OH = | 5,205361E-08 | 1,096864E-06 | 0,0000 | 0,0000 |
| NH2 = | 3,680131E-08 | 7,754704E-07 | 0,0000 | 0,0000 |
| C2H4 = | 2,227419E-08 | 4,693575E-07 | 0,0000 | 0,0000 |
| NO = | 1,024723E-08 | 2,159277E-07 | 0,0000 | 0,0000 |
| C2H6 = | 1,023325E-09 | 2,156331E-08 | 0,0000 | 0,0000 |
| BH2 = | 4,111571E-10 | 8,663825E-09 | 0,0000 | 0,0000 |
| CNO = | 9,440370E-12 | 1,989257E-10 | 0,0000 | 0,0000 |
| H2O2 = | 3,290217E-12 | 6,933083E-11 | 0,0000 | 0,0000 |
| N = | 1,194330E-12 | 2,516671E-11 | 0,0000 | 0,0000 |
| BH = | 5,867394E-15 | 1,236366E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 9,031196E-16 | 1,903037E-14 | 0,0000 | 0,0000 |
| BN = | 7,403521E-16 | 1,560056E-14 | 0,0000 | 0,0000 |
| NO2 = | 6,233833E-16 | 1,313581E-14 | 0,0000 | 0,0000 |
| B = | 1,953901E-16 | 4,117224E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 9,408557E-17 | 1,982553E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,663407E-18 | 1,193383E-16 | 0,0000 | 0,0000 |
| BN(s) = | 4,994174E-18 | 1,052363E-16 | 0,0000 | 0,0000 |
| C(gr) = | 3,464029E-18 | 7,299336E-17 | 0,0000 | 0,0000 |
| B(s) = | 3,416337E-21 | 7,198840E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,407212E-21 | 2,965250E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,070029E-22 | 2,254744E-21 | 0,0000 | 0,0000 |
| N2O3 = | 5,292522E-24 | 1,115230E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,657298E-25 | 1,613531E-23 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -5751,47 kJ/kg
- Entropy of combustion products = 12,64 kJ/K kg
- Temperature at nozzle exit = 769,24 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 59,693 mol/kg expl.
- Total mole number of products = 60,396 mol/kg expl.
- Volume of gaseous products (at SATP) = 1479,72 L/kg expl.
- Mass of gaseous products = 951,0 g/kg expl.
- Mass of condensed products = 48,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,932 g
- Mean molecular mass of all products = 16,557 g
- Density of products = 0,262 kg/m3
- Specific gas constant = 496,284 J/kg K
- Specific heat capacity at p=const. (Cp) = 2086,77 J/kgK
- Specific heat capacity at V=const. (Cv) = 1590,49 J/molK
- Specific heat ratio (Cp/Cv) = 1,312

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 237,4 s
- Vacuum-specific impulse (pa=0) = 253,8 s
- Exhaust (or nozzle exit) velocity = 2328,1 m/s
- Characteristic exhaust velocity (c*) = 1504,5 m/s
- Thrust coefficient (Cf) = 1,547
- Nozzle area expansion ratio (Ae/At) = 7,63
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 694,03 m/s
- Mach number at nozzle exit = 3,354

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 1,233264E+00 | 2,598711E+01 | 43,0281 | 5,2390 | |
| CO = | 7,979009E-01 | 1,681322E+01 | 27,8384 | 47,0938 | |
| H2O = | 4,720519E-01 | 9,946988E+00 | | 16,4697 | 17,9198 |
| N2 = | 1,883720E-01 | 3,969339E+00 | 6,5722 | 11,1193 | |
| CO2 = | 8,169780E-02 | 1,721521E+00 | | 2,8504 | 7,5764 |
| BHO2 = | 4,009629E-02 | 8,449014E-01 | | 1,3989 | 3,7005 |
| B2O3(l) = | 3,337075E-02 | 7,031822E-01 | | 1,1643 | 4,8948 |
| B(OH)3 = | 1,845987E-02 | 3,889829E-01 | | 0,6441 | 2,4051 |
| NH3 = | 3,266431E-04 | 6,882962E-03 | | 0,0114 | 0,0117 |
| CH4 = | 2,582404E-04 | 5,441592E-03 | | 0,0090 | 0,0087 |
| BHO = | 1,593972E-04 | 3,358788E-03 | | 0,0056 | 0,0093 |
| B2O3 = | 1,212232E-04 | 2,554393E-03 | | 0,0042 | 0,0178 |
| H = | 6,269399E-05 | 1,321076E-03 | 0,0022 | 0,0001 | |
| HCN = | 2,796836E-05 | 5,893440E-04 | | 0,0010 | 0,0016 |
| CH2O = | 1,347977E-05 | 2,840433E-04 | | 0,0005 | 0,0009 |
| HCNO = | 1,206398E-06 | 2,542098E-05 | | 0,0000 | 0,0001 |
| BO = | 1,525985E-07 | 3,215528E-06 | 0,0000 | 0,0000 | |
| BO2 = | 1,226424E-07 | 2,584298E-06 | | 0,0000 | 0,0000 |
| B2O2 = | 8,629303E-08 | 1,818350E-06 | | 0,0000 | 0,0000 |
| CH3OH = | 5,205361E-08 | 1,096864E-06 | | 0,0000 | 0,0000 |
| NH2 = | 3,680131E-08 | 7,754704E-07 | | 0,0000 | 0,0000 |
| C2H4 = | 2,227419E-08 | 4,693575E-07 | | 0,0000 | 0,0000 |
| NO = | 1,024723E-08 | 2,159277E-07 | | 0,0000 | 0,0000 |
| C2H6 = | 1,023325E-09 | 2,156331E-08 | | 0,0000 | 0,0000 |
| BH2 = | 4,111571E-10 | 8,663825E-09 | | 0,0000 | 0,0000 |
| CNO = | 9,440370E-12 | 1,989257E-10 | | 0,0000 | 0,0000 |
| H2O2 = | 3,290217E-12 | 6,933083E-11 | | 0,0000 | 0,0000 |
| N = | 1,194330E-12 | 2,516671E-11 | 0,0000 | 0,0000 | |
| BH = | 5,867394E-15 | 1,236366E-13 | 0,0000 | 0,0000 | |
| B4C(l) = | 9,031196E-16 | 1,903037E-14 | | 0,0000 | 0,0000 |
| BN = | 7,403521E-16 | 1,560056E-14 | 0,0000 | 0,0000 | |
| NO2 = | 6,233833E-16 | 1,313581E-14 | | 0,0000 | 0,0000 |
| B = | 1,953901E-16 | 4,117224E-15 | 0,0000 | 0,0000 | |
| B2O3(s) = | 9,408557E-17 | 1,982553E-15 | | 0,0000 | 0,0000 |
| BHO2(s) = | 5,663407E-18 | 1,193383E-16 | | 0,0000 | 0,0000 |
| BN(s) = | 4,994174E-18 | 1,052363E-16 | | 0,0000 | 0,0000 |
| C(gr) = | 3,464029E-18 | 7,299336E-17 | | 0,0000 | 0,0000 |
| B(s) = | 3,416337E-21 | 7,198840E-20 | | 0,0000 | 0,0000 |
| B(l) = | 1,407212E-21 | 2,965250E-20 | | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,070029E-22 | 2,254744E-21 | | 0,0000 | 0,0000 |
| N2O3 = | 5,292522E-24 | 1,115230E-22 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,657298E-25 | 1,613531E-23 | | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | | 0,0000 | 0,0000 |

Excluded products(12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 10

**Combustion conditions (Number 10):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 33.34 %**
2. **Hydrogen peroxide ($H_2O_2$), 63.33 %**
3. **Water ($H_2O$, liquid), 3.33 %**

C(0,682) H(3,168) N(0,292) O(1,724) B(0,097)

Molecular weight = 44,1
Oxygen balance = -49,68447 %
Enthalpy of formation = -3539,17 kJ/kg
Internal energy of formation = -3348,97 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -4165,4 kJ/kg
- Total enthalpy of combustion prod. = -3539,59 kJ/kg
- Entropy of combustion products = 12,58 kJ/K kg
- Isobaric combustion temperature = 2248,63 K
- Mole number of gaseous products = 55,639 mol/kg expl.
- Total mole number of products = 55,639 mol/kg expl.
- Volume of gaseous products (at SATP) = 1379,23 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,972 g
- Mean molecular mass of all products = 17,972 g
- Density of products = 6,729 kg/m3
- Specific gas constant = 462,582 J/kg K
- Specific heat capacity at p=const. (Cp) = 2425,21 J/kgK
- Specific heat capacity at V=const. (Cv) = 1962,63 J/molK
- Specific heat ratio (Cp/Cv) = 1,2357

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 7,833699E-01 | 1,776289E+01 | 31,9253 | 3,5810 | |
| H2O = | 7,449523E-01 | 1,689178E+01 | | 30,3596 | 30,4310 |
| CO = | 5,844003E-01 | 1,325126E+01 | 23,8165 | 37,1168 | |
| N2 = | 1,459728E-01 | 3,309931E+00 | 5,9489 | 9,2721 | |
| CO2 = | 9,711143E-02 | 2,201999E+00 | | 3,9577 | 9,6910 |
| BHO2 = | 8,756814E-02 | 1,985606E+00 | | 3,5687 | 8,6966 |
| B(OH)3 = | 7,174023E-03 | 1,626708E-01 | | 0,2924 | 1,0058 |
| H = | 1,280625E-03 | 2,903813E-02 | 0,0522 | 0,0029 | |
| BHO = | 8,815714E-04 | 1,998961E-02 | | 0,0359 | 0,0556 |
| B2O3 = | 8,471233E-04 | 1,920850E-02 | | 0,0345 | 0,1337 |
| NH3 = | 1,266727E-04 | 2,872301E-03 | | 0,0052 | 0,0049 |
| BO2 = | 2,280794E-05 | 5,171696E-04 | | 0,0009 | 0,0022 |
| BO = | 1,652863E-05 | 3,747863E-04 | 0,0007 | 0,0010 | |
| HCN = | 1,179252E-05 | 2,673950E-04 | | 0,0005 | 0,0007 |
| CH2O = | 1,115258E-05 | 2,528846E-04 | | 0,0005 | 0,0008 |
| NO = | 3,723486E-06 | 8,442996E-05 | | 0,0002 | 0,0003 |
| CH4 = | 3,683147E-06 | 8,351527E-05 | | 0,0002 | 0,0001 |
| B2O2 = | 1,883613E-06 | 4,271088E-05 | | 0,0001 | 0,0002 |
| HCNO = | 1,565915E-06 | 3,550709E-05 | | 0,0001 | 0,0002 |
| NH2 = | 5,579165E-07 | 1,265074E-05 | | 0,0000 | 0,0000 |
| CH3OH = | 1,413908E-08 | 3,206034E-07 | | 0,0000 | 0,0000 |
| BH2 = | 1,128354E-08 | 2,558540E-07 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| H2O2 = | 4,075148E-09 | 9,240389E-08 | 0,0000 | 0,0000 |
| N = | 1,522409E-09 | 3,452059E-08 | 0,0000 | 0,0000 |
| CNO = | 7,465092E-10 | 1,692708E-08 | 0,0000 | 0,0000 |
| C2H4 = | 1,804609E-10 | 4,091948E-09 | 0,0000 | 0,0000 |
| NO2 = | 1,203410E-11 | 2,728728E-10 | 0,0000 | 0,0000 |
| BH = | 6,472097E-12 | 1,467547E-10 | 0,0000 | 0,0000 |
| BN = | 1,577098E-12 | 3,576066E-11 | 0,0000 | 0,0000 |
| B = | 1,306640E-12 | 2,962803E-11 | 0,0000 | 0,0000 |
| C2H6 = | 1,171481E-12 | 2,656330E-11 | 0,0000 | 0,0000 |
| B4C(l) = | 6,584734E-17 | 1,493087E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 4,095329E-17 | 9,286149E-16 | 0,0000 | 0,0000 |
| B4C(s) = | 3,114280E-17 | 7,061624E-16 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,440066E-18 | 5,532845E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 9,583132E-19 | 2,172973E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,567828E-19 | 8,090042E-18 | 0,0000 | 0,0000 |
| BN(s) = | 2,462600E-19 | 5,583941E-18 | 0,0000 | 0,0000 |
| B(s) = | 7,008293E-21 | 1,589129E-19 | 0,0000 | 0,0000 |
| B(l) = | 6,442083E-21 | 1,460741E-19 | 0,0000 | 0,0000 |
| N2O3 = | 7,934126E-22 | 1,799061E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 5,484985E-23 | 1,243719E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,067922E-23 | 2,421511E-22 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -4118,22 kJ/kg
- Entropy of combustion products = 12,58 kJ/K kg
- Temperature at nozzle throat = 2020,07 K
- Pressure at nozzle throat = 3,892322 MPa
- Mole number of gaseous products = 55,535 mol/kg expl.
- Total mole number of products = 55,535 mol/kg expl.
- Volume of gaseous products (at SATP) = 1376,66 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 18,006 g
- Mean molecular mass of all products = 18,006 g
- Density of products = 4,173 kg/m3
- Specific gas constant = 461,717 J/kg K
- Specific heat capacity at p=const. (Cp) = 2378,14 J/kgK
- Specific heat capacity at V=const. (Cv) = 1916,42 J/molK
- Specific heat ratio (Cp/Cv) = 1,2409

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1075,8 m/s
- Sound velocity at throat) = 1075,8 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,556
- Pressure ratio (pc/pt) = 1,798

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = | 7,947536E-01 | 1,802102E+01 | 32,4499 | 3,6330 |
| H2O = | 7,295653E-01 | 1,654288E+01 | 29,7883 | 29,8025 |
| CO = | 5,739493E-01 | 1,301429E+01 | 23,4344 | 36,4530 |
| N2 = | 1,459907E-01 | 3,310336E+00 | 5,9608 | 9,2732 |
| CO2 = | 1,075756E-01 | 2,439275E+00 | 4,3923 | 10,7353 |
| BHO2 = | 8,436973E-02 | 1,913082E+00 | 3,4448 | 8,3789 |
| B(OH)3 = | 1,137913E-02 | 2,580216E-01 | 0,4646 | 1,5953 |
| B2O3 = | 5,831646E-04 | 1,322324E-02 | 0,0238 | 0,0920 |
| BHO = | 4,384892E-04 | 9,942732E-03 | 0,0179 | 0,0277 |
| H = | 4,367710E-04 | 9,903773E-03 | 0,0178 | 0,0010 |
| NH3 = | 1,004558E-04 | 2,277833E-03 | 0,0041 | 0,0039 |
| HCN = | 6,786682E-06 | 1,538879E-04 | 0,0003 | 0,0004 |
| CH2O = | 6,564483E-06 | 1,488495E-04 | 0,0003 | 0,0004 |

| | | | | |
|---|---|---|---|---|
| BO2 = | 5,115260E-06 | 1,159884E-04 | 0,0002 | 0,0005 |
| CH4 = | 4,677681E-06 | 1,060663E-04 | 0,0002 | 0,0002 |
| BO = | 3,364179E-06 | 7,628269E-05 | 0,0001 | 0,0002 |
| HCNO = | 8,002956E-07 | 1,814668E-05 | 0,0000 | 0,0001 |
| B2O2 = | 6,192357E-07 | 1,404116E-05 | 0,0000 | 0,0001 |
| NO = | 5,995184E-07 | 1,359407E-05 | 0,0000 | 0,0000 |
| NH2 = | 1,390619E-07 | 3,153225E-06 | 0,0000 | 0,0000 |
| CH3OH = | 7,945849E-09 | 1,801719E-07 | 0,0000 | 0,0000 |
| BH2 = | 1,782788E-09 | 4,042467E-08 | 0,0000 | 0,0000 |
| H2O2 = | 4,321941E-10 | 9,799991E-09 | 0,0000 | 0,0000 |
| C2H4 = | 1,336721E-10 | 3,031012E-09 | 0,0000 | 0,0000 |
| N = | 1,116554E-10 | 2,531783E-09 | 0,0000 | 0,0000 |
| CNO = | 1,009689E-10 | 2,289468E-09 | 0,0000 | 0,0000 |
| C2H6 = | 1,143063E-12 | 2,591893E-11 | 0,0000 | 0,0000 |
| NO2 = | 5,832193E-13 | 1,322449E-11 | 0,0000 | 0,0000 |
| BH = | 3,181781E-13 | 7,214682E-12 | 0,0000 | 0,0000 |
| BN = | 6,226029E-14 | 1,411751E-12 | 0,0000 | 0,0000 |
| B = | 4,077628E-14 | 9,246012E-13 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,615818E-16 | 3,663862E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 1,024871E-16 | 2,323893E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 9,638352E-18 | 2,185494E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,759862E-18 | 3,990483E-17 | 0,0000 | 0,0000 |
| BN(s) = | 4,066867E-19 | 9,221612E-18 | 0,0000 | 0,0000 |
| C(gr) = | 3,971433E-19 | 9,005216E-18 | 0,0000 | 0,0000 |
| B(s) = | 3,443910E-21 | 7,809057E-20 | 0,0000 | 0,0000 |
| B(l) = | 2,334382E-21 | 5,293205E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 5,124011E-23 | 1,161868E-21 | 0,0000 | 0,0000 |
| N2O3 = | 4,165673E-24 | 9,445654E-23 | 0,0000 | 0,0000 |
| B4C(s) = | 1,390931E-27 | 3,153933E-26 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,914310E-28 | 8,875688E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -6526,06 kJ/kg
- Entropy of combustion products = 12,58 kJ/K kg
- Temperature at nozzle exit = 937,63 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 55,535 mol/kg expl.
- Total mole number of products = 55,535 mol/kg expl.
- Volume of gaseous products (at SATP) = 1376,66 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 18,006 g
- Mean molecular mass of all products = 18,006 g
- Density of products = 0,231 kg/m3
- Specific gas constant = 461,717 J/kg K
- Specific heat capacity at p=const. (Cp) = 2038,41 J/kgK
- Specific heat capacity at V=const. (Cv) = 1576,69 J/molK
- Specific heat ratio (Cp/Cv) = 1,2928

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 249,21 s
- Vacuum-specific impulse (pa=0) = 266,93 s
- Exhaust (or nozzle exit) velocity = 2444,0 m/s
- Characteristic exhaust velocity (c*) = 1559,3 m/s
- Thrust coefficient (Cf) = 1,567
- Nozzle area expansion ratio (Ae/At) = 7,95
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 732,95 m/s
- Mach number at nozzle exit = 3,334

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | | |
|---|---|---|---|---|---|
| H2 = | 7,947536E-01 | 1,802102E+01 | 32,4499 | 3,6330 | |
| H2O = | 7,295653E-01 | 1,654288E+01 | 29,7883 | 29,8025 | |
| CO = | 5,739493E-01 | 1,301429E+01 | 23,4344 | 36,4530 | |
| N2 = | 1,459907E-01 | 3,310336E+00 | 5,9608 | 9,2732 | |
| CO2 = | 1,075756E-01 | 2,439275E+00 | 4,3923 | 10,7353 | |
| BHO2 = | 8,436973E-02 | 1,913082E+00 | 3,4448 | 8,3789 | |
| B(OH)3 = | 1,137913E-02 | 2,580216E-01 | 0,4646 | 1,5953 | |
| B2O3 = | 5,831646E-04 | 1,322324E-02 | 0,0238 | 0,0920 | |
| BHO = | 4,384892E-04 | 9,942732E-03 | 0,0179 | 0,0277 | |
| H = | 4,367710E-04 | 9,903773E-03 | 0,0178 | 0,0010 | |
| NH3 = | 1,004558E-04 | 2,277833E-03 | 0,0041 | 0,0039 | |
| HCN = | 6,786682E-06 | 1,538879E-04 | 0,0003 | 0,0004 | |
| CH2O = | 6,564483E-06 | 1,488495E-04 | 0,0003 | 0,0004 | |
| BO2 = | 5,115260E-06 | 1,159884E-04 | 0,0002 | 0,0005 | |
| CH4 = | 4,677681E-06 | 1,060663E-04 | 0,0002 | 0,0002 | |
| BO = | 3,364179E-06 | 7,628269E-05 | 0,0001 | 0,0002 | |
| HCNO = | 8,002956E-07 | 1,814668E-05 | 0,0000 | 0,0001 | |
| B2O2 = | 6,192357E-07 | 1,404116E-05 | 0,0000 | 0,0001 | |
| NO = | 5,995184E-07 | 1,359407E-05 | 0,0000 | 0,0000 | |
| NH2 = | 1,390619E-07 | 3,153225E-06 | 0,0000 | 0,0000 | |
| CH3OH = | 7,945849E-09 | 1,801719E-07 | 0,0000 | 0,0000 | |
| BH2 = | 1,782788E-09 | 4,042467E-08 | 0,0000 | 0,0000 | |
| H2O2 = | 4,321941E-10 | 9,799991E-09 | 0,0000 | 0,0000 | |
| C2H4 = | 1,336721E-10 | 3,031012E-09 | 0,0000 | 0,0000 | |
| N = | 1,116554E-10 | 2,531783E-09 | 0,0000 | 0,0000 | |
| CNO = | 1,009689E-10 | 2,289468E-09 | 0,0000 | 0,0000 | |
| C2H6 = | 1,143063E-12 | 2,591893E-11 | 0,0000 | 0,0000 | |
| NO2 = | 5,832193E-13 | 1,322449E-11 | 0,0000 | 0,0000 | |
| BH = | 3,181781E-13 | 7,214682E-12 | 0,0000 | 0,0000 | |
| BN = | 6,226029E-14 | 1,411751E-12 | 0,0000 | 0,0000 | |
| B = | 4,077628E-14 | 9,246012E-13 | 0,0000 | 0,0000 | |
| B2O3(l) = | 1,615818E-16 | 3,663862E-15 | 0,0000 | 0,0000 | |
| B4C(l) = | 1,024871E-16 | 2,323893E-15 | 0,0000 | 0,0000 | |
| B2O3(s) = | 9,638352E-18 | 2,185494E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = | 1,759862E-18 | 3,990483E-17 | 0,0000 | 0,0000 | |
| BN(s) = | 4,066867E-19 | 9,221612E-18 | 0,0000 | 0,0000 | |
| C(gr) = | 3,971433E-19 | 9,005216E-18 | 0,0000 | 0,0000 | |
| B(s) = | 3,443910E-21 | 7,809057E-20 | 0,0000 | 0,0000 | |
| B(l) = | 2,334382E-21 | 5,293205E-20 | 0,0000 | 0,0000 | |
| B(OH)3(s) = | 5,124011E-23 | 1,161868E-21 | 0,0000 | 0,0000 | |
| N2O3 = | 4,165673E-24 | 9,445654E-23 | 0,0000 | 0,0000 | |
| B4C(s) = | 1,390931E-27 | 3,153933E-26 | 0,0000 | 0,0000 | |
| B3H3O3(s) = | 3,914310E-28 | 8,875688E-27 | 0,0000 | 0,0000 | |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 11

**Combustion conditions (Number 11):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 25.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 71.25 %**
3. **Water ($H_2O$, liquid), 3.75 %**

C(0,469) H(2,805) N(0,201) O(1,782) B(0,067)

Molecular weight = 40,51
Oxygen balance = -26,07909 %
Enthalpy of formation = -4163,42 kJ/kg
Internal energy of formation = -3974,06 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5183,4 kJ/kg
- Total enthalpy of combustion prod. = -4164,12 kJ/kg
- Entropy of combustion products = 12,3 kJ/K kg
- Isobaric combustion temperature = 2749,02 K
- Mole number of gaseous products = 49,573 mol/kg expl.
- Total mole number of products = 49,573 mol/kg expl.
- Volume of gaseous products (at SATP) = 1228,86 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,172 g
- Mean molecular mass of all products = 20,172 g
- Density of products = 6,178 kg/m3
- Specific gas constant = 412,148 J/kg K
- Specific heat capacity at p=const. (Cp) = 2445,58 J/kgK
- Specific heat capacity at V=const. (Cv) = 2033,44 J/molK
- Specific heat ratio (Cp/Cv) = 1,2027

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,034947E+00 | 2,554694E+01 | | 51,5342 | 46,0236 |
| H2 = | 3,296536E-01 | 8,137272E+00 | 16,4148 | 1,6405 | |
| CO = | 3,269986E-01 | 8,071735E+00 | 16,2826 | 22,6089 | |
| CO2 = | 1,424510E-01 | 3,516305E+00 | | 7,0932 | 15,4753 |
| N2 = | 1,004526E-01 | 2,479603E+00 | 5,0019 | 6,9461 | |
| BHO2 = | 6,339435E-02 | 1,564846E+00 | | 3,1567 | 6,8537 |
| H = | 6,949128E-03 | 1,715344E-01 | 0,3460 | 0,0173 | |
| B(OH)3 = | 1,519044E-03 | 3,749656E-02 | | 0,0756 | 0,2318 |
| BHO = | 5,904800E-04 | 1,457559E-02 | | 0,0294 | 0,0405 |
| B2O3 = | 5,375902E-04 | 1,327004E-02 | | 0,0268 | 0,0924 |
| BO2 = | 3,815136E-04 | 9,417400E-03 | | 0,0190 | 0,0403 |
| NO = | 2,654390E-04 | 6,552178E-03 | | 0,0132 | 0,0197 |
| BO = | 1,011251E-04 | 2,496204E-03 | 0,0050 | 0,0067 | |
| NH3 = | 2,091893E-05 | 5,163694E-04 | | 0,0010 | 0,0009 |
| CH2O = | 2,981051E-06 | 7,358519E-05 | | 0,0001 | 0,0002 |
| HCN = | 1,320686E-06 | 3,260021E-05 | | 0,0001 | 0,0001 |
| NH2 = | 1,293211E-06 | 3,192202E-05 | | 0,0001 | 0,0001 |
| B2O2 = | 1,246993E-06 | 3,078116E-05 | | 0,0001 | 0,0002 |
| HCNO = | 6,652504E-07 | 1,642125E-05 | | 0,0000 | 0,0001 |
| H2O2 = | 6,375493E-07 | 1,573746E-05 | | 0,0000 | 0,0001 |
| N = | 1,236620E-07 | 3,052512E-06 | 0,0000 | 0,0000 | |
| CH4 = | 1,895683E-08 | 4,679363E-07 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| NO2 = | 1,868932E-08 | 4,613329E-07 | 0,0000 | 0,0000 |
| BH2 = | 6,948636E-09 | 1,715223E-07 | 0,0000 | 0,0000 |
| CNO = | 5,945107E-09 | 1,467509E-07 | 0,0000 | 0,0000 |
| CH3OH = | 8,651930E-10 | 2,135669E-08 | 0,0000 | 0,0000 |
| BH = | 5,670636E-11 | 1,399757E-09 | 0,0000 | 0,0000 |
| B = | 5,265615E-11 | 1,299781E-09 | 0,0000 | 0,0000 |
| BN = | 2,489751E-11 | 6,145778E-10 | 0,0000 | 0,0000 |
| N2H4 = | 5,102505E-13 | 1,259518E-11 | 0,0000 | 0,0000 |
| C2H4 = | 1,873786E-13 | 4,625311E-12 | 0,0000 | 0,0000 |
| C2H6 = | 1,644780E-16 | 4,060025E-15 | 0,0000 | 0,0000 |
| N2O3 = | 8,154896E-17 | 2,012980E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 2,606929E-17 | 6,435024E-16 | 0,0000 | 0,0000 |
| B4C(l) = | 2,567626E-17 | 6,338006E-16 | 0,0000 | 0,0000 |
| B2O3(l) = | 9,327204E-19 | 2,302356E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,260245E-19 | 3,110827E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 5,432162E-20 | 1,340892E-18 | 0,0000 | 0,0000 |
| C(gr) = | 2,545512E-20 | 6,283420E-19 | 0,0000 | 0,0000 |
| BN(s) = | 4,740421E-21 | 1,170140E-19 | 0,0000 | 0,0000 |
| B(l) = | 2,482492E-21 | 6,127860E-20 | 0,0000 | 0,0000 |
| B(s) = | 1,663727E-21 | 4,106796E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,642528E-23 | 4,054466E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 6,884676E-29 | 1,699435E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -4785,96 kJ/kg
- Entropy of combustion products = 12,3 kJ/K kg
- Temperature at nozzle throat = 2504,71 K
- Pressure at nozzle throat = 3,93874 MPa
- Mole number of gaseous products = 49,517 mol/kg expl.
- Total mole number of products = 49,517 mol/kg expl.
- Volume of gaseous products (at SATP) = 1227,48 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,195 g
- Mean molecular mass of all products = 20,195 g
- Density of products = 3,82 kg/m3
- Specific gas constant = 411,685 J/kg K
- Specific heat capacity at p=const. (Cp) = 2406,42 J/kgK
- Specific heat capacity at V=const. (Cv) = 1994,73 J/molK
- Specific heat ratio (Cp/Cv) = 1,2064

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1115,2 m/s
- Sound velocity at throat ) = 1115,3 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,563
- Pressure ratio (pc/pt) = 1,777

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,027823E+00 | 2,537109E+01 | 51,2371 | 45,7068 |
| H2 = | 3,379309E-01 | 8,341591E+00 | 16,8459 | 1,6817 |
| CO = | 3,203882E-01 | 7,908562E+00 | 15,9714 | 22,1519 |
| CO2 = | 1,490641E-01 | 3,679543E+00 | 7,4309 | 16,1937 |
| N2 = | 1,005498E-01 | 2,482003E+00 | 5,0124 | 6,9528 |
| BHO2 = | 6,378875E-02 | 1,574581E+00 | 3,1799 | 6,8964 |
| H = | 3,530530E-03 | 8,714869E-02 | 0,1760 | 0,0088 |
| B(OH)3 = | 1,842016E-03 | 4,546889E-02 | 0,0918 | 0,2811 |
| B2O3 = | 4,359952E-04 | 1,076224E-02 | 0,0217 | 0,0749 |
| BHO = | 3,761759E-04 | 9,285643E-03 | 0,0188 | 0,0258 |
| BO2 = | 1,475546E-04 | 3,642283E-03 | 0,0074 | 0,0156 |
| NO = | 7,856750E-05 | 1,939384E-03 | 0,0039 | 0,0058 |

| | | | | |
|---|---|---|---|---|
| BO = 3,731975E-05 | 9,212123E-04 | 0,0019 | 0,0025 | |
| NH3 = 1,529398E-05 | 3,775212E-04 | 0,0008 | 0,0006 | |
| CH2O = 1,735258E-06 | 4,283363E-05 | 0,0001 | 0,0001 | |
| HCN = 7,579807E-07 | 1,871023E-05 | 0,0000 | 0,0001 | |
| B2O2 = 6,079972E-07 | 1,500799E-05 | 0,0000 | 0,0001 | |
| NH2 = 4,532044E-07 | 1,118704E-05 | 0,0000 | 0,0000 | |
| HCNO = 3,478048E-07 | 8,585321E-06 | 0,0000 | 0,0000 | |
| H2O2 = 1,304525E-07 | 3,220130E-06 | 0,0000 | 0,0000 | |
| N = 2,112759E-08 | 5,215200E-07 | 0,0000 | 0,0000 | |
| CH4 = 1,640946E-08 | 4,050563E-07 | 0,0000 | 0,0000 | |
| NO2 = 2,339689E-09 | 5,775360E-08 | 0,0000 | 0,0000 | |
| BH2 = 1,845485E-09 | 4,555453E-08 | 0,0000 | 0,0000 | |
| CNO = 1,309949E-09 | 3,233519E-08 | 0,0000 | 0,0000 | |
| CH3OH = 4,119976E-10 | 1,016988E-08 | 0,0000 | 0,0000 | |
| BH = 7,178726E-12 | 1,772019E-10 | 0,0000 | 0,0000 | |
| B = 5,197408E-12 | 1,282944E-10 | 0,0000 | 0,0000 | |
| BN = 2,679267E-12 | 6,613586E-11 | 0,0000 | 0,0000 | |
| N2H4 = 1,082142E-13 | 2,671192E-12 | 0,0000 | 0,0000 | |
| C2H4 = 9,313630E-14 | 2,299005E-12 | 0,0000 | 0,0000 | |
| B4C(l) = 2,926564E-16 | 7,224021E-15 | 0,0000 | 0,0000 | |
| C2H6 = 8,434792E-17 | 2,082070E-15 | 0,0000 | 0,0000 | |
| B2O3(l) = 1,937643E-18 | 4,782937E-17 | 0,0000 | 0,0000 | |
| N2O3 = 1,916589E-18 | 4,730968E-17 | 0,0000 | 0,0000 | |
| B4C(s) = 1,737187E-18 | 4,288127E-17 | 0,0000 | 0,0000 | |
| BHO2(s) = 1,625301E-19 | 4,011942E-18 | 0,0000 | 0,0000 | |
| B2O3(s) = 1,132426E-19 | 2,795315E-18 | 0,0000 | 0,0000 | |
| C(gr) = 2,303521E-20 | 5,686083E-19 | 0,0000 | 0,0000 | |
| BN(s) = 5,894029E-21 | 1,454900E-19 | 0,0000 | 0,0000 | |
| B(l) = 1,148548E-21 | 2,835111E-20 | 0,0000 | 0,0000 | |
| B(s) = 9,501687E-22 | 2,345426E-20 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 9,533839E-24 | 2,353362E-22 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 2,721519E-29 | 6,717881E-28 | 0,0000 | 0,0000 | |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7564,02 kJ/kg
- Entropy of combustion products = 12,3 kJ/K kg
- Temperature at nozzle exit = 1275,65 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 49,517 mol/kg expl.
- Total mole number of products = 49,517 mol/kg expl.
- Volume of gaseous products (at SATP) = 1227,48 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,195 g
- Mean molecular mass of all products = 20,195 g
- Density of products = 0,19 kg/m3
- Specific gas constant = 411,685 J/kg K
- Specific heat capacity at p=const. (Cp) = 2073,1 J/kgK
- Specific heat capacity at V=const. (Cv) = 1661,41 J/molK
- Specific heat ratio (Cp/Cv) = 1,2478

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 265,91 s
- Vacuum-specific impulse (pa=0) = 286,05 s
- Exhaust (or nozzle exit) velocity = 2607,6 m/s
- Characteristic exhaust velocity (c*) = 1643,3 m/s
- Thrust coefficient (Cf) = 1,587
- Nozzle area expansion ratio (Ae/At) = 8,58
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 795,96 m/s
- Mach number at nozzle exit = 3,276

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,027823E+00 | 2,537109E+01 | | 51,2371 | 45,7068 |
| H2 = | 3,379309E-01 | 8,341591E+00 | 16,8459 | 1,6817 | |
| CO = | 3,203882E-01 | 7,908562E+00 | 15,9714 | 22,1519 | |
| CO2 = | 1,490641E-01 | 3,679543E+00 | | 7,4309 | 16,1937 |
| N2 = | 1,005498E-01 | 2,482003E+00 | 5,0124 | 6,9528 | |
| BHO2 = | 6,378875E-02 | 1,574581E+00 | | 3,1799 | 6,8964 |
| H = | 3,530530E-03 | 8,714869E-02 | 0,1760 | 0,0088 | |
| B(OH)3 = | 1,842016E-03 | 4,546889E-02 | | 0,0918 | 0,2811 |
| B2O3 = | 4,359952E-04 | 1,076224E-02 | | 0,0217 | 0,0749 |
| BHO = | 3,761759E-04 | 9,285643E-03 | | 0,0188 | 0,0258 |
| BO2 = | 1,475546E-04 | 3,642283E-03 | | 0,0074 | 0,0156 |
| NO = | 7,856750E-05 | 1,939384E-03 | | 0,0039 | 0,0058 |
| BO = | 3,731975E-05 | 9,212123E-04 | 0,0019 | 0,0025 | |
| NH3 = | 1,529398E-05 | 3,775212E-04 | | 0,0008 | 0,0006 |
| CH2O = | 1,735258E-06 | 4,283363E-05 | | 0,0001 | 0,0001 |
| HCN = | 7,579807E-07 | 1,871023E-05 | | 0,0000 | 0,0001 |
| B2O2 = | 6,079972E-07 | 1,500799E-05 | | 0,0000 | 0,0001 |
| NH2 = | 4,532044E-07 | 1,118704E-05 | | 0,0000 | 0,0000 |
| HCNO = | 3,478048E-07 | 8,585321E-06 | | 0,0000 | 0,0000 |
| H2O2 = | 1,304525E-07 | 3,220130E-06 | | 0,0000 | 0,0000 |
| N = | 2,112759E-08 | 5,215200E-07 | 0,0000 | 0,0000 | |
| CH4 = | 1,640946E-08 | 4,050563E-07 | | 0,0000 | 0,0000 |
| NO2 = | 2,339689E-09 | 5,775360E-08 | | 0,0000 | 0,0000 |
| BH2 = | 1,845485E-09 | 4,555453E-08 | | 0,0000 | 0,0000 |
| CNO = | 1,309949E-09 | 3,233519E-08 | | 0,0000 | 0,0000 |
| CH3OH = | 4,119976E-10 | 1,016988E-08 | | 0,0000 | 0,0000 |
| BH = | 7,178726E-12 | 1,772019E-10 | 0,0000 | 0,0000 | |
| B = | 5,197408E-12 | 1,282944E-10 | 0,0000 | 0,0000 | |
| BN = | 2,679267E-12 | 6,613586E-11 | 0,0000 | 0,0000 | |
| N2H4 = | 1,082142E-13 | 2,671192E-12 | | 0,0000 | 0,0000 |
| C2H4 = | 9,313630E-14 | 2,299005E-12 | | 0,0000 | 0,0000 |
| B4C(l) = | 2,926564E-16 | 7,224021E-15 | | 0,0000 | 0,0000 |
| C2H6 = | 8,434792E-17 | 2,082070E-15 | | 0,0000 | 0,0000 |
| B2O3(l) = | 1,937643E-18 | 4,782937E-17 | | 0,0000 | 0,0000 |
| N2O3 = | 1,916589E-18 | 4,730968E-17 | | 0,0000 | 0,0000 |
| B4C(s) = | 1,737187E-18 | 4,288127E-17 | | 0,0000 | 0,0000 |
| BHO2(s) = | 1,625301E-19 | 4,011942E-18 | | 0,0000 | 0,0000 |
| B2O3(s) = | 1,132426E-19 | 2,795315E-18 | | 0,0000 | 0,0000 |
| C(gr) = | 2,303521E-20 | 5,686083E-19 | | 0,0000 | 0,0000 |
| BN(s) = | 5,894029E-21 | 1,454900E-19 | | 0,0000 | 0,0000 |
| B(l) = | 1,148548E-21 | 2,835111E-20 | | 0,0000 | 0,0000 |
| B(s) = | 9,501687E-22 | 2,345426E-20 | | 0,0000 | 0,0000 |
| B(OH)3(s) = | 9,533839E-24 | 2,353362E-22 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,721519E-29 | 6,717881E-28 | | 0,0000 | 0,0000 |

Excluded products(11):

- ---

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 12

**Combustion conditions (Number 12):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 22.22 %**
2. **Hydrogen peroxide ($H_2O_2$), 73.89 %**
3. **Water ($H_2O$, liquid), 3.89 %**

C(0,406) H(2,696) N(0,174) O(1,799) B(0,058)

Molecular weight = 39,44
Oxygen balance = -18,21063 %
Enthalpy of formation = -4371,51 kJ/kg
Internal energy of formation = -4182,42 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5434,75 kJ/kg
- Total enthalpy of combustion prod. = -4372,18 kJ/kg
- Entropy of combustion products = 12,16 kJ/K kg
- Isobaric combustion temperature = 2878,91 K
- Mole number of gaseous products = 47,707 mol/kg expl.
- Total mole number of products = 47,707 mol/kg expl.
- Volume of gaseous products (at SATP) = 1182,6 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,961 g
- Mean molecular mass of all products = 20,961 g
- Density of products = 6,13 kg/m3
- Specific gas constant = 396,632 J/kg K
- Specific heat capacity at p=const. (Cp) = 2444,04 J/kgK
- Specific heat capacity at V=const. (Cv) = 2047,41 J/molK
- Specific heat ratio (Cp/Cv) = 1,1937

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,096247E+00 | 2,779435E+01 | | 58,2611 | 50,0724 |
| CO = | 2,408924E-01 | 6,107606E+00 | 12,8025 | 17,1074 | |
| H2 = | 2,123267E-01 | 5,383350E+00 | 11,2843 | 1,0853 | |
| CO2 = | 1,653341E-01 | 4,191894E+00 | | 8,7868 | 18,4485 |
| N2 = | 8,665493E-02 | 2,197057E+00 | 4,6054 | 6,1546 | |
| BHO2 = | 5,492582E-02 | 1,392594E+00 | | 2,9191 | 6,0993 |
| OH = | 1,225060E-02 | 3,106027E-01 | | 0,6511 | 0,5282 |
| H = | 8,489769E-03 | 2,152503E-01 | 0,4512 | 0,0217 | |
| B(OH)3 = | 1,045316E-03 | 2,650303E-02 | | 0,0556 | 0,1639 |
| NO = | 7,761742E-04 | 1,967919E-02 | | 0,0413 | 0,0590 |
| O2 = | 7,269671E-04 | 1,843159E-02 | 0,0386 | 0,0590 | |
| BO2 = | 7,044850E-04 | 1,786157E-02 | | 0,0374 | 0,0765 |
| B2O3 = | 4,237678E-04 | 1,074425E-02 | | 0,0225 | 0,0748 |
| BHO = | 3,898751E-04 | 9,884925E-03 | | 0,0207 | 0,0275 |
| O = | 2,881119E-04 | 7,304813E-03 | 0,0153 | 0,0117 | |
| BO = | 1,174883E-04 | 2,978808E-03 | 0,0062 | 0,0080 | |
| NH3 = | 9,688499E-06 | 2,456430E-04 | | 0,0005 | 0,0004 |
| H2O2 = | 2,274169E-06 | 5,765947E-05 | | 0,0001 | 0,0002 |
| CH2O = | 1,493412E-06 | 3,786409E-05 | | 0,0001 | 0,0001 |
| NH2 = | 1,151227E-06 | 2,918832E-05 | | 0,0001 | 0,0000 |
| B2O2 = | 7,669916E-07 | 1,944637E-05 | | 0,0000 | 0,0001 |
| HCN = | 4,729665E-07 | 1,199163E-05 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| HCNO = | 4,032052E-07 | 1,022290E-05 | 0,0000 | 0,0000 |
| N = | 2,878716E-07 | 7,298722E-06 | 0,0000 | 0,0000 |
| NO2 = | 1,320580E-07 | 3,348210E-06 | 0,0000 | 0,0000 |
| CNO = | 7,358513E-09 | 1,865684E-07 | 0,0000 | 0,0000 |
| BH2 = | 3,098952E-09 | 7,857108E-08 | 0,0000 | 0,0000 |
| CH4 = | 2,604146E-09 | 6,602574E-08 | 0,0000 | 0,0000 |
| B = | 6,953106E-11 | 1,762896E-09 | 0,0000 | 0,0000 |
| BH = | 4,871911E-11 | 1,235228E-09 | 0,0000 | 0,0000 |
| BN = | 2,654656E-11 | 6,730637E-10 | 0,0000 | 0,0000 |
| N2H4 = | 2,581601E-13 | 6,545413E-12 | 0,0000 | 0,0000 |
| N2O3 = | 1,705601E-15 | 4,324396E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 1,153645E-16 | 2,924962E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 1,054777E-16 | 2,674290E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 3,929107E-19 | 9,961892E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 8,030194E-20 | 2,035982E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,321347E-20 | 5,885563E-19 | 0,0000 | 0,0000 |
| C(gr) = | 9,851522E-21 | 2,497763E-19 | 0,0000 | 0,0000 |
| BN(s) = | 1,339092E-21 | 3,395146E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,318399E-21 | 3,342679E-20 | 0,0000 | 0,0000 |
| B(s) = | 8,028774E-22 | 2,035622E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,314546E-23 | 3,332911E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,593123E-29 | 4,039217E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5000,13 kJ/kg
- Entropy of combustion products = 12,16 kJ/K kg
- Temperature at nozzle throat = 2656,17 K
- Pressure at nozzle throat = 3,946689 MPa
- Mole number of gaseous products = 47,552 mol/kg expl.
- Total mole number of products = 47,552 mol/kg expl.
- Volume of gaseous products (at SATP) = 1178,76 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,03 g
- Mean molecular mass of all products = 21,03 g
- Density of products = 3,758 kg/m3
- Specific gas constant = 395,344 J/kg K
- Specific heat capacity at p=const. (Cp) = 2411,64 J/kgK
- Specific heat capacity at V=const. (Cv) = 2016,29 J/molK
- Specific heat ratio (Cp/Cv) = 1,1961

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1120,7 m/s
- Sound velocity at throat ) = 1120,7 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,564
- Pressure ratio (pc/pt) = 1,774

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,097683E+00 | 2,783076E+01 | 58,5275 | 50,1379 |
| CO = | 2,345873E-01 | 5,947747E+00 | 12,5080 | 16,6596 |
| H2 = | 2,154275E-01 | 5,461968E+00 | 11,4864 | 1,1011 |
| CO2 = | 1,716406E-01 | 4,351790E+00 | 9,1517 | 19,1522 |
| N2 = | 8,689331E-02 | 2,203100E+00 | 4,6331 | 6,1715 |
| BHO2 = | 5,553009E-02 | 1,407915E+00 | 2,9608 | 6,1664 |
| OH = | 5,893873E-03 | 1,494337E-01 | 0,3143 | 0,2541 |
| H = | 5,090872E-03 | 1,290744E-01 | 0,2714 | 0,0130 |
| B(OH)3 = | 1,121543E-03 | 2,843569E-02 | 0,0598 | 0,1758 |
| B2O3 = | 3,582028E-04 | 9,081903E-03 | 0,0191 | 0,0632 |
| BO2 = | 3,420717E-04 | 8,672916E-03 | 0,0182 | 0,0371 |
| NO = | 3,038819E-04 | 7,704647E-03 | 0,0162 | 0,0231 |

| | | | | |
|---|---|---|---|---|
| BHO = | 2,674428E-04 | 6,780766E-03 | 0,0143 | 0,0189 |
| O2 = | 2,129321E-04 | 5,398698E-03 | 0,0114 | 0,0173 |
| O = | 8,434886E-05 | 2,138588E-03 | 0,0045 | 0,0034 |
| BO = | 5,435430E-05 | 1,378104E-03 | 0,0029 | 0,0037 |
| NH3 = | 6,717865E-06 | 1,703253E-04 | 0,0004 | 0,0003 |
| CH2O = | 8,517371E-07 | 2,159502E-05 | 0,0000 | 0,0001 |
| H2O2 = | 6,295964E-07 | 1,596284E-05 | 0,0000 | 0,0001 |
| NH2 = | 4,603566E-07 | 1,167192E-05 | 0,0000 | 0,0000 |
| B2O2 = | 4,218111E-07 | 1,069464E-05 | 0,0000 | 0,0001 |
| HCN = | 2,642923E-07 | 6,700890E-06 | 0,0000 | 0,0000 |
| HCNO = | 2,113146E-07 | 5,357688E-06 | 0,0000 | 0,0000 |
| N = | 7,079591E-08 | 1,794965E-06 | 0,0000 | 0,0000 |
| NO2 = | 2,578240E-08 | 6,536891E-07 | 0,0000 | 0,0000 |
| CNO = | 1,998066E-09 | 5,065915E-08 | 0,0000 | 0,0000 |
| CH4 = | 1,827227E-09 | 4,632768E-08 | 0,0000 | 0,0000 |
| BH2 = | 9,708530E-10 | 2,461509E-08 | 0,0000 | 0,0000 |
| B = | 1,073845E-11 | 2,722637E-10 | 0,0000 | 0,0000 |
| BH = | 8,765615E-12 | 2,222441E-10 | 0,0000 | 0,0000 |
| BN = | 4,194730E-12 | 1,063535E-10 | 0,0000 | 0,0000 |
| N2H4 = | 5,826827E-14 | 1,477339E-12 | 0,0000 | 0,0000 |
| B4C(l) = | 2,208163E-16 | 5,598595E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 9,073305E-17 | 2,300454E-15 | 0,0000 | 0,0000 |
| N2O3 = | 8,108043E-17 | 2,055720E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 6,437076E-19 | 1,632062E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 8,928752E-20 | 2,263803E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 3,737823E-20 | 9,476909E-19 | 0,0000 | 0,0000 |
| C(gr) = | 8,013143E-21 | 2,031659E-19 | 0,0000 | 0,0000 |
| BN(s) = | 1,423670E-21 | 3,609586E-20 | 0,0000 | 0,0000 |
| B(l) = | 6,528625E-22 | 1,655273E-20 | 0,0000 | 0,0000 |
| B(s) = | 4,715360E-22 | 1,195536E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,233748E-24 | 1,580510E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 8,383084E-31 | 2,125454E-29 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7867,23 kJ/kg
- Entropy of combustion products = 12,16 kJ/K kg
- Temperature at nozzle exit = 1394,21 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 47,552 mol/kg expl.
- Total mole number of products = 47,552 mol/kg expl.
- Volume of gaseous products (at SATP) = 1178,76 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,03 g
- Mean molecular mass of all products = 21,03 g
- Density of products = 0,181 kg/m3
- Specific gas constant = 395,344 J/kg K
- Specific heat capacity at p=const. (Cp) = 2089,73 J/kgK
- Specific heat capacity at V=const. (Cv) = 1694,39 J/molK
- Specific heat ratio (Cp/Cv) = 1,2333

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 269,6 s
- Vacuum-specific impulse (pa=0) = 290,45 s
- Exhaust (or nozzle exit) velocity = 2643,9 m/s
- Characteristic exhaust velocity (c*) = 1662,0 m/s
- Thrust coefficient (Cf) = 1,591
- Nozzle area expansion ratio (Ae/At) = 8,78
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 811,95 m/s
- Mach number at nozzle exit = 3,256

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,097683E+00 | 2,783076E+01 | | 58,5275 | 50,1379 |
| CO = | 2,345873E-01 | 5,947747E+00 | 12,5080 | 16,6596 | |
| H2 = | 2,154275E-01 | 5,461968E+00 | 11,4864 | 1,1011 | |
| CO2 = | 1,716406E-01 | 4,351790E+00 | | 9,1517 | 19,1522 |
| N2 = | 8,689331E-02 | 2,203100E+00 | 4,6331 | 6,1715 | |
| BHO2 = | 5,553009E-02 | 1,407915E+00 | | 2,9608 | 6,1664 |
| OH = | 5,893873E-03 | 1,494337E-01 | | 0,3143 | 0,2541 |
| H = | 5,090872E-03 | 1,290744E-01 | 0,2714 | 0,0130 | |
| B(OH)3 = | 1,121543E-03 | 2,843569E-02 | | 0,0598 | 0,1758 |
| B2O3 = | 3,582028E-04 | 9,081903E-03 | | 0,0191 | 0,0632 |
| BO2 = | 3,420717E-04 | 8,672916E-03 | | 0,0182 | 0,0371 |
| NO = | 3,038819E-04 | 7,704647E-03 | | 0,0162 | 0,0231 |
| BHO = | 2,674428E-04 | 6,780766E-03 | | 0,0143 | 0,0189 |
| O2 = | 2,129321E-04 | 5,398698E-03 | 0,0114 | 0,0173 | |
| O = | 8,434886E-05 | 2,138588E-03 | 0,0045 | 0,0034 | |
| BO = | 5,435430E-05 | 1,378104E-03 | 0,0029 | 0,0037 | |
| NH3 = | 6,717865E-06 | 1,703253E-04 | | 0,0004 | 0,0003 |
| CH2O = | 8,517371E-07 | 2,159502E-05 | | 0,0000 | 0,0001 |
| H2O2 = | 6,295964E-07 | 1,596284E-05 | | 0,0000 | 0,0001 |
| NH2 = | 4,603566E-07 | 1,167192E-05 | | 0,0000 | 0,0000 |
| B2O2 = | 4,218111E-07 | 1,069464E-05 | | 0,0000 | 0,0001 |
| HCN = | 2,642923E-07 | 6,700890E-06 | | 0,0000 | 0,0000 |
| HCNO = | 2,113146E-07 | 5,357688E-06 | | 0,0000 | 0,0000 |
| N = | 7,079591E-08 | 1,794965E-06 | 0,0000 | 0,0000 | |
| NO2 = | 2,578240E-08 | 6,536891E-07 | | 0,0000 | 0,0000 |
| CNO = | 1,998066E-09 | 5,065915E-08 | | 0,0000 | 0,0000 |
| CH4 = | 1,827227E-09 | 4,632768E-08 | | 0,0000 | 0,0000 |
| BH2 = | 9,708530E-10 | 2,461509E-08 | | 0,0000 | 0,0000 |
| B = | 1,073845E-11 | 2,722637E-10 | 0,0000 | 0,0000 | |
| BH = | 8,765615E-12 | 2,222441E-10 | 0,0000 | 0,0000 | |
| BN = | 4,194730E-12 | 1,063535E-10 | 0,0000 | 0,0000 | |
| N2H4 = | 5,826827E-14 | 1,477339E-12 | | 0,0000 | 0,0000 |
| B4C(l) = | 2,208163E-16 | 5,598595E-15 | | 0,0000 | 0,0000 |
| B4C(s) = | 9,073305E-17 | 2,300454E-15 | | 0,0000 | 0,0000 |
| N2O3 = | 8,108043E-17 | 2,055720E-15 | | 0,0000 | 0,0000 |
| B2O3(l) = | 6,437076E-19 | 1,632062E-17 | | 0,0000 | 0,0000 |
| BHO2(s) = | 8,928752E-20 | 2,263803E-18 | | 0,0000 | 0,0000 |
| B2O3(s) = | 3,737823E-20 | 9,476909E-19 | | 0,0000 | 0,0000 |
| C(gr) = | 8,013143E-21 | 2,031659E-19 | | 0,0000 | 0,0000 |
| BN(s) = | 1,423670E-21 | 3,609586E-20 | | 0,0000 | 0,0000 |
| B(l) = | 6,528625E-22 | 1,655273E-20 | | 0,0000 | 0,0000 |
| B(s) = | 4,715360E-22 | 1,195536E-20 | | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,233748E-24 | 1,580510E-22 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 8,383084E-31 | 2,125454E-29 | | 0,0000 | 0,0000 |

Excluded products(11):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 13

**Combustion conditions (Number 13):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit

Reactant information:

---

1. **[EMIM][$BH_3CN$], 20.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 76.00 %**
3. **Water ($H_2O$, liquid), 4.00 %**

C(0,358) H(2,614) N(0,153) O(1,812) B(0,051)

Molecular weight = 38,63
Oxygen balance = -11,92633 %
Enthalpy of formation = -4537,49 kJ/kg
Internal energy of formation = -4348,63 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5601,76 kJ/kg
- Total enthalpy of combustion prod. = -4537,15 kJ/kg
- Entropy of combustion products = 12,03 kJ/K kg
- Isobaric combustion temperature = 2968,46 K
- Mole number of gaseous products = 46,288 mol/kg expl.
- Total mole number of products = 46,288 mol/kg expl.
- Volume of gaseous products (at SATP) = 1147,42 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,604 g
- Mean molecular mass of all products = 21,604 g
- Density of products = 6,128 kg/m3
- Specific gas constant = 384,835 J/kg K
- Specific heat capacity at p=const. (Cp) = 2440,72 J/kgK
- Specific heat capacity at V=const. (Cv) = 2055,89 J/molK
- Specific heat ratio (Cp/Cv) = 1,1872

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 1,132158E+00 | 2,930984E+01 | 63,3212 | 52,8026 |
| CO2 = | 1,872174E-01 | 4,846772E+00 | 10,4710 | 21,3306 |
| CO = | 1,708765E-01 | 4,423731E+00 | 9,5571 | 12,3909 |
| H2 = | 1,337686E-01 | 3,463066E+00 | 7,4816 | 0,6982 |
| N2 = | 7,583438E-02 | 1,963236E+00 | 4,2414 | 5,4996 |
| BHO2 = | 4,823291E-02 | 1,248676E+00 | 2,6976 | 5,4690 |
| OH = | 2,234380E-02 | 5,784469E-01 | 1,2497 | 0,9838 |
| H = | 8,773864E-03 | 2,271420E-01 | 0,4907 | 0,0229 |
| O2 = | 3,511679E-03 | 9,091202E-02 | 0,1964 | 0,2909 |
| NO = | 1,793744E-03 | 4,643730E-02 | 0,1003 | 0,1393 |
| BO2 = | 1,092951E-03 | 2,829482E-02 | 0,0611 | 0,1211 |
| O = | 8,530243E-04 | 2,208350E-02 | 0,0477 | 0,0353 |
| B(OH)3 = | 7,969504E-04 | 2,063183E-02 | 0,0446 | 0,1276 |
| B2O3 = | 3,387328E-04 | 8,769274E-03 | 0,0189 | 0,0610 |
| BHO = | 2,412109E-04 | 6,244583E-03 | 0,0135 | 0,0174 |
| BO = | 1,135357E-04 | 2,939265E-03 | 0,0064 | 0,0079 |
| H2O2 = | 6,084631E-06 | 1,575218E-04 | 0,0003 | 0,0005 |
| NH3 = | 4,474920E-06 | 1,158489E-04 | 0,0003 | 0,0002 |
| NH2 = | 8,790026E-07 | 2,275604E-05 | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| CH2O = | 6,981847E-07 | 1,807494E-05 | 0,0000 | 0,0001 |
| NO2 = | 6,398272E-07 | 1,656415E-05 | 0,0000 | 0,0001 |
| N = | 4,820964E-07 | 1,248074E-05 | 0,0000 | 0,0000 |
| B2O2 = | 4,384343E-07 | 1,135040E-05 | 0,0000 | 0,0001 |
| HCNO = | 2,285493E-07 | 5,916794E-06 | 0,0000 | 0,0000 |
| HCN = | 1,605608E-07 | 4,156674E-06 | 0,0000 | 0,0000 |
| CNO = | 7,169632E-09 | 1,856108E-07 | 0,0000 | 0,0000 |
| BH2 = | 1,147880E-09 | 2,971687E-08 | 0,0000 | 0,0000 |
| B = | 6,112628E-11 | 1,582466E-09 | 0,0000 | 0,0000 |
| BH = | 2,987042E-11 | 7,732996E-10 | 0,0000 | 0,0000 |
| BN = | 2,005848E-11 | 5,192835E-10 | 0,0000 | 0,0000 |
| N2H4 = | 1,142522E-13 | 2,957814E-12 | 0,0000 | 0,0000 |
| N2O3 = | 1,944440E-14 | 5,033858E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 4,666131E-16 | 1,207990E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 4,116214E-16 | 1,065625E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 2,133085E-19 | 5,522231E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,868201E-20 | 1,519188E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,279749E-20 | 3,313075E-19 | 0,0000 | 0,0000 |
| C(gr) = | 3,924020E-21 | 1,015869E-19 | 0,0000 | 0,0000 |
| B(l) = | 6,551383E-22 | 1,696053E-20 | 0,0000 | 0,0000 |
| BN(s) = | 4,380649E-22 | 1,134083E-20 | 0,0000 | 0,0000 |
| B(s) = | 3,755948E-22 | 9,723576E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,063836E-23 | 2,754110E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,610831E-27 | 4,170195E-26 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5166,81 kJ/kg
- Entropy of combustion products = 12,03 kJ/K kg
- Temperature at nozzle throat = 2766,26 K
- Pressure at nozzle throat = 3,951361 MPa
- Mole number of gaseous products = 46,042 mol/kg expl.
- Total mole number of products = 46,042 mol/kg expl.
- Volume of gaseous products (at SATP) = 1141,32 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,719 g
- Mean molecular mass of all products = 21,719 g
- Density of products = 3,732 kg/m3
- Specific gas constant = 382,789 J/kg K
- Specific heat capacity at p=const. (Cp) = 2413,58 J/kgK
- Specific heat capacity at V=const. (Cv) = 2030,79 J/molK
- Specific heat ratio (Cp/Cv) = 1,1885

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1122,2 m/s
- Sound velocity at throat ) = 1121,8 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,564
- Pressure ratio (pc/pt) = 1,772

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,139777E+00 | 2,950708E+01 | 64,0880 | 53,1579 |
| CO2 = | 1,945794E-01 | 5,037363E+00 | 10,9409 | 22,1694 |
| CO = | 1,635153E-01 | 4,233161E+00 | 9,1942 | 11,8571 |
| H2 = | 1,320999E-01 | 3,419864E+00 | 7,4278 | 0,6894 |
| N2 = | 7,629507E-02 | 1,975163E+00 | 4,2900 | 5,5330 |
| BHO2 = | 4,891971E-02 | 1,266457E+00 | 2,7507 | 5,5468 |
| OH = | 1,280117E-02 | 3,314027E-01 | 0,7198 | 0,5636 |
| H = | 5,867410E-03 | 1,518983E-01 | 0,3299 | 0,0153 |
| O2 = | 1,440003E-03 | 3,727949E-02 | 0,0810 | 0,1193 |
| NO = | 8,754346E-04 | 2,266367E-02 | 0,0492 | 0,0680 |

| | | | | |
|---|---|---|---|---|
| B(OH)3 = | 7,835295E-04 | 2,028438E-02 | 0,0441 | 0,1254 |
| BO2 = | 6,304838E-04 | 1,632226E-02 | 0,0355 | 0,0699 |
| O = | 3,391902E-04 | 8,781117E-03 | 0,0191 | 0,0140 |
| B2O3 = | 2,950196E-04 | 7,637608E-03 | 0,0166 | 0,0532 |
| BHO = | 1,710802E-04 | 4,429006E-03 | 0,0096 | 0,0123 |
| BO = | 6,110035E-05 | 1,581795E-03 | 0,0034 | 0,0042 |
| NH3 = | 2,906462E-06 | 7,524388E-05 | 0,0002 | 0,0001 |
| H2O2 = | 2,131760E-06 | 5,518801E-05 | 0,0001 | 0,0002 |
| CH2O = | 3,801567E-07 | 9,841676E-06 | 0,0000 | 0,0000 |
| NH2 = | 3,793154E-07 | 9,819898E-06 | 0,0000 | 0,0000 |
| B2O2 = | 2,578151E-07 | 6,674439E-06 | 0,0000 | 0,0000 |
| NO2 = | 1,787037E-07 | 4,626367E-06 | 0,0000 | 0,0000 |
| N = | 1,540611E-07 | 3,988406E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,175225E-07 | 3,042477E-06 | 0,0000 | 0,0000 |
| HCN = | 8,456205E-08 | 2,189182E-06 | 0,0000 | 0,0000 |
| CNO = | 2,235780E-09 | 5,788093E-08 | 0,0000 | 0,0000 |
| BH2 = | 3,856017E-10 | 9,982639E-09 | 0,0000 | 0,0000 |
| B = | 1,262747E-11 | 3,269058E-10 | 0,0000 | 0,0000 |
| BH = | 6,645276E-12 | 1,720361E-10 | 0,0000 | 0,0000 |
| BN = | 4,055940E-12 | 1,050021E-10 | 0,0000 | 0,0000 |
| N2H4 = | 2,604904E-14 | 6,743698E-13 | 0,0000 | 0,0000 |
| N2O3 = | 1,627029E-15 | 4,212129E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 1,387817E-15 | 3,592846E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 9,043974E-16 | 2,341347E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 2,960506E-19 | 7,664299E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,884428E-20 | 1,523389E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,727320E-20 | 4,471768E-19 | 0,0000 | 0,0000 |
| C(gr) = | 2,866429E-21 | 7,420746E-20 | 0,0000 | 0,0000 |
| BN(s) = | 4,054961E-22 | 1,049768E-20 | 0,0000 | 0,0000 |
| B(l) = | 3,313534E-22 | 8,578234E-21 | 0,0000 | 0,0000 |
| B(s) = | 2,191434E-22 | 5,673287E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,668906E-24 | 1,208708E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,936415E-25 | 5,013082E-24 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8086,5 kJ/kg
- Entropy of combustion products = 12,03 kJ/K kg
- Temperature at nozzle exit = 1485,48 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 46,042 mol/kg expl.
- Total mole number of products = 46,042 mol/kg expl.
- Volume of gaseous products (at SATP) = 1141,32 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,719 g
- Mean molecular mass of all products = 21,719 g
- Density of products = 0,176 kg/m3
- Specific gas constant = 382,789 J/kg K
- Specific heat capacity at p=const. (Cp) = 2102,7 J/kgK
- Specific heat capacity at V=const. (Cv) = 1719,91 J/molK
- Specific heat ratio (Cp/Cv) = 1,2226

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 271,69 s
- Vacuum-specific impulse (pa=0) = 293,03 s
- Exhaust (or nozzle exit) velocity = 2664,3 m/s
- Characteristic exhaust velocity (c*) = 1671,6 m/s
- Thrust coefficient (Cf) = 1,594
- Nozzle area expansion ratio (Ae/At) = 8,94
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 822,08 m/s
- Mach number at nozzle exit = 3,241

Composition of combustion products at the nozzle exit:

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,139777E+00 | 2,950708E+01 | | 64,0880 | 53,1579 |
| CO2 = | 1,945794E-01 | 5,037363E+00 | | 10,9409 | 22,1694 |
| CO = | 1,635153E-01 | 4,233161E+00 | 9,1942 | 11,8571 | |
| H2 = | 1,320999E-01 | 3,419864E+00 | 7,4278 | 0,6894 | |
| N2 = | 7,629507E-02 | 1,975163E+00 | 4,2900 | 5,5330 | |
| BHO2 = | 4,891971E-02 | 1,266457E+00 | | 2,7507 | 5,5468 |
| OH = | 1,280117E-02 | 3,314027E-01 | | 0,7198 | 0,5636 |
| H = | 5,867410E-03 | 1,518983E-01 | 0,3299 | 0,0153 | |
| O2 = | 1,440003E-03 | 3,727949E-02 | 0,0810 | 0,1193 | |
| NO = | 8,754346E-04 | 2,266367E-02 | | 0,0492 | 0,0680 |
| B(OH)3 = | 7,835295E-04 | 2,028438E-02 | | 0,0441 | 0,1254 |
| BO2 = | 6,304838E-04 | 1,632226E-02 | | 0,0355 | 0,0699 |
| O = | 3,391902E-04 | 8,781117E-03 | 0,0191 | 0,0140 | |
| B2O3 = | 2,950196E-04 | 7,637608E-03 | | 0,0166 | 0,0532 |
| BHO = | 1,710802E-04 | 4,429006E-03 | | 0,0096 | 0,0123 |
| BO = | 6,110035E-05 | 1,581795E-03 | 0,0034 | 0,0042 | |
| NH3 = | 2,906462E-06 | 7,524388E-05 | | 0,0002 | 0,0001 |
| H2O2 = | 2,131760E-06 | 5,518801E-05 | | 0,0001 | 0,0002 |
| CH2O = | 3,801567E-07 | 9,841676E-06 | | 0,0000 | 0,0000 |
| NH2 = | 3,793154E-07 | 9,819898E-06 | | 0,0000 | 0,0000 |
| B2O2 = | 2,578151E-07 | 6,674439E-06 | | 0,0000 | 0,0000 |
| NO2 = | 1,787037E-07 | 4,626367E-06 | | 0,0000 | 0,0000 |
| N = | 1,540611E-07 | 3,988406E-06 | 0,0000 | 0,0000 | |
| HCNO = | 1,175225E-07 | 3,042477E-06 | | 0,0000 | 0,0000 |
| HCN = | 8,456205E-08 | 2,189182E-06 | | 0,0000 | 0,0000 |
| CNO = | 2,235780E-09 | 5,788093E-08 | | 0,0000 | 0,0000 |
| BH2 = | 3,856017E-10 | 9,982639E-09 | | 0,0000 | 0,0000 |
| B = | 1,262747E-11 | 3,269058E-10 | 0,0000 | 0,0000 | |
| BH = | 6,645276E-12 | 1,720361E-10 | 0,0000 | 0,0000 | |
| BN = | 4,055940E-12 | 1,050021E-10 | 0,0000 | 0,0000 | |
| N2H4 = | 2,604904E-14 | 6,743698E-13 | | 0,0000 | 0,0000 |
| N2O3 = | 1,627029E-15 | 4,212129E-14 | | 0,0000 | 0,0000 |
| B4C(s) = | 1,387817E-15 | 3,592846E-14 | | 0,0000 | 0,0000 |
| B4C(l) = | 9,043974E-16 | 2,341347E-14 | | 0,0000 | 0,0000 |
| B2O3(l) = | 2,960506E-19 | 7,664299E-18 | | 0,0000 | 0,0000 |
| BHO2(s) = | 5,884428E-20 | 1,523389E-18 | | 0,0000 | 0,0000 |
| B2O3(s) = | 1,727320E-20 | 4,471768E-19 | | 0,0000 | 0,0000 |
| C(gr) = | 2,866429E-21 | 7,420746E-20 | | 0,0000 | 0,0000 |
| BN(s) = | 4,054961E-22 | 1,049768E-20 | | 0,0000 | 0,0000 |
| B(l) = | 3,313534E-22 | 8,578234E-21 | | 0,0000 | 0,0000 |
| B(s) = | 2,191434E-22 | 5,673287E-21 | | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,668906E-24 | 1,208708E-22 | | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,936415E-25 | 5,013082E-24 | | 0,0000 | 0,0000 |

Excluded products (12):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; CH4; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 14

**Combustion conditions (Number 14):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion to throat and frozen from throat to exit**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 18.18 %**
2. **Hydrogen peroxide ($H_2O_2$), 77.73 %**
3. **Water ($H_2O$, liquid), 4.09 %**

C(0,320) H(2,549) N(0,137) O(1,822) B(0,046)

Molecular weight = 37,98
Oxygen balance = -6,774266 %
Enthalpy of formation = -4673,54 kJ/kg
Internal energy of formation = -4484,87 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5651,4 kJ/kg
- Total enthalpy of combustion prod. = -4673,05 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Isobaric combustion temperature = 3005,03 K
- Mole number of gaseous products = 45,292 mol/kg expl.
- Total mole number of products = 45,292 mol/kg expl.
- Volume of gaseous products (at SATP) = 1122,75 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,079 g
- Mean molecular mass of all products = 22,079 g
- Density of products = 6,186 kg/m3
- Specific gas constant = 376,56 J/kg K
- Specific heat capacity at p=const. (Cp) = 2432,97 J/kgK
- Specific heat capacity at V=const. (Cv) = 2056,41 J/molK
- Specific heat ratio (Cp/Cv) = 1,1831

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,147549E+00 | 3,021098E+01 | | 66,7023 | 54,4260 |
| CO2 = | 2,034536E-01 | 5,356226E+00 | | 11,8259 | 23,5728 |
| CO = | 1,166381E-01 | 3,070675E+00 | 6,7797 | 8,6010 | |
| H2 = | 8,430096E-02 | 2,219352E+00 | 4,9001 | 0,4474 | |
| N2 = | 6,701113E-02 | 1,764171E+00 | 3,8951 | 4,9420 | |
| BHO2 = | 4,288442E-02 | 1,128998E+00 | | 2,4927 | 4,9448 |
| OH = | 3,225761E-02 | 8,492310E-01 | | 1,8750 | 1,4443 |
| O2 = | 1,121626E-02 | 2,952853E-01 | 0,6520 | 0,9449 | |
| H = | 7,652135E-03 | 2,014542E-01 | 0,4448 | 0,0203 | |
| NO = | 3,154681E-03 | 8,305181E-02 | | 0,1834 | 0,2492 |
| O = | 1,697347E-03 | 4,468527E-02 | 0,0987 | 0,0715 | |
| BO2 = | 1,384688E-03 | 3,645403E-02 | | 0,0805 | 0,1561 |
| B(OH)3 = | 6,836757E-04 | 1,799881E-02 | | 0,0397 | 0,1113 |
| B2O3 = | 2,713296E-04 | 7,143168E-03 | | 0,0158 | 0,0497 |
| BHO = | 1,410687E-04 | 3,713849E-03 | | 0,0082 | 0,0103 |
| BO = | 9,012655E-05 | 2,372719E-03 | 0,0052 | 0,0064 | |
| H2O2 = | 1,186459E-05 | 3,123536E-04 | | 0,0007 | 0,0011 |
| NH3 = | 2,133502E-06 | 5,616772E-05 | | 0,0001 | 0,0001 |
| NO2 = | 1,993198E-06 | 5,247400E-05 | | 0,0001 | 0,0002 |
| NH2 = | 5,816591E-07 | 1,531307E-05 | | 0,0000 | 0,0000 |
| N = | 5,639392E-07 | 1,484656E-05 | 0,0000 | 0,0000 | |
| CH2O = | 3,114654E-07 | 8,199804E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 2,323952E-07 | 6,118160E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,220778E-07 | 3,213884E-06 | 0,0000 | 0,0000 |
| HCN = | 5,293242E-08 | 1,393527E-06 | 0,0000 | 0,0000 |
| CNO = | 5,397282E-09 | 1,420917E-07 | 0,0000 | 0,0000 |
| BH2 = | 3,633757E-10 | 9,566421E-09 | 0,0000 | 0,0000 |
| B = | 3,527397E-11 | 9,286412E-10 | 0,0000 | 0,0000 |
| BH = | 1,312971E-11 | 3,456597E-10 | 0,0000 | 0,0000 |
| BN = | 1,062567E-11 | 2,797371E-10 | 0,0000 | 0,0000 |
| N2O3 = | 1,092951E-13 | 2,877360E-12 | 0,0000 | 0,0000 |
| N2H4 = | 4,577206E-14 | 1,205020E-12 | 0,0000 | 0,0000 |
| B4C(s) = | 6,346011E-17 | 1,670684E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 5,587324E-17 | 1,470948E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,496730E-19 | 3,940370E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,949497E-20 | 1,303031E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 9,049283E-21 | 2,382362E-19 | 0,0000 | 0,0000 |
| C(gr) = | 1,642806E-21 | 4,324937E-20 | 0,0000 | 0,0000 |
| B(l) = | 3,082327E-22 | 8,114697E-21 | 0,0000 | 0,0000 |
| B(s) = | 1,725843E-22 | 4,543545E-21 | 0,0000 | 0,0000 |
| BN(s) = | 1,702110E-22 | 4,481065E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,035467E-23 | 2,726025E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,526928E-26 | 4,019872E-25 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5298,05 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Temperature at nozzle throat = 2825,34 K
- Pressure at nozzle throat = 3,952973 MPa
- Mole number of gaseous products = 44,954 mol/kg expl.
- Total mole number of products = 44,954 mol/kg expl.
- Volume of gaseous products (at SATP) = 1114,36 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,245 g
- Mean molecular mass of all products = 22,245 g
- Density of products = 3,743 kg/m3
- Specific gas constant = 373,747 J/kg K
- Specific heat capacity at p=const. (Cp) = 2410,13 J/kgK
- Specific heat capacity at V=const. (Cv) = 2036,38 J/molK
- Specific heat ratio (Cp/Cv) = 1,1835

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1118,0 m/s
- Sound velocity at throat ) = 1117,9 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,565
- Pressure ratio (pc/pt) = 1,771

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,159803E+00 | 3,053359E+01 | 67,9220 | 55,0072 |
| CO2 = | 2,134930E-01 | 5,620531E+00 | 12,5029 | 24,7360 |
| CO = | 1,065991E-01 | 2,806383E+00 | 6,2428 | 7,8607 |
| H2 = | 7,829996E-02 | 2,061366E+00 | 4,5855 | 0,4156 |
| N2 = | 6,764120E-02 | 1,780758E+00 | 3,9613 | 4,9884 |
| BHO2 = | 4,353694E-02 | 1,146177E+00 | 2,5497 | 5,0200 |
| OH = | 2,153812E-02 | 5,670239E-01 | 1,2613 | 0,9643 |
| O2 = | 6,446899E-03 | 1,697245E-01 | 0,3776 | 0,5431 |
| H = | 5,450463E-03 | 1,434918E-01 | 0,3192 | 0,0145 |
| NO = | 1,897443E-03 | 4,995310E-02 | 0,1111 | 0,1499 |
| BO2 = | 9,279376E-04 | 2,442938E-02 | 0,0543 | 0,1046 |
| O = | 8,876577E-04 | 2,336895E-02 | 0,0520 | 0,0374 |
| B(OH)3 = | 6,284072E-04 | 1,654378E-02 | 0,0368 | 0,1023 |
| B2O3 = | 2,411543E-04 | 6,348757E-03 | 0,0141 | 0,0442 |

| | | | | |
|---|---|---|---|---|
| BHO = | 9,840095E-05 | 2,590555E-03 | 0,0058 | 0,0072 |
| BO = | 5,321241E-05 | 1,400898E-03 | 0,0031 | 0,0038 |
| H2O2 = | 5,178952E-06 | 1,363438E-04 | 0,0003 | 0,0005 |
| NH3 = | 1,241969E-06 | 3,269674E-05 | 0,0001 | 0,0001 |
| NO2 = | 7,937007E-07 | 2,089538E-05 | 0,0000 | 0,0001 |
| NH2 = | 2,555995E-07 | 6,729048E-06 | 0,0000 | 0,0000 |
| N = | 2,201777E-07 | 5,796515E-06 | 0,0000 | 0,0000 |
| CH2O = | 1,522896E-07 | 4,009257E-06 | 0,0000 | 0,0000 |
| B2O2 = | 1,376886E-07 | 3,624862E-06 | 0,0000 | 0,0000 |
| HCNO = | 5,876411E-08 | 1,547055E-06 | 0,0000 | 0,0000 |
| HCN = | 2,430656E-08 | 6,399073E-07 | 0,0000 | 0,0000 |
| CNO = | 1,812721E-09 | 4,772265E-08 | 0,0000 | 0,0000 |
| BH2 = | 1,161549E-10 | 3,057955E-09 | 0,0000 | 0,0000 |
| B = | 8,542474E-12 | 2,248937E-10 | 0,0000 | 0,0000 |
| BH = | 3,159981E-12 | 8,319132E-11 | 0,0000 | 0,0000 |
| BN = | 2,435850E-12 | 6,412748E-11 | 0,0000 | 0,0000 |
| N2O3 = | 1,592582E-14 | 4,192716E-13 | 0,0000 | 0,0000 |
| N2H4 = | 9,726899E-15 | 2,560755E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 1,669456E-16 | 4,395099E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 4,684807E-17 | 1,233347E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,833648E-19 | 4,827358E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,595620E-20 | 1,209867E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,075996E-20 | 2,832723E-19 | 0,0000 | 0,0000 |
| C(gr) = | 1,028912E-21 | 2,708769E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,489854E-22 | 3,922270E-21 | 0,0000 | 0,0000 |
| BN(s) = | 1,336030E-22 | 3,517303E-21 | 0,0000 | 0,0000 |
| B(s) = | 9,426365E-23 | 2,481635E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,361388E-24 | 1,148202E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,144782E-32 | 8,279119E-31 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8228,62 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Temperature at nozzle exit = 1539,92 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 44,954 mol/kg expl.
- Total mole number of products = 44,954 mol/kg expl.
- Volume of gaseous products (at SATP) = 1114,36 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,245 g
- Mean molecular mass of all products = 22,245 g
- Density of products = 0,174 kg/m3
- Specific gas constant = 373,747 J/kg K
- Specific heat capacity at p=const. (Cp) = 2106,91 J/kgK
- Specific heat capacity at V=const. (Cv) = 1733,17 J/molK
- Specific heat ratio (Cp/Cv) = 1,2156

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 271,93 s
- Vacuum-specific impulse (pa=0) = 293,51 s
- Exhaust (or nozzle exit) velocity = 2666,7 m/s
- Characteristic exhaust velocity (c*) = 1672,5 m/s
- Thrust coefficient (Cf) = 1,594
- Nozzle area expansion ratio (Ae/At) = 9,03
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 825,33 m/s
- Mach number at nozzle exit = 3,231

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 1,159803E+00 | 3,053359E+01 | 67,9220 | 55,0072 |

| | | | | |
|---|---|---|---|---|
| CO2 = | 2,134930E-01 | 5,620531E+00 | 12,5029 | 24,7360 |
| CO = | 1,065991E-01 | 2,806383E+00 | 6,2428 | 7,8607 |
| H2 = | 7,829996E-02 | 2,061366E+00 | 4,5855 | 0,4156 |
| N2 = | 6,764120E-02 | 1,780758E+00 | 3,9613 | 4,9884 |
| BHO2 = | 4,353694E-02 | 1,146177E+00 | 2,5497 | 5,0200 |
| OH = | 2,153812E-02 | 5,670239E-01 | 1,2613 | 0,9643 |
| O2 = | 6,446899E-03 | 1,697245E-01 | 0,3776 | 0,5431 |
| H = | 5,450463E-03 | 1,434918E-01 | 0,3192 | 0,0145 |
| NO = | 1,897443E-03 | 4,995310E-02 | 0,1111 | 0,1499 |
| BO2 = | 9,279376E-04 | 2,442938E-02 | 0,0543 | 0,1046 |
| O = | 8,876577E-04 | 2,336895E-02 | 0,0520 | 0,0374 |
| B(OH)3 = | 6,284072E-04 | 1,654378E-02 | 0,0368 | 0,1023 |
| B2O3 = | 2,411543E-04 | 6,348757E-03 | 0,0141 | 0,0442 |
| BHO = | 9,840095E-05 | 2,590555E-03 | 0,0058 | 0,0072 |
| BO = | 5,321241E-05 | 1,400898E-03 | 0,0031 | 0,0038 |
| H2O2 = | 5,178952E-06 | 1,363438E-04 | 0,0003 | 0,0005 |
| NH3 = | 1,241969E-06 | 3,269674E-05 | 0,0001 | 0,0001 |
| NO2 = | 7,937007E-07 | 2,089538E-05 | 0,0000 | 0,0001 |
| NH2 = | 2,555995E-07 | 6,729048E-06 | 0,0000 | 0,0000 |
| N = | 2,201777E-07 | 5,796515E-06 | 0,0000 | 0,0000 |
| CH2O = | 1,522896E-07 | 4,009257E-06 | 0,0000 | 0,0000 |
| B2O2 = | 1,376886E-07 | 3,624862E-06 | 0,0000 | 0,0000 |
| HCNO = | 5,876411E-08 | 1,547055E-06 | 0,0000 | 0,0000 |
| HCN = | 2,430656E-08 | 6,399073E-07 | 0,0000 | 0,0000 |
| CNO = | 1,812721E-09 | 4,772265E-08 | 0,0000 | 0,0000 |
| BH2 = | 1,161549E-10 | 3,057955E-09 | 0,0000 | 0,0000 |
| B = | 8,542474E-12 | 2,248937E-10 | 0,0000 | 0,0000 |
| BH = | 3,159981E-12 | 8,319132E-11 | 0,0000 | 0,0000 |
| BN = | 2,435850E-12 | 6,412748E-11 | 0,0000 | 0,0000 |
| N2O3 = | 1,592582E-14 | 4,192716E-13 | 0,0000 | 0,0000 |
| N2H4 = | 9,726899E-15 | 2,560755E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 1,669456E-16 | 4,395099E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 4,684807E-17 | 1,233347E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,833648E-19 | 4,827358E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,595620E-20 | 1,209867E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,075996E-20 | 2,832723E-19 | 0,0000 | 0,0000 |
| C(gr) = | 1,028912E-21 | 2,708769E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,489854E-22 | 3,922270E-21 | 0,0000 | 0,0000 |
| BN(s) = | 1,336030E-22 | 3,517303E-21 | 0,0000 | 0,0000 |
| B(s) = | 9,426365E-23 | 2,481635E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,361388E-24 | 1,148202E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,144782E-32 | 8,279119E-31 | 0,0000 | 0,0000 |

Excluded products(12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; CH4; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 15

**Combustion conditions (Number 15):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 66.67 %**
2. **Hydrogen peroxide ($H_2O_2$), 31.67 %**
3. **Water ($H_2O$, liquid), 1.66 %**

C(2,110) H(5,617) N(0,904) O(1,334) B(0,301)

Molecular weight = 68,27
Oxygen balance = -144,0251 %
Enthalpy of formation = -1045,30 kJ/kg
Internal energy of formation = -851,73 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -2799,48 kJ/kg
- Total enthalpy of combustion prod. = -1045,07 kJ/kg
- Entropy of combustion products = 11,65 kJ/K kg
- Isobaric combustion temperature = 1516,85 K
- Mole number of gaseous products = 56,506 mol/kg expl.
- Total mole number of products = 64,162 mol/kg expl.
- Volume of gaseous products (at SATP) = 1400,73 L/kg expl.
- Mass of gaseous products = 851,6 g/kg expl.
- Mass of condensed products = 148,4 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,072 g
- Mean molecular mass of all products = 15,586 g
- Density of products = 9,823 kg/m3
- Specific gas constant = 469,792 J/kg K
- Specific heat capacity at p=const. (Cp) = 2617,27 J/kgK
- Specific heat capacity at V=const. (Cv) = 2147,48 J/molK
- Specific heat ratio (Cp/Cv) = 1,2188

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 1,660478E+00 | 2,432117E+01 | 37,9056 | 4,9031 |
| CO = | 1,309843E+00 | 1,918538E+01 | 29,9013 | 53,7383 |
| CH4 = | 5,569519E-01 | 8,157725E+00 | 12,7142 | 13,0874 |
| BN(s) = | 3,007939E-01 | 4,405755E+00 | 6,8666 | 10,9333 |
| N2 = | 2,989807E-01 | 4,379196E+00 | 6,8252 | 12,2674 |
| C(gr) = | 2,219225E-01 | 3,250518E+00 | 5,0661 | 3,9042 |
| H2O = | 1,480914E-02 | 2,169107E-01 | 0,3381 | 0,3908 |
| C2H4 = | 4,848086E-03 | 7,101035E-02 | 0,1107 | 0,1992 |
| CO2 = | 4,153328E-03 | 6,083416E-02 | 0,0948 | 0,2677 |
| HCN = | 3,970928E-03 | 5,816253E-02 | 0,0906 | 0,1572 |
| C2H6 = | 1,637900E-03 | 2,399047E-02 | 0,0374 | 0,0721 |
| NH3 = | 1,497152E-03 | 2,192892E-02 | 0,0342 | 0,0373 |
| BHO2 = | 5,228707E-04 | 7,658535E-03 | 0,0119 | 0,0335 |
| B(OH)3 = | 6,289525E-05 | 9,212324E-04 | 0,0014 | 0,0057 |
| CH2O = | 4,488142E-05 | 6,573822E-04 | 0,0010 | 0,0020 |
| BHO = | 2,846004E-05 | 4,168568E-04 | 0,0006 | 0,0012 |
| H = | 6,823341E-06 | 9,994209E-05 | 0,0002 | 0,0000 |
| HCNO = | 3,526847E-06 | 5,165804E-05 | 0,0001 | 0,0002 |
| CH3OH = | 7,620501E-07 | 1,116182E-05 | 0,0000 | 0,0000 |
| B2O3 = | 3,944005E-07 | 5,776820E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,180199E-08 | 1,728649E-07 | 0,0000 | 0,0000 |
| B2O2 = | 3,354291E-09 | 4,913060E-08 | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| BO = 2,905957E-09 | 4,256381E-08 | 0,0000 | 0,0000 | |
| BH2 = 9,736942E-10 | 1,426179E-08 | 0,0000 | 0,0000 | |
| BO2 = 7,042463E-11 | 1,031516E-09 | 0,0000 | 0,0000 | |
| NO = 8,863020E-12 | 1,298174E-10 | 0,0000 | 0,0000 | |
| CNO = 1,486916E-12 | 2,177899E-11 | 0,0000 | 0,0000 | |
| N = 1,162135E-14 | 1,702190E-13 | 0,0000 | 0,0000 | |
| N2O3 = 1,054623E-15 | 1,544715E-14 | 0,0000 | 0,0000 | |
| BH = 9,534218E-16 | 1,396485E-14 | 0,0000 | 0,0000 | |
| B2O3(l) = 2,283694E-16 | 3,344947E-15 | 0,0000 | 0,0000 | |
| BN = 9,254120E-17 | 1,355459E-15 | 0,0000 | 0,0000 | |
| H2O2 = 6,970799E-17 | 1,021019E-15 | 0,0000 | 0,0000 | |
| B2O3(s) = 2,116608E-17 | 3,100214E-16 | 0,0000 | 0,0000 | |
| B = 7,131678E-18 | 1,044583E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = 8,136443E-19 | 1,191752E-17 | 0,0000 | 0,0000 | |
| B(s) = 4,036447E-20 | 5,912220E-19 | 0,0000 | 0,0000 | |
| B(l) = 1,014679E-20 | 1,486210E-19 | 0,0000 | 0,0000 | |
| NO2 = 1,916140E-21 | 2,806588E-20 | 0,0000 | 0,0000 | |
| B4C(l) = 3,139688E-23 | 4,598729E-22 | 0,0000 | 0,0000 | |
| B4C(s) = 1,314951E-23 | 1,926020E-22 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 1,187474E-26 | 1,739304E-25 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 4,970793E-27 | 7,280765E-26 | 0,0000 | 0,0000 | |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -1441,0 kJ/kg
- Entropy of combustion products = 11,65 kJ/K kg
- Temperature at nozzle throat = 1398,3 K
- Pressure at nozzle throat = 3,911012 MPa
- Mole number of gaseous products = 55,804 mol/kg expl.
- Total mole number of products = 62,94 mol/kg expl.
- Volume of gaseous products (at SATP) = 1383,32 L/kg expl.
- Mass of gaseous products = 857,9 g/kg expl.
- Mass of condensed products = 142,1 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,373 g
- Mean molecular mass of all products = 15,888 g
- Density of products = 6,029 kg/m3
- Specific gas constant = 463,952 J/kg K
- Specific heat capacity at p=const. (Cp) = 2567,13 J/kgK
- Specific heat capacity at V=const. (Cv) = 2103,18 J/molK
- Specific heat ratio (Cp/Cv) = 1,2206

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 889,9 m/s
- Sound velocity at throat ) = 889,9 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,559
- Pressure ratio (pc/pt) = 1,79

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = 1,571251E+00 | 2,301425E+01 | 36,5654 | 4,6397 | |
| CO = 1,303792E+00 | 1,909675E+01 | 30,3412 | 53,4900 | |
| CH4 = 6,041949E-01 | 8,849697E+00 | 14,0605 | 14,1976 | |
| BN(s) = 3,008913E-01 | 4,407182E+00 | 7,0022 | 10,9369 | |
| N2 = 3,001800E-01 | 4,396763E+00 | 6,9856 | 12,3167 | |
| C(gr) = 1,863218E-01 | 2,729072E+00 | 4,3360 | 3,2779 | |
| H2O = 1,702725E-02 | 2,493996E-01 | 0,3962 | 0,4493 | |
| CO2 = 6,144023E-03 | 8,999206E-02 | 0,1430 | 0,3961 | |
| C2H4 = 2,561118E-03 | 3,751292E-02 | 0,0596 | 0,1052 | |
| HCN = 1,833256E-03 | 2,685186E-02 | 0,0427 | 0,0726 | |
| C2H6 = 1,213139E-03 | 1,776895E-02 | 0,0282 | 0,0534 | |
| NH3 = 1,140519E-03 | 1,670528E-02 | 0,0265 | 0,0285 | |
| BHO2 = 3,996717E-04 | 5,854027E-03 | 0,0093 | 0,0256 | |
| B(OH)3 = 1,094926E-04 | 1,603748E-03 | 0,0025 | 0,0099 | |

| | | | | |
|---|---|---|---|---|
| CH2O = | 2,600383E-05 | 3,808805E-04 | 0,0006 | 0,0011 |
| BHO = | 8,195305E-06 | 1,200374E-04 | 0,0002 | 0,0003 |
| H = | 1,949824E-06 | 2,855924E-05 | 0,0000 | 0,0000 |
| HCNO = | 1,825279E-06 | 2,673502E-05 | 0,0000 | 0,0001 |
| CH3OH = | 4,367140E-07 | 6,396590E-06 | 0,0000 | 0,0000 |
| B2O3 = | 1,419544E-07 | 2,079219E-06 | 0,0000 | 0,0000 |
| NH2 = | 2,443054E-09 | 3,578363E-08 | 0,0000 | 0,0000 |
| B2O2 = | 4,134333E-10 | 6,055594E-09 | 0,0000 | 0,0000 |
| BO = | 3,024908E-10 | 4,430610E-09 | 0,0000 | 0,0000 |
| BH2 = | 6,184293E-11 | 9,058189E-10 | 0,0000 | 0,0000 |
| BO2 = | 1,073268E-11 | 1,572025E-10 | 0,0000 | 0,0000 |
| NO = | 1,438640E-12 | 2,107189E-11 | 0,0000 | 0,0000 |
| CNO = | 1,756584E-13 | 2,572884E-12 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,020571E-15 | 1,494839E-14 | 0,0000 | 0,0000 |
| N = | 6,223920E-16 | 9,116232E-15 | 0,0000 | 0,0000 |
| N2O3 = | 2,866225E-16 | 4,198185E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 7,281453E-17 | 1,066521E-15 | 0,0000 | 0,0000 |
| BH = | 1,621902E-17 | 2,375614E-16 | 0,0000 | 0,0000 |
| H2O2 = | 8,761712E-18 | 1,283336E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,524422E-18 | 2,232834E-17 | 0,0000 | 0,0000 |
| BN = | 1,282186E-18 | 1,878029E-17 | 0,0000 | 0,0000 |
| B = | 7,333878E-20 | 1,074200E-18 | 0,0000 | 0,0000 |
| B(s) = | 9,959382E-21 | 1,458760E-19 | 0,0000 | 0,0000 |
| B(l) = | 1,801868E-21 | 2,639212E-20 | 0,0000 | 0,0000 |
| NO2 = | 1,052889E-22 | 1,542177E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,913639E-27 | 1,159118E-25 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,774724E-28 | 9,922999E-27 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(l) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -3349,94 kJ/kg
- Entropy of combustion products = 11,65 kJ/K kg
- Temperature at nozzle exit = 991,73 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 50,069 mol/kg expl.
- Total mole number of products = 60,502 mol/kg expl.
- Volume of gaseous products (at SATP) = 1241,16 L/kg expl.
- Mass of gaseous products = 747,6 g/kg expl.
- Mass of condensed products = 252,4 g/kg expl.
- Mean molecular mass of gaseous prod. = 14,931 g
- Mean molecular mass of all products = 16,528 g
- Density of products = 0,242 kg/m3
- Specific gas constant = 416,272 J/kg K
- Specific heat capacity at p=const. (Cp) = 2443,66 J/kgK
- Specific heat capacity at V=const. (Cv) = 2027,39 J/molK
- Specific heat ratio (Cp/Cv) = 1,2053

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 218,94 s
- Vacuum-specific impulse (pa=0) = 238,16 s
- Exhaust (or nozzle exit) velocity = 2147,0 m/s
- Characteristic exhaust velocity (c*) = 1304,8 m/s
- Thrust coefficient (Cf) = 1,645
- Nozzle area expansion ratio (Ae/At) = 10,32
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 709,86 m/s
- Mach number at nozzle exit = 3,025

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 1,401972E+00 | 2,053482E+01 | 33,9409 | 4,1398 |

| | | | | |
|---|---|---|---|---|
| CO = 8,401330E-01 | 1,230550E+01 | 20,3391 | 34,4677 | |
| CH4 = 6,947392E-01 | 1,017591E+01 | 16,8192 | 16,3252 | |
| C(gr) = 5,616031E-01 | 8,225850E+00 | 13,5961 | 9,8801 | |
| N2 = 4,519734E-01 | 6,620095E+00 | 10,9420 | 18,5449 | |
| B2O3(l) = 1,506797E-01 | 2,207019E+00 | 3,6479 | 15,3628 | |
| H2O = 1,604206E-02 | 2,349695E-01 | 0,3884 | 0,4233 | |
| CO2 = 1,295796E-02 | 1,897964E-01 | 0,3137 | 0,8353 | |
| NH3 = 2,389654E-04 | 3,500147E-03 | 0,0058 | 0,0060 | |
| C2H6 = 1,268469E-04 | 1,857938E-03 | 0,0031 | 0,0056 | |
| C2H4 = 6,701469E-05 | 9,815702E-04 | 0,0016 | 0,0028 | |
| B(OH)3 = 4,198531E-05 | 6,149626E-04 | 0,0010 | 0,0038 | |
| HCN = 4,100744E-05 | 6,006396E-04 | 0,0010 | 0,0016 | |
| BHO2 = 7,582717E-06 | 1,110647E-04 | 0,0002 | 0,0005 | |
| CH2O = 6,624919E-07 | 9,703578E-06 | 0,0000 | 0,0000 | |
| HCNO = 2,949892E-08 | 4,320733E-07 | 0,0000 | 0,0000 | |
| CH3OH = 7,214572E-09 | 1,056725E-07 | 0,0000 | 0,0000 | |
| H = 4,166947E-09 | 6,103365E-08 | 0,0000 | 0,0000 | |
| BHO = 2,379404E-09 | 3,485135E-08 | 0,0000 | 0,0000 | |
| B2O3 = 9,233917E-12 | 1,352500E-10 | 0,0000 | 0,0000 | |
| NH2 = 6,670751E-13 | 9,770709E-12 | 0,0000 | 0,0000 | |
| N2O3 = 1,115329E-15 | 1,633633E-14 | 0,0000 | 0,0000 | |
| B2O3(s) = 5,785052E-16 | 8,473417E-15 | 0,0000 | 0,0000 | |
| BN(s) = 5,220101E-16 | 7,645929E-15 | 0,0000 | 0,0000 | |
| BO = 4,992132E-16 | 7,312021E-15 | 0,0000 | 0,0000 | |
| B2O2 = 2,434015E-16 | 3,565124E-15 | 0,0000 | 0,0000 | |
| NO = 6,708917E-17 | 9,826610E-16 | 0,0000 | 0,0000 | |
| BO2 = 5,537472E-17 | 8,110784E-16 | 0,0000 | 0,0000 | |
| BH2 = 1,344588E-17 | 1,969431E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = 2,243792E-18 | 3,286502E-17 | 0,0000 | 0,0000 | |
| CNO = 1,527748E-18 | 2,237706E-17 | 0,0000 | 0,0000 | |
| B4C(l) = 7,503967E-22 | 1,099113E-20 | 0,0000 | 0,0000 | |
| B4C(s) = 4,655001E-22 | 6,818222E-21 | 0,0000 | 0,0000 | |
| N = 2,239054E-22 | 3,279562E-21 | 0,0000 | 0,0000 | |
| H2O2 = 3,057946E-23 | 4,479001E-22 | 0,0000 | 0,0000 | |
| B = 1,243821E-23 | 1,821835E-22 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 3,948788E-25 | 5,783826E-24 | 0,0000 | 0,0000 | |
| B(l) = 1,922967E-25 | 2,816587E-24 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 7,578658E-26 | 1,110053E-24 | 0,0000 | 0,0000 | |
| B(s) = 5,054077E-26 | 7,402752E-25 | 0,0000 | 0,0000 | |
| BH = 3,780188E-27 | 5,536875E-26 | 0,0000 | 0,0000 | |
| NO2 = 6,648950E-30 | 9,738777E-29 | 0,0000 | 0,0000 | |
| BN = 3,143471E-30 | 4,604270E-29 | 0,0000 | 0,0000 | |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 16

**Combustion conditions (Number 16):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 50.00 %**
**2. Hydrogen peroxide ($H_2O_2$), 47.50 %**
**3. Water ($H_2O$, liquid), 2.50 %**

C(1,242) H(4,129) N(0,532) O(1,571) B(0,177)

Molecular weight = 53,58
Oxygen balance = -96,84287 %
Enthalpy of formation = -2293,11 kJ/kg
Internal energy of formation = -2101,21 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -2883,85 kJ/kg
- Total enthalpy of combustion prod. = -2292,61 kJ/kg
- Entropy of combustion products = 12,46 kJ/K kg
- Isobaric combustion temperature = 1567,09 K
- Mole number of gaseous products = 64,175 mol/kg expl.
- Total mole number of products = 65,762 mol/kg expl.
- Volume of gaseous products (at SATP) = 1590,83 L/kg expl.
- Mass of gaseous products = 889,5 g/kg expl.
- Mass of condensed products = 110,5 g/kg expl.
- Mean molecular mass of gaseous prod. = 13,861 g
- Mean molecular mass of all products = 15,206 g
- Density of products = 8,372 kg/m3
- Specific gas constant = 533,55 J/kg K
- Specific heat capacity at p=const. (Cp) = 2476,54 J/kgK
- Specific heat capacity at V=const. (Cv) = 1942,99 J/molK
- Specific heat ratio (Cp/Cv) = 1,2746

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 1,820717E+00 | 3,398091E+01 | 51,6724 | 6,8506 | |
| CO = | 1,153461E+00 | 2,152760E+01 | 32,7355 | 60,2988 | |
| N2 = | 2,650067E-01 | 4,945947E+00 | 7,5210 | 13,8551 | |
| H2O = | 1,022323E-01 | 1,908011E+00 | | 2,9014 | 3,4373 |
| B2O3(l) = | 8,504468E-02 | 1,587230E+00 | | 2,4136 | 11,0485 |
| CH4 = | 6,607920E-02 | 1,233268E+00 | | 1,8753 | 1,9785 |
| CO2 = | 2,136859E-02 | 3,988123E-01 | | 0,6064 | 1,7552 |
| BHO2 = | 4,584276E-03 | 8,555854E-02 | | 0,1301 | 0,3747 |
| B(OH)3 = | 2,662100E-03 | 4,968405E-02 | | 0,0756 | 0,3072 |
| NH3 = | 1,573647E-03 | 2,936972E-02 | | 0,0447 | 0,0500 |
| HCN = | 6,094177E-04 | 1,137385E-02 | | 0,0173 | 0,0307 |
| C2H4 = | 8,863675E-05 | 1,654270E-03 | | 0,0025 | 0,0046 |
| BHO = | 5,323638E-05 | 9,935760E-04 | | 0,0015 | 0,0028 |
| CH2O = | 4,712824E-05 | 8,795769E-04 | | 0,0013 | 0,0026 |
| C2H6 = | 2,561251E-05 | 4,780185E-04 | | 0,0007 | 0,0014 |
| H = | 1,195107E-05 | 2,230486E-04 | 0,0003 | 0,0000 | |
| B2O3 = | 5,006906E-06 | 9,344628E-05 | | 0,0001 | 0,0007 |
| HCNO = | 3,515896E-06 | 6,561885E-05 | | 0,0001 | 0,0003 |
| CH3OH = | 7,812306E-07 | 1,458048E-05 | | 0,0000 | 0,0000 |
| NH2 = | 2,059354E-08 | 3,843471E-07 | | 0,0000 | 0,0000 |
| B2O2 = | 9,414077E-09 | 1,756994E-07 | | 0,0000 | 0,0000 |
| BO = | 8,097401E-09 | 1,511257E-07 | 0,0000 | 0,0000 | |

| | | | | |
|---|---|---|---|---|
| BO2 = | 1,153823E-09 | 2,153436E-08 | 0,0000 | 0,0000 |
| BH2 = | 4,688501E-10 | 8,750373E-09 | 0,0000 | 0,0000 |
| NO = | 1,184622E-10 | 2,210916E-09 | 0,0000 | 0,0000 |
| CNO = | 2,630526E-12 | 4,909476E-11 | 0,0000 | 0,0000 |
| N = | 3,485327E-14 | 6,504832E-13 | 0,0000 | 0,0000 |
| H2O2 = | 7,542515E-15 | 1,407696E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 8,687263E-16 | 1,621345E-14 | 0,0000 | 0,0000 |
| BH = | 7,661481E-16 | 1,429899E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 7,371963E-16 | 1,375865E-14 | 0,0000 | 0,0000 |
| BN(s) = | 1,654419E-16 | 3,087722E-15 | 0,0000 | 0,0000 |
| C(gr) = | 1,330528E-16 | 2,483227E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,160819E-16 | 2,166492E-15 | 0,0000 | 0,0000 |
| BN = | 7,307114E-17 | 1,363762E-15 | 0,0000 | 0,0000 |
| B = | 7,037124E-18 | 1,313372E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,638441E-18 | 8,656944E-17 | 0,0000 | 0,0000 |
| NO2 = | 2,616587E-19 | 4,883461E-18 | 0,0000 | 0,0000 |
| N2O3 = | 9,306108E-20 | 1,736843E-18 | 0,0000 | 0,0000 |
| B(s) = | 1,083494E-20 | 2,022177E-19 | 0,0000 | 0,0000 |
| B(l) = | 3,096007E-21 | 5,778227E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,765046E-23 | 5,160538E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,377622E-24 | 4,437470E-23 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -2769,14 kJ/kg
- Entropy of combustion products = 12,46 kJ/K kg
- Temperature at nozzle throat = 1422,34 K
- Pressure at nozzle throat = 3,832146 MPa
- Mole number of gaseous products = 63,224 mol/kg expl.
- Total mole number of products = 64,836 mol/kg expl.
- Volume of gaseous products (at SATP) = 1567,27 L/kg expl.
- Mass of gaseous products = 887,8 g/kg expl.
- Mass of condensed products = 112,2 g/kg expl.
- Mean molecular mass of gaseous prod. = 14,042 g
- Mean molecular mass of all products = 15,423 g
- Density of products = 5,126 kg/m3
- Specific gas constant = 525,647 J/kg K
- Specific heat capacity at p=const. (Cp) = 2439,82 J/kgK
- Specific heat capacity at V=const. (Cv) = 1914,18 J/molK
- Specific heat ratio (Cp/Cv) = 1,2746

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 976,2 m/s
- Sound velocity at throat ) = 976,2 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,547
- Pressure ratio (pc/pt) = 1,827

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = | 1,756547E+00 | 3,278328E+01 | 50,5633 | 6,6091 |
| CO = | 1,118885E+00 | 2,088229E+01 | 32,2078 | 58,4913 |
| N2 = | 2,653179E-01 | 4,951754E+00 | 7,6373 | 13,8713 |
| H2O = | 1,180445E-01 | 2,203121E+00 | 3,3980 | 3,9690 |
| CH4 = | 9,114993E-02 | 1,701175E+00 | 2,6238 | 2,7292 |
| B2O3(l) = | 8,635999E-02 | 1,611778E+00 | 2,4859 | 11,2194 |
| CO2 = | 3,128974E-02 | 5,839753E-01 | 0,9007 | 2,5701 |
| B(OH)3 = | 2,872269E-03 | 5,360653E-02 | 0,0827 | 0,3314 |
| BHO2 = | 1,800155E-03 | 3,359715E-02 | 0,0518 | 0,1471 |
| NH3 = | 1,286980E-03 | 2,401953E-02 | 0,0370 | 0,0409 |
| HCN = | 2,765870E-04 | 5,162075E-03 | 0,0080 | 0,0140 |
| C2H4 = | 5,828634E-05 | 1,087826E-03 | 0,0017 | 0,0031 |
| C2H6 = | 2,761539E-05 | 5,153992E-04 | 0,0008 | 0,0015 |
| CH2O = | 2,699559E-05 | 5,038315E-04 | 0,0008 | 0,0015 |

| | | | | |
|---|---|---|---|---|
| BHO = | 7,049193E-06 | 1,315625E-04 | 0,0002 | 0,0004 |
| H = | 2,721282E-06 | 5,078859E-05 | 0,0001 | 0,0000 |
| HCNO = | 1,737335E-06 | 3,242471E-05 | 0,0001 | 0,0001 |
| CH3OH = | 4,889661E-07 | 9,125807E-06 | 0,0000 | 0,0000 |
| B2O3 = | 4,474644E-07 | 8,351242E-06 | 0,0000 | 0,0001 |
| NH2 = | 3,522557E-09 | 6,574316E-08 | 0,0000 | 0,0000 |
| BO = | 3,126054E-10 | 5,834305E-09 | 0,0000 | 0,0000 |
| B2O2 = | 2,541019E-10 | 4,742425E-09 | 0,0000 | 0,0000 |
| BO2 = | 6,602123E-11 | 1,232186E-09 | 0,0000 | 0,0000 |
| NO = | 1,313402E-11 | 2,451264E-10 | 0,0000 | 0,0000 |
| BH2 = | 1,183259E-11 | 2,208373E-10 | 0,0000 | 0,0000 |
| CNO = | 2,217946E-13 | 4,139458E-12 | 0,0000 | 0,0000 |
| N = | 1,116595E-15 | 2,083955E-14 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,725107E-16 | 1,441774E-14 | 0,0000 | 0,0000 |
| H2O2 = | 6,338197E-16 | 1,182928E-14 | 0,0000 | 0,0000 |
| C(gr) = | 1,482680E-16 | 2,767197E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,481284E-16 | 2,764592E-15 | 0,0000 | 0,0000 |
| BN(s) = | 9,715111E-17 | 1,813178E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,525315E-18 | 1,031216E-16 | 0,0000 | 0,0000 |
| BH = | 3,977944E-18 | 7,424227E-17 | 0,0000 | 0,0000 |
| BN = | 2,941844E-19 | 5,490503E-18 | 0,0000 | 0,0000 |
| B = | 1,932962E-20 | 3,607579E-19 | 0,0000 | 0,0000 |
| NO2 = | 7,856240E-21 | 1,466248E-19 | 0,0000 | 0,0000 |
| B(s) = | 1,287616E-21 | 2,403140E-20 | 0,0000 | 0,0000 |
| B(l) = | 2,488197E-22 | 4,643842E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,544814E-23 | 4,749507E-22 | 0,0000 | 0,0000 |
| N2O3 = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |
| B4C(l) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -4837,64 kJ/kg
- Entropy of combustion products = 12,46 kJ/K kg
- Temperature at nozzle exit = 938,92 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 55,844 mol/kg expl.
- Total mole number of products = 57,483 mol/kg expl.
- Volume of gaseous products (at SATP) = 1384,33 L/kg expl.
- Mass of gaseous products = 885,9 g/kg expl.
- Mass of condensed products = 114,1 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,864 g
- Mean molecular mass of all products = 17,396 g
- Density of products = 0,229 kg/m3
- Specific gas constant = 464,291 J/kg K
- Specific heat capacity at p=const. (Cp) = 2260,61 J/kgK
- Specific heat capacity at V=const. (Cv) = 1796,32 J/molK
- Specific heat ratio (Cp/Cv) = 1,2585

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 230,06 s
- Vacuum-specific impulse (pa=0) = 249,38 s
- Exhaust (or nozzle exit) velocity = 2256,1 m/s
- Characteristic exhaust velocity (c*) = 1398,9 m/s
- Thrust coefficient (Cf) = 1,613
- Nozzle area expansion ratio (Ae/At) = 9,67
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 745,42 m/s
- Mach number at nozzle exit = 3,027

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 1,308172E+00 | 2,441504E+01 | 42,4732 | 4,9221 |

| | | | | |
|---|---|---|---|---|
| CO = 7,767409E-01 | 1,449669E+01 | 25,2189 | 40,6052 | |
| CH4 = 2,894537E-01 | 5,402212E+00 | 9,3979 | 8,6668 | |
| N2 = 2,659621E-01 | 4,963778E+00 | 8,6352 | 13,9050 | |
| CO2 = 1,755703E-01 | 3,276753E+00 | 5,7003 | 14,4210 | |
| H2O = 1,742163E-01 | 3,251483E+00 | 5,6564 | 5,8576 | |
| B2O3(l) = 8,780765E-02 | 1,638796E+00 | 2,8509 | 11,4075 | |
| B(OH)3 = 1,760727E-03 | 3,286129E-02 | 0,0572 | 0,2032 | |
| NH3 = 2,739888E-04 | 5,113583E-03 | 0,0089 | 0,0087 | |
| C2H6 = 1,428184E-05 | 2,665488E-04 | 0,0005 | 0,0008 | |
| B2O3(s) = 8,616170E-06 | 1,608077E-04 | 0,0003 | 0,0011 | |
| BHO2 = 7,071772E-06 | 1,319839E-04 | 0,0002 | 0,0006 | |
| HCN = 2,801756E-06 | 5,229051E-05 | 0,0001 | 0,0001 | |
| C2H4 = 2,666657E-06 | 4,976910E-05 | 0,0001 | 0,0001 | |
| CH2O = 7,092104E-07 | 1,323633E-05 | 0,0000 | 0,0000 | |
| HCNO = 2,195393E-08 | 4,097366E-07 | 0,0000 | 0,0000 | |
| CH3OH = 1,538640E-08 | 2,871638E-07 | 0,0000 | 0,0000 | |
| H = 8,277816E-10 | 1,544928E-08 | 0,0000 | 0,0000 | |
| BHO = 8,546756E-11 | 1,595122E-09 | 0,0000 | 0,0000 | |
| B2O3 = 5,286225E-13 | 9,865934E-12 | 0,0000 | 0,0000 | |
| NH2 = 1,438431E-13 | 2,684612E-12 | 0,0000 | 0,0000 | |
| C(gr) = 2,483094E-16 | 4,634317E-15 | 0,0000 | 0,0000 | |
| N2O3 = 7,489944E-17 | 1,397884E-15 | 0,0000 | 0,0000 | |
| NO = 5,535755E-17 | 1,033164E-15 | 0,0000 | 0,0000 | |
| BHO2(s) = 1,149303E-17 | 2,144998E-16 | 0,0000 | 0,0000 | |
| BN(s) = 7,252630E-18 | 1,353593E-16 | 0,0000 | 0,0000 | |
| BO2 = 7,230387E-18 | 1,349442E-16 | 0,0000 | 0,0000 | |
| BO = 4,465414E-18 | 8,334016E-17 | 0,0000 | 0,0000 | |
| B2O2 = 4,829963E-19 | 9,014392E-18 | 0,0000 | 0,0000 | |
| CNO = 1,808078E-19 | 3,374502E-18 | 0,0000 | 0,0000 | |
| BH2 = 1,524166E-20 | 2,844623E-19 | 0,0000 | 0,0000 | |
| H2O2 = 3,443448E-22 | 6,426671E-21 | 0,0000 | 0,0000 | |
| N = 6,240731E-24 | 1,164737E-22 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 7,328085E-26 | 1,367676E-24 | 0,0000 | 0,0000 | |
| B(l) = 2,487042E-28 | 4,641686E-27 | 0,0000 | 0,0000 | |
| NO2 = 1,772966E-29 | 3,308971E-28 | 0,0000 | 0,0000 | |
| B(s) = 1,080434E-29 | 2,016466E-28 | 0,0000 | 0,0000 | |
| BH = 6,957250E-31 | 1,298465E-29 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 1,068264E-33 | 1,993753E-32 | 0,0000 | 0,0000 | |
| BN = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |
| B4C(s) = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |
| B4C(l) = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |
| B = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 17

**Combustion conditions (Number 17):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 40.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 57.00 %**
3. **Water ($H_2O$, liquid), 3.00 %**

C(0,880) H(3,508) N(0,377) O(1,670) B(0,126)

Molecular weight = 47,46
Oxygen balance = -68,53736 %
Enthalpy of formation = -3041,23 kJ/kg
Internal energy of formation = -2850,35 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3474,46 kJ/kg
- Total enthalpy of combustion prod. = -3041,51 kJ/kg
- Entropy of combustion products = 12,64 kJ/K kg
- Isobaric combustion temperature = 1897,61 K
- Mole number of gaseous products = 60,087 mol/kg expl.
- Total mole number of products = 60,344 mol/kg expl.
- Volume of gaseous products (at SATP) = 1489,49 L/kg expl.
- Mass of gaseous products = 982,0 g/kg expl.
- Mass of condensed products = 17,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 16,344 g
- Mean molecular mass of all products = 16,571 g
- Density of products = 7,384 kg/m3
- Specific gas constant = 499,56 J/kg K
- Specific heat capacity at p=const. (Cp) = 2417,87 J/kgK
- Specific heat capacity at V=const. (Cv) = 1918,31 J/molK
- Specific heat ratio (Cp/Cv) = 1,2604

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 1,220357E+00 | 2,571514E+01 | 42,6141 | 5,1842 | |
| CO = | 8,102332E-01 | 1,707308E+01 | 28,2928 | 47,8217 | |
| H2O = | 4,617497E-01 | 9,729902E+00 | | 16,1240 | 17,5287 |
| N2 = | 1,883157E-01 | 3,968153E+00 | 6,5759 | 11,1160 | |
| BHO2 = | 7,837998E-02 | 1,651608E+00 | | 2,7370 | 7,2337 |
| CO2 = | 6,937490E-02 | 1,461855E+00 | | 2,4225 | 6,4336 |
| B(OH)3 = | 2,092774E-02 | 4,409854E-01 | | 0,7308 | 2,7266 |
| B2O3(l) = | 1,222689E-02 | 2,576427E-01 | | 0,4270 | 1,7934 |
| B2O3 = | 6,497488E-04 | 1,369138E-02 | | 0,0227 | 0,0953 |
| BHO = | 6,344033E-04 | 1,336803E-02 | | 0,0222 | 0,0372 |
| NH3 = | 4,149608E-04 | 8,743976E-03 | | 0,0145 | 0,0149 |
| CH4 = | 2,152092E-04 | 4,534848E-03 | | 0,0075 | 0,0073 |
| H = | 1,821914E-04 | 3,839102E-03 | 0,0064 | 0,0004 | |
| HCN = | 5,093100E-05 | 1,073209E-03 | | 0,0018 | 0,0029 |
| CH2O = | 2,289633E-05 | 4,824672E-04 | | 0,0008 | 0,0014 |
| HCNO = | 2,350822E-06 | 4,953609E-05 | | 0,0001 | 0,0002 |
| BO = | 1,489597E-06 | 3,138850E-05 | 0,0001 | 0,0001 | |
| B2O2 = | 1,021481E-06 | 2,152445E-05 | | 0,0000 | 0,0001 |
| BO2 = | 1,020731E-06 | 2,150864E-05 | | 0,0000 | 0,0001 |
| NH2 = | 1,488368E-07 | 3,136261E-06 | | 0,0000 | 0,0000 |
| CH3OH = | 9,225007E-08 | 1,943876E-06 | | 0,0000 | 0,0000 |
| NO = | 6,020294E-08 | 1,268585E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| C2H4 = | 3,324098E-08 | 7,004477E-07 | 0,0000 | 0,0000 |
| BH2 = | 5,447236E-09 | 1,147831E-07 | 0,0000 | 0,0000 |
| C2H6 = | 1,159284E-09 | 2,442822E-08 | 0,0000 | 0,0000 |
| CNO = | 6,906044E-11 | 1,455229E-09 | 0,0000 | 0,0000 |
| H2O2 = | 2,816004E-11 | 5,933830E-10 | 0,0000 | 0,0000 |
| N = | 1,614372E-11 | 3,401774E-10 | 0,0000 | 0,0000 |
| BH = | 2,502229E-13 | 5,272650E-12 | 0,0000 | 0,0000 |
| BN = | 3,922319E-14 | 8,265036E-13 | 0,0000 | 0,0000 |
| B = | 1,302283E-14 | 2,744146E-13 | 0,0000 | 0,0000 |
| NO2 = | 1,153912E-14 | 2,431502E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,872034E-15 | 3,944714E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 8,035240E-17 | 1,693171E-15 | 0,0000 | 0,0000 |
| BN(s) = | 6,235044E-18 | 1,313837E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,616702E-18 | 1,183541E-16 | 0,0000 | 0,0000 |
| B4C(s) = | 4,483659E-18 | 9,447882E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,246655E-18 | 6,841291E-17 | 0,0000 | 0,0000 |
| B(s) = | 1,429386E-20 | 3,011976E-19 | 0,0000 | 0,0000 |
| B(l) = | 7,983137E-21 | 1,682192E-19 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,813325E-25 | 3,821004E-24 | 0,0000 | 0,0000 |
| N2O3 = | 1,446558E-26 | 3,048159E-25 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,781518E-27 | 3,753981E-26 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -3583,51 kJ/kg
- Entropy of combustion products = 12,64 kJ/K kg
- Temperature at nozzle throat = 1732,16 K
- Pressure at nozzle throat = 3,841721 MPa
- Mole number of gaseous products = 59,693 mol/kg expl.
- Total mole number of products = 60,396 mol/kg expl.
- Volume of gaseous products (at SATP) = 1479,72 L/kg expl.
- Mass of gaseous products = 951,0 g/kg expl.
- Mass of condensed products = 48,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,932 g
- Mean molecular mass of all products = 16,557 g
- Density of products = 4,469 kg/m3
- Specific gas constant = 496,284 J/kg K
- Specific heat capacity at p=const. (Cp) = 2392,62 J/kgK
- Specific heat capacity at V=const. (Cv) = 1896,33 J/molK
- Specific heat ratio (Cp/Cv) = 1,2617

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1041,2 m/s
- Sound velocity at throat ) = 1041,5 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,549
- Pressure ratio (pc/pt) = 1,822

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = | 1,233264E+00 | 2,598711E+01 | 43,0281 | 5,2390 |
| CO = | 7,979009E-01 | 1,681322E+01 | 27,8384 | 47,0938 |
| H2O = | 4,720519E-01 | 9,946988E+00 | 16,4697 | 17,9198 |
| N2 = | 1,883720E-01 | 3,969339E+00 | 6,5722 | 11,1193 |
| CO2 = | 8,169780E-02 | 1,721521E+00 | 2,8504 | 7,5764 |
| BHO2 = | 4,009629E-02 | 8,449014E-01 | 1,3989 | 3,7005 |
| B2O3(l) = | 3,337075E-02 | 7,031822E-01 | 1,1643 | 4,8948 |
| B(OH)3 = | 1,845987E-02 | 3,889829E-01 | 0,6441 | 2,4051 |
| NH3 = | 3,266431E-04 | 6,882962E-03 | 0,0114 | 0,0117 |
| CH4 = | 2,582404E-04 | 5,441592E-03 | 0,0090 | 0,0087 |
| BHO = | 1,593972E-04 | 3,358788E-03 | 0,0056 | 0,0093 |
| B2O3 = | 1,212232E-04 | 2,554393E-03 | 0,0042 | 0,0178 |
| H = | 6,269399E-05 | 1,321076E-03 | 0,0022 | 0,0001 |

| | | | | |
|---|---|---|---|---|
| HCN = | 2,796836E-05 | 5,893440E-04 | 0,0010 | 0,0016 |
| CH2O = | 1,347977E-05 | 2,840433E-04 | 0,0005 | 0,0009 |
| HCNO = | 1,206398E-06 | 2,542098E-05 | 0,0000 | 0,0001 |
| BO = | 1,525985E-07 | 3,215528E-06 | 0,0000 | 0,0000 |
| BO2 = | 1,226424E-07 | 2,584298E-06 | 0,0000 | 0,0000 |
| B2O2 = | 8,629303E-08 | 1,818350E-06 | 0,0000 | 0,0000 |
| CH3OH = | 5,205361E-08 | 1,096864E-06 | 0,0000 | 0,0000 |
| NH2 = | 3,680131E-08 | 7,754704E-07 | 0,0000 | 0,0000 |
| C2H4 = | 2,227419E-08 | 4,693575E-07 | 0,0000 | 0,0000 |
| NO = | 1,024723E-08 | 2,159277E-07 | 0,0000 | 0,0000 |
| C2H6 = | 1,023325E-09 | 2,156331E-08 | 0,0000 | 0,0000 |
| BH2 = | 4,111571E-10 | 8,663825E-09 | 0,0000 | 0,0000 |
| CNO = | 9,440370E-12 | 1,989257E-10 | 0,0000 | 0,0000 |
| H2O2 = | 3,290217E-12 | 6,933083E-11 | 0,0000 | 0,0000 |
| N = | 1,194330E-12 | 2,516671E-11 | 0,0000 | 0,0000 |
| BH = | 5,867394E-15 | 1,236366E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 9,031196E-16 | 1,903037E-14 | 0,0000 | 0,0000 |
| BN = | 7,403521E-16 | 1,560056E-14 | 0,0000 | 0,0000 |
| NO2 = | 6,233833E-16 | 1,313581E-14 | 0,0000 | 0,0000 |
| B = | 1,953901E-16 | 4,117224E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 9,408557E-17 | 1,982553E-15 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,663407E-18 | 1,193383E-16 | 0,0000 | 0,0000 |
| BN(s) = | 4,994174E-18 | 1,052363E-16 | 0,0000 | 0,0000 |
| C(gr) = | 3,464029E-18 | 7,299336E-17 | 0,0000 | 0,0000 |
| B(s) = | 3,416337E-21 | 7,198840E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,407212E-21 | 2,965250E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,070029E-22 | 2,254744E-21 | 0,0000 | 0,0000 |
| N2O3 = | 5,292522E-24 | 1,115230E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,657298E-25 | 1,613531E-23 | 0,0000 | 0,0000 |
| B4C(s) = | 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -5877,95 kJ/kg
- Entropy of combustion products = 12,64 kJ/K kg
- Temperature at nozzle exit = 960,13 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 57,126 mol/kg expl.
- Total mole number of products = 58,389 mol/kg expl.
- Volume of gaseous products (at SATP) = 1416,1 L/kg expl.
- Mass of gaseous products = 912,1 g/kg expl.
- Mass of condensed products = 87,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 15,966 g
- Mean molecular mass of all products = 17,126 g
- Density of products = 0,219 kg/m3
- Specific gas constant = 474,948 J/kg K
- Specific heat capacity at p=const. (Cp) = 2196,83 J/kgK
- Specific heat capacity at V=const. (Cv) = 1721,88 J/molK
- Specific heat ratio (Cp/Cv) = 1,2758

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 242,87 s
- Vacuum-specific impulse (pa=0) = 262,02 s
- Exhaust (or nozzle exit) velocity = 2381,8 m/s
- Characteristic exhaust velocity (c*) = 1504,5 m/s
- Thrust coefficient (Cf) = 1,583
- Nozzle area expansion ratio (Ae/At) = 8,91
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 758,52 m/s
- Mach number at nozzle exit = 3,14

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | |
|---|---|---|---|---|
| H2 = 1,254103E+00 | 2,642622E+01 | 45,2586 | 5,3275 | |
| CO = 5,615211E-01 | 1,183227E+01 | 20,2644 | 33,1422 | |
| H2O = 3,825589E-01 | 8,061209E+00 | 13,8060 | 14,5225 | |
| CO2 = 2,641161E-01 | 5,565404E+00 | 9,5315 | 24,4933 | |
| N2 = 1,884471E-01 | 3,970922E+00 | 6,8008 | 11,1237 | |
| B2O3(l) = 5,993288E-02 | 1,262894E+00 | 2,1629 | 8,7909 | |
| CH4 = 5,425914E-02 | 1,143338E+00 | 1,9581 | 1,8343 | |
| B(OH)3 = 5,799775E-03 | 1,222118E-01 | 0,2093 | 0,7556 | |
| NH3 = 2,047695E-04 | 4,314864E-03 | 0,0074 | 0,0073 | |
| BHO2 = 1,640050E-05 | 3,455883E-04 | 0,0006 | 0,0015 | |
| B2O3(s) = 8,993927E-06 | 1,895183E-04 | 0,0003 | 0,0013 | |
| HCN = 7,992317E-07 | 1,684126E-05 | 0,0000 | 0,0000 | |
| C2H6 = 6,444902E-07 | 1,358058E-05 | 0,0000 | 0,0000 | |
| CH2O = 5,242699E-07 | 1,104732E-05 | 0,0000 | 0,0000 | |
| C2H4 = 1,704891E-07 | 3,592514E-06 | 0,0000 | 0,0000 | |
| HCNO = 1,474079E-08 | 3,106151E-07 | 0,0000 | 0,0000 | |
| CH3OH = 9,286092E-09 | 1,956748E-07 | 0,0000 | 0,0000 | |
| H = 1,446004E-09 | 3,046992E-08 | 0,0000 | 0,0000 | |
| BHO = 1,207298E-10 | 2,543995E-09 | 0,0000 | 0,0000 | |
| B2O3 = 1,487926E-12 | 3,135329E-11 | 0,0000 | 0,0000 | |
| NH2 = 2,062596E-13 | 4,346264E-12 | 0,0000 | 0,0000 | |
| NO = 2,653373E-16 | 5,591137E-15 | 0,0000 | 0,0000 | |
| B4C(l) = 1,439186E-16 | 3,032626E-15 | 0,0000 | 0,0000 | |
| C(gr) = 5,267212E-17 | 1,109897E-15 | 0,0000 | 0,0000 | |
| BO2 = 3,635387E-17 | 7,660419E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = 1,544088E-17 | 3,253674E-16 | 0,0000 | 0,0000 | |
| B4C(s) = 1,346375E-17 | 2,837055E-16 | 0,0000 | 0,0000 | |
| BO = 1,077347E-17 | 2,270165E-16 | 0,0000 | 0,0000 | |
| BN(s) = 1,826671E-18 | 3,849126E-17 | 0,0000 | 0,0000 | |
| B2O2 = 8,651793E-19 | 1,823089E-17 | 0,0000 | 0,0000 | |
| CNO = 2,496983E-19 | 5,261595E-18 | 0,0000 | 0,0000 | |
| N2O3 = 2,652253E-20 | 5,588778E-19 | 0,0000 | 0,0000 | |
| BH2 = 1,484875E-20 | 3,128901E-19 | 0,0000 | 0,0000 | |
| H2O2 = 4,721022E-21 | 9,948048E-20 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 2,716556E-23 | 5,724277E-22 | 0,0000 | 0,0000 | |
| N = 1,923852E-23 | 4,053904E-22 | 0,0000 | 0,0000 | |
| NO2 = 3,311481E-28 | 6,977890E-27 | 0,0000 | 0,0000 | |
| B(s) = 1,614185E-28 | 3,401379E-27 | 0,0000 | 0,0000 | |
| B(l) = 4,166161E-30 | 8,778856E-29 | 0,0000 | 0,0000 | |
| BH = 1,630583E-30 | 3,435933E-29 | 0,0000 | 0,0000 | |
| BN = 3,952561E-32 | 8,328762E-31 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 4,795790E-34 | 1,010560E-32 | 0,0000 | 0,0000 | |
| B = 0,000000E+00 | 0,000000E+00 | 0,0000 | 0,0000 | |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 18

**Combustion conditions (Number 18):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 33.34 %**
2. **Hydrogen peroxide ($H_2O_2$), 63.33 %**
3. **Water ($H_2O$, liquid), 3.33 %**

C(0,682) H(3,168) N(0,292) O(1,724) B(0,097)

Molecular weight = 44,1
Oxygen balance = -49,68447 %
Enthalpy of formation = -3539,17 kJ/kg
Internal energy of formation = -3348,97 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -4165,4 kJ/kg
- Total enthalpy of combustion prod. = -3539,59 kJ/kg
- Entropy of combustion products = 12,58 kJ/K kg
- Isobaric combustion temperature = 2248,63 K
- Mole number of gaseous products = 55,639 mol/kg expl.
- Total mole number of products = 55,639 mol/kg expl.
- Volume of gaseous products (at SATP) = 1379,23 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,972 g
- Mean molecular mass of all products = 17,972 g
- Density of products = 6,729 kg/m3
- Specific gas constant = 462,582 J/kg K
- Specific heat capacity at p=const. (Cp) = 2425,21 J/kgK
- Specific heat capacity at V=const. (Cv) = 1962,63 J/molK
- Specific heat ratio (Cp/Cv) = 1,2357

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2 = | 7,833699E-01 | 1,776289E+01 | 31,9253 | 3,5810 | |
| H2O = | 7,449523E-01 | 1,689178E+01 | | 30,3596 | 30,4310 |
| CO = | 5,844003E-01 | 1,325126E+01 | 23,8165 | 37,1168 | |
| N2 = | 1,459728E-01 | 3,309931E+00 | 5,9489 | 9,2721 | |
| CO2 = | 9,711143E-02 | 2,201999E+00 | | 3,9577 | 9,6910 |
| BHO2 = | 8,756814E-02 | 1,985606E+00 | | 3,5687 | 8,6966 |
| B(OH)3 = | 7,174023E-03 | 1,626708E-01 | | 0,2924 | 1,0058 |
| H = | 1,280625E-03 | 2,903813E-02 | 0,0522 | 0,0029 | |
| BHO = | 8,815714E-04 | 1,998961E-02 | | 0,0359 | 0,0556 |
| B2O3 = | 8,471233E-04 | 1,920850E-02 | | 0,0345 | 0,1337 |
| NH3 = | 1,266727E-04 | 2,872301E-03 | | 0,0052 | 0,0049 |
| BO2 = | 2,280794E-05 | 5,171696E-04 | | 0,0009 | 0,0022 |
| BO = | 1,652863E-05 | 3,747863E-04 | 0,0007 | 0,0010 | |
| HCN = | 1,179252E-05 | 2,673950E-04 | | 0,0005 | 0,0007 |
| CH2O = | 1,115258E-05 | 2,528846E-04 | | 0,0005 | 0,0008 |
| NO = | 3,723486E-06 | 8,442996E-05 | | 0,0002 | 0,0003 |
| CH4 = | 3,683147E-06 | 8,351527E-05 | | 0,0002 | 0,0001 |
| B2O2 = | 1,883613E-06 | 4,271088E-05 | | 0,0001 | 0,0002 |
| HCNO = | 1,565915E-06 | 3,550709E-05 | | 0,0001 | 0,0002 |
| NH2 = | 5,579165E-07 | 1,265074E-05 | | 0,0000 | 0,0000 |
| CH3OH = | 1,413908E-08 | 3,206034E-07 | | 0,0000 | 0,0000 |
| BH2 = | 1,128354E-08 | 2,558540E-07 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| H2O2 = | 4,075148E-09 | 9,240389E-08 | 0,0000 | 0,0000 |
| N = | 1,522409E-09 | 3,452059E-08 | 0,0000 | 0,0000 |
| CNO = | 7,465092E-10 | 1,692708E-08 | 0,0000 | 0,0000 |
| C2H4 = | 1,804609E-10 | 4,091948E-09 | 0,0000 | 0,0000 |
| NO2 = | 1,203410E-11 | 2,728728E-10 | 0,0000 | 0,0000 |
| BH = | 6,472097E-12 | 1,467547E-10 | 0,0000 | 0,0000 |
| BN = | 1,577098E-12 | 3,576066E-11 | 0,0000 | 0,0000 |
| B = | 1,306640E-12 | 2,962803E-11 | 0,0000 | 0,0000 |
| C2H6 = | 1,171481E-12 | 2,656330E-11 | 0,0000 | 0,0000 |
| B4C(l) = | 6,584734E-17 | 1,493087E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 4,095329E-17 | 9,286149E-16 | 0,0000 | 0,0000 |
| B4C(s) = | 3,114280E-17 | 7,061624E-16 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,440066E-18 | 5,532845E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 9,583132E-19 | 2,172973E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,567828E-19 | 8,090042E-18 | 0,0000 | 0,0000 |
| BN(s) = | 2,462600E-19 | 5,583941E-18 | 0,0000 | 0,0000 |
| B(s) = | 7,008293E-21 | 1,589129E-19 | 0,0000 | 0,0000 |
| B(l) = | 6,442083E-21 | 1,460741E-19 | 0,0000 | 0,0000 |
| N2O3 = | 7,934126E-22 | 1,799061E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 5,484985E-23 | 1,243719E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,067922E-23 | 2,421511E-22 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -4118,22 kJ/kg
- Entropy of combustion products = 12,58 kJ/K kg
- Temperature at nozzle throat = 2020,07 K
- Pressure at nozzle throat = 3,892322 MPa
- Mole number of gaseous products = 55,535 mol/kg expl.
- Total mole number of products = 55,535 mol/kg expl.
- Volume of gaseous products (at SATP) = 1376,66 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 18,006 g
- Mean molecular mass of all products = 18,006 g
- Density of products = 4,173 kg/m3
- Specific gas constant = 461,717 J/kg K
- Specific heat capacity at p=const. (Cp) = 2378,14 J/kgK
- Specific heat capacity at V=const. (Cv) = 1916,42 J/molK
- Specific heat ratio (Cp/Cv) = 1,2409

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1075,8 m/s
- Sound velocity at throat ) = 1075,8 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,556
- Pressure ratio (pc/pt) = 1,798

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2 = | 7,947536E-01 | 1,802102E+01 | 32,4499 | 3,6330 |
| H2O = | 7,295653E-01 | 1,654288E+01 | 29,7883 | 29,8025 |
| CO = | 5,739493E-01 | 1,301429E+01 | 23,4344 | 36,4530 |
| N2 = | 1,459907E-01 | 3,310336E+00 | 5,9608 | 9,2732 |
| CO2 = | 1,075756E-01 | 2,439275E+00 | 4,3923 | 10,7353 |
| BHO2 = | 8,436973E-02 | 1,913082E+00 | 3,4448 | 8,3789 |
| B(OH)3 = | 1,137913E-02 | 2,580216E-01 | 0,4646 | 1,5953 |
| B2O3 = | 5,831646E-04 | 1,322324E-02 | 0,0238 | 0,0920 |
| BHO = | 4,384892E-04 | 9,942732E-03 | 0,0179 | 0,0277 |
| H = | 4,367710E-04 | 9,903773E-03 | 0,0178 | 0,0010 |
| NH3 = | 1,004558E-04 | 2,277833E-03 | 0,0041 | 0,0039 |
| HCN = | 6,786682E-06 | 1,538879E-04 | 0,0003 | 0,0004 |
| CH2O = | 6,564483E-06 | 1,488495E-04 | 0,0003 | 0,0004 |
| BO2 = | 5,115260E-06 | 1,159884E-04 | 0,0002 | 0,0005 |

| | | | | |
|---|---|---|---|---|
| CH4 = | 4,677681E-06 | 1,060663E-04 | 0,0002 | 0,0002 |
| BO = | 3,364179E-06 | 7,628269E-05 | 0,0001 | 0,0002 |
| HCNO = | 8,002956E-07 | 1,814668E-05 | 0,0000 | 0,0001 |
| B2O2 = | 6,192357E-07 | 1,404116E-05 | 0,0000 | 0,0001 |
| NO = | 5,995184E-07 | 1,359407E-05 | 0,0000 | 0,0000 |
| NH2 = | 1,390619E-07 | 3,153225E-06 | 0,0000 | 0,0000 |
| CH3OH = | 7,945849E-09 | 1,801719E-07 | 0,0000 | 0,0000 |
| BH2 = | 1,782788E-09 | 4,042467E-08 | 0,0000 | 0,0000 |
| H2O2 = | 4,321941E-10 | 9,799991E-09 | 0,0000 | 0,0000 |
| C2H4 = | 1,336721E-10 | 3,031012E-09 | 0,0000 | 0,0000 |
| N = | 1,116554E-10 | 2,531783E-09 | 0,0000 | 0,0000 |
| CNO = | 1,009689E-10 | 2,289468E-09 | 0,0000 | 0,0000 |
| C2H6 = | 1,143063E-12 | 2,591893E-11 | 0,0000 | 0,0000 |
| NO2 = | 5,832193E-13 | 1,322449E-11 | 0,0000 | 0,0000 |
| BH = | 3,181781E-13 | 7,214682E-12 | 0,0000 | 0,0000 |
| BN = | 6,226029E-14 | 1,411751E-12 | 0,0000 | 0,0000 |
| B = | 4,077628E-14 | 9,246012E-13 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,615818E-16 | 3,663862E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 1,024871E-16 | 2,323893E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 9,638352E-18 | 2,185494E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,759862E-18 | 3,990483E-17 | 0,0000 | 0,0000 |
| BN(s) = | 4,066867E-19 | 9,221612E-18 | 0,0000 | 0,0000 |
| C(gr) = | 3,971433E-19 | 9,005216E-18 | 0,0000 | 0,0000 |
| B(s) = | 3,443910E-21 | 7,809057E-20 | 0,0000 | 0,0000 |
| B(l) = | 2,334382E-21 | 5,293205E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 5,124011E-23 | 1,161868E-21 | 0,0000 | 0,0000 |
| N2O3 = | 4,165673E-24 | 9,445654E-23 | 0,0000 | 0,0000 |
| B4C(s) = | 1,390931E-27 | 3,153933E-26 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,914310E-28 | 8,875688E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -6657,24 kJ/kg
- Entropy of combustion products = 12,58 kJ/K kg
- Temperature at nozzle exit = 1093,52 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 54,552 mol/kg expl.
- Total mole number of products = 55,536 mol/kg expl.
- Volume of gaseous products (at SATP) = 1352,29 L/kg expl.
- Mass of gaseous products = 931,5 g/kg expl.
- Mass of condensed products = 68,5 g/kg expl.
- Mean molecular mass of gaseous prod. = 17,076 g
- Mean molecular mass of all products = 18,006 g
- Density of products = 0,202 kg/m3
- Specific gas constant = 453,546 J/kg K
- Specific heat capacity at p=const. (Cp) = 2161,89 J/kgK
- Specific heat capacity at V=const. (Cv) = 1708,35 J/molK
- Specific heat ratio (Cp/Cv) = 1,2655

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 254,63 s
- Vacuum-specific impulse (pa=0) = 274,49 s
- Exhaust (or nozzle exit) velocity = 2497,1 m/s
- Characteristic exhaust velocity (c*) = 1559,3 m/s
- Thrust coefficient (Cf) = 1,601
- Nozzle area expansion ratio (Ae/At) = 8,92
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 784,51 m/s
- Mach number at nozzle exit = 3,183

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2 = | 9,449548E-01 | 2,142683E+01 | 38,5818 | 4,3196 |

| | | | | |
|---|---|---|---|---|
| H2O = | 6,226907E-01 | 1,411950E+01 | 25,4240 | 25,4367 |
| CO = | 4,227576E-01 | 9,586019E+00 | 17,2609 | 26,8504 |
| CO2 = | 2,583454E-01 | 5,857975E+00 | 10,5481 | 25,7809 |
| N2 = | 1,460163E-01 | 3,310915E+00 | 5,9617 | 9,2749 |
| B2O3(l) = | 4,339738E-02 | 9,840345E-01 | 1,7719 | 6,8498 |
| B(OH)3 = | 1,028159E-02 | 2,331348E-01 | 0,4198 | 1,4415 |
| CH4 = | 4,383497E-04 | 9,939569E-03 | 0,0179 | 0,0159 |
| BHO2 = | 2,826121E-04 | 6,408224E-03 | 0,0115 | 0,0281 |
| NH3 = | 5,733552E-05 | 1,300082E-03 | 0,0023 | 0,0022 |
| CH2O = | 2,776923E-07 | 6,296667E-06 | 0,0000 | 0,0000 |
| HCN = | 2,305969E-07 | 5,228780E-06 | 0,0000 | 0,0000 |
| H = | 3,538610E-08 | 8,023790E-07 | 0,0000 | 0,0000 |
| HCNO = | 1,070959E-08 | 2,428397E-07 | 0,0000 | 0,0000 |
| BHO = | 5,793712E-09 | 1,313723E-07 | 0,0000 | 0,0000 |
| CH3OH = | 1,026873E-09 | 2,328432E-08 | 0,0000 | 0,0000 |
| B2O3 = | 5,786061E-10 | 1,311988E-08 | 0,0000 | 0,0000 |
| C2H4 = | 4,817599E-10 | 1,092389E-08 | 0,0000 | 0,0000 |
| C2H6 = | 1,732028E-10 | 3,927370E-09 | 0,0000 | 0,0000 |
| NH2 = | 2,467677E-12 | 5,595453E-11 | 0,0000 | 0,0000 |
| NO = | 8,542937E-14 | 1,937109E-12 | 0,0000 | 0,0000 |
| BO2 = | 5,210989E-14 | 1,181591E-12 | 0,0000 | 0,0000 |
| BO = | 1,174377E-14 | 2,662897E-13 | 0,0000 | 0,0000 |
| B2O2 = | 1,183454E-15 | 2,683479E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 3,614130E-16 | 8,195031E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 1,719766E-16 | 3,899564E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 3,118844E-17 | 7,071972E-16 | 0,0000 | 0,0000 |
| CNO = | 1,130793E-17 | 2,564071E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 9,208593E-18 | 2,088046E-16 | 0,0000 | 0,0000 |
| H2O2 = | 3,767643E-18 | 8,543121E-17 | 0,0000 | 0,0000 |
| C(gr) = | 3,400206E-18 | 7,709959E-17 | 0,0000 | 0,0000 |
| BH2 = | 3,062772E-18 | 6,944829E-17 | 0,0000 | 0,0000 |
| BN(s) = | 5,035544E-19 | 1,141808E-17 | 0,0000 | 0,0000 |
| N = | 2,316205E-20 | 5,251989E-19 | 0,0000 | 0,0000 |
| N2O3 = | 4,029447E-21 | 9,136762E-20 | 0,0000 | 0,0000 |
| NO2 = | 4,082688E-24 | 9,257486E-23 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 6,360254E-25 | 1,442186E-23 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,283084E-25 | 9,711883E-24 | 0,0000 | 0,0000 |
| BH = | 1,520883E-26 | 3,448599E-25 | 0,0000 | 0,0000 |
| B(s) = | 6,284387E-27 | 1,424983E-25 | 0,0000 | 0,0000 |
| BN = | 4,685092E-28 | 1,062343E-26 | 0,0000 | 0,0000 |
| B(l) = | 8,601876E-30 | 1,950473E-28 | 0,0000 | 0,0000 |
| B = | 4,651945E-32 | 1,054827E-30 | 0,0000 | 0,0000 |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 19

**Combustion conditions (Number 19):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 28.57 %**
**2. Hydrogen peroxide ($H_2O_2$), 67.86 %**
**3. Water ($H_2O$, liquid), 3.57 %**

C(0,556) H(2,953) N(0,238) O(1,758) B(0,079)

Molecular weight = 41,97
Oxygen balance = -36,18345 %
Enthalpy of formation = -3896,19 kJ/kg
Internal energy of formation = -3706,46 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -4744,11 kJ/kg
- Total enthalpy of combustion prod. = -3895,62 kJ/kg
- Entropy of combustion products = 12,45 kJ/K kg
- Isobaric combustion temperature = 2533,69 K
- Mole number of gaseous products = 52,181 mol/kg expl.
- Total mole number of products = 52,181 mol/kg expl.
- Volume of gaseous products (at SATP) = 1293,52 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,164 g
- Mean molecular mass of all products = 19,164 g
- Density of products = 6,368 kg/m3
- Specific gas constant = 433,836 J/kg K
- Specific heat capacity at p=const. (Cp) = 2438,38 J/kgK
- Specific heat capacity at V=const. (Cv) = 2004,54 J/molK
- Specific heat ratio (Cp/Cv) = 1,2164

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 9,226746E-01 | 2,198193E+01 | 42,1260 | 39,6011 |
| H2 = | 5,099918E-01 | 1,215012E+01 | 23,2844 | 2,4495 |
| CO = | 4,365720E-01 | 1,040095E+01 | 19,9323 | 29,1331 |
| CO2 = | 1,192797E-01 | 2,841736E+00 | 5,4459 | 12,5065 |
| N2 = | 1,190621E-01 | 2,836552E+00 | 5,4360 | 7,9460 |
| BHO2 = | 7,424461E-02 | 1,768814E+00 | 3,3897 | 7,7471 |
| H = | 3,853485E-03 | 9,180597E-02 | 0,1759 | 0,0093 |
| B(OH)3 = | 2,837852E-03 | 6,760939E-02 | 0,1296 | 0,4180 |
| BHO = | 7,838540E-04 | 1,867465E-02 | 0,0358 | 0,0519 |
| B2O3 = | 6,775022E-04 | 1,614091E-02 | 0,0309 | 0,1124 |
| BO2 = | 1,283549E-04 | 3,057945E-03 | 0,0059 | 0,0131 |
| BO = | 5,515043E-05 | 1,313912E-03 | 0,0025 | 0,0035 |
| NH3 = | 4,878757E-05 | 1,162322E-03 | 0,0022 | 0,0020 |
| NO = | 4,816551E-05 | 1,147502E-03 | 0,0022 | 0,0034 |
| CH2O = | 5,785085E-06 | 1,378247E-04 | 0,0003 | 0,0004 |
| HCN = | 3,779587E-06 | 9,004541E-05 | 0,0002 | 0,0002 |
| B2O2 = | 1,702944E-06 | 4,057119E-05 | 0,0001 | 0,0002 |
| NH2 = | 1,050459E-06 | 2,502629E-05 | 0,0000 | 0,0000 |
| HCNO = | 1,039768E-06 | 2,477158E-05 | 0,0000 | 0,0001 |
| CH4 = | 2,008390E-07 | 4,784818E-06 | 0,0000 | 0,0000 |
| H2O2 = | 8,498509E-08 | 2,024697E-06 | 0,0000 | 0,0000 |
| N = | 2,346149E-08 | 5,589498E-07 | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| BH2 = | 1,098985E-08 | 2,618239E-07 | 0,0000 | 0,0000 |
| CH3OH = | 3,224389E-09 | 7,681830E-08 | 0,0000 | 0,0000 |
| CNO = | 2,892312E-09 | 6,890686E-08 | 0,0000 | 0,0000 |
| NO2 = | 9,489159E-10 | 2,260711E-08 | 0,0000 | 0,0000 |
| BH = | 3,108496E-11 | 7,405726E-10 | 0,0000 | 0,0000 |
| B = | 1,535784E-11 | 3,658873E-10 | 0,0000 | 0,0000 |
| BN = | 1,047700E-11 | 2,496056E-10 | 0,0000 | 0,0000 |
| C2H4 = | 4,244547E-12 | 1,011227E-10 | 0,0000 | 0,0000 |
| C2H6 = | 8,759646E-15 | 2,086911E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 4,053206E-17 | 9,656416E-16 | 0,0000 | 0,0000 |
| B4C(s) = | 3,432119E-17 | 8,176729E-16 | 0,0000 | 0,0000 |
| B2O3(l) = | 4,037992E-18 | 9,620169E-17 | 0,0000 | 0,0000 |
| N2O3 = | 7,636610E-19 | 1,819357E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 2,767736E-19 | 6,593893E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,348574E-19 | 5,595277E-18 | 0,0000 | 0,0000 |
| C(gr) = | 8,091108E-20 | 1,927637E-18 | 0,0000 | 0,0000 |
| BN(s) = | 2,542269E-20 | 6,056738E-19 | 0,0000 | 0,0000 |
| B(l) = | 4,204942E-21 | 1,001791E-19 | 0,0000 | 0,0000 |
| B(s) = | 3,385103E-21 | 8,064717E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,530143E-23 | 6,027850E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 6,471110E-28 | 1,541686E-26 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -4502,02 kJ/kg
- Entropy of combustion products = 12,45 kJ/K kg
- Temperature at nozzle throat = 2292,58 K
- Pressure at nozzle throat = 3,919854 MPa
- Mole number of gaseous products = 52,129 mol/kg expl.
- Total mole number of products = 52,129 mol/kg expl.
- Volume of gaseous products (at SATP) = 1292,24 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,183 g
- Mean molecular mass of all products = 19,183 g
- Density of products = 3,945 kg/m3
- Specific gas constant = 433,404 J/kg K
- Specific heat capacity at p=const. (Cp) = 2394,75 J/kgK
- Specific heat capacity at V=const. (Cv) = 1961,35 J/molK
- Specific heat ratio (Cp/Cv) = 1,221

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1101,3 m/s
- Sound velocity at throat ) = 1101,4 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,56
- Pressure ratio (pc/pt) = 1,786

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 9,125299E-01 | 2,174024E+01 | 41,7044 | 39,1657 |
| H2 = | 5,200098E-01 | 1,238879E+01 | 23,7655 | 2,4976 |
| CO = | 4,279495E-01 | 1,019553E+01 | 19,5581 | 28,5577 |
| CO2 = | 1,279075E-01 | 3,047287E+00 | 5,8456 | 13,4111 |
| N2 = | 1,190881E-01 | 2,837172E+00 | 5,4426 | 7,9478 |
| BHO2 = | 7,398658E-02 | 1,762667E+00 | 3,3813 | 7,7201 |
| B(OH)3 = | 3,867812E-03 | 9,214729E-02 | 0,1768 | 0,5697 |
| H = | 1,663928E-03 | 3,964166E-02 | 0,0760 | 0,0040 |
| B2O3 = | 5,213947E-04 | 1,242178E-02 | 0,0238 | 0,0865 |
| BHO = | 4,541895E-04 | 1,082068E-02 | 0,0208 | 0,0301 |
| BO2 = | 4,013251E-05 | 9,561226E-04 | 0,0018 | 0,0041 |
| NH3 = | 3,676261E-05 | 8,758376E-04 | 0,0017 | 0,0015 |
| BO = | 1,610156E-05 | 3,836058E-04 | 0,0007 | 0,0010 |
| NO = | 1,116070E-05 | 2,658941E-04 | 0,0005 | 0,0008 |

| | | | | |
|---|---|---|---|---|
| CH2O = | 3,373496E-06 | 8,037065E-05 | 0,0002 | 0,0002 |
| HCN = | 2,161230E-06 | 5,148946E-05 | 0,0001 | 0,0001 |
| B2O2 = | 7,161223E-07 | 1,706100E-05 | 0,0000 | 0,0001 |
| HCNO = | 5,372414E-07 | 1,279931E-05 | 0,0000 | 0,0001 |
| NH2 = | 3,201865E-07 | 7,628170E-06 | 0,0000 | 0,0000 |
| CH4 = | 2,017068E-07 | 4,805491E-06 | 0,0000 | 0,0000 |
| H2O2 = | 1,336341E-08 | 3,183717E-07 | 0,0000 | 0,0000 |
| N = 2,843403E-09 | 6,774164E-08 | 0,0000 | 0,0000 | |
| BH2 = | 2,369542E-09 | 5,645231E-08 | 0,0000 | 0,0000 |
| CH3OH = | 1,633382E-09 | 3,891394E-08 | 0,0000 | 0,0000 |
| CNO = | 5,218734E-10 | 1,243319E-08 | 0,0000 | 0,0000 |
| NO2 = | 8,118227E-11 | 1,934098E-09 | 0,0000 | 0,0000 |
| BH = 2,691400E-12 | 6,412030E-11 | 0,0000 | 0,0000 | |
| C2H4 = | 2,453089E-12 | 5,844273E-11 | 0,0000 | 0,0000 |
| B = 9,543954E-13 | 2,273765E-11 | 0,0000 | 0,0000 | |
| BN = 7,537892E-13 | 1,795838E-11 | 0,0000 | 0,0000 | |
| C2H6 = | 5,754710E-15 | 1,371010E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,085505E-16 | 2,586123E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,057210E-17 | 2,518713E-16 | 0,0000 | 0,0000 |
| B2O3(s) = | 6,388705E-19 | 1,522054E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,136154E-19 | 9,854031E-18 | 0,0000 | 0,0000 |
| C(gr) = | 7,931069E-20 | 1,889509E-18 | 0,0000 | 0,0000 |
| BN(s) = | 3,554316E-20 | 8,467853E-19 | 0,0000 | 0,0000 |
| N2O3 = | 9,809000E-21 | 2,336910E-19 | 0,0000 | 0,0000 |
| B(s) = | 1,825020E-21 | 4,347954E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,766577E-21 | 4,208718E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,839646E-23 | 4,382798E-22 | 0,0000 | 0,0000 |
| B4C(s) = | 8,145049E-27 | 1,940488E-25 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 4,129679E-28 | 9,838605E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7206,29 kJ/kg
- Entropy of combustion products = 12,45 kJ/K kg
- Temperature at nozzle exit = 1269,36 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 51,151 mol/kg expl.
- Total mole number of products = 51,893 mol/kg expl.
- Volume of gaseous products (at SATP) = 1267,99 L/kg expl.
- Mass of gaseous products = 948,4 g/kg expl.
- Mass of condensed products = 51,6 g/kg expl.
- Mean molecular mass of gaseous prod. = 18,541 g
- Mean molecular mass of all products = 19,271 g
- Density of products = 0,185 kg/m3
- Specific gas constant = 425,271 J/kg K
- Specific heat capacity at p=const. (Cp) = 2154,4 J/kgK
- Specific heat capacity at V=const. (Cv) = 1729,13 J/molK
- Specific heat ratio (Cp/Cv) = 1,2459

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 262,39 s
- Vacuum-specific impulse (pa=0) = 283,37 s
- Exhaust (or nozzle exit) velocity = 2573,2 m/s
- Characteristic exhaust velocity (c*) = 1611,2 m/s
- Thrust coefficient (Cf) = 1,597
- Nozzle area expansion ratio (Ae/At) = 9,11
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 811,85 m/s
- Mach number at nozzle exit = 3,17

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 8,243235E-01 | 1,963880E+01 | 37,8449 | 35,3799 |

| | | | | |
|---|---|---|---|---|
| H2 = 6,305817E-01 | 1,502307E+01 | 28,9502 | 3,0287 | |
| CO = 3,186738E-01 | 7,592131E+00 | 14,6304 | 21,2656 | |
| CO2 = 2,371854E-01 | 5,650739E+00 | 10,8892 | 24,8689 | |
| N2 = 1,191067E-01 | 2,837615E+00 | 5,4682 | 7,9490 | |
| B2O3(l) = 3,113335E-02 | 7,417253E-01 | 1,4293 | 5,1631 | |
| B(OH)3 = 1,294460E-02 | 3,083941E-01 | 0,5943 | 1,9068 | |
| BHO2 = 4,196021E-03 | 9,996661E-02 | 0,1926 | 0,4378 | |
| NH3 = 1,353507E-05 | 3,224614E-04 | 0,0006 | 0,0005 | |
| CH4 = 2,958126E-06 | 7,047482E-05 | 0,0001 | 0,0001 | |
| H = 8,191454E-07 | 1,951544E-05 | 0,0000 | 0,0000 | |
| BHO = 2,576360E-07 | 6,137957E-06 | 0,0000 | 0,0000 | |
| B2O3 = 2,071964E-07 | 4,936277E-06 | 0,0000 | 0,0000 | |
| CH2O = 1,292108E-07 | 3,078336E-06 | 0,0000 | 0,0000 | |
| HCN = 6,917995E-08 | 1,648153E-06 | 0,0000 | 0,0000 | |
| HCNO = 7,514618E-09 | 1,790293E-07 | 0,0000 | 0,0000 | |
| CH3OH = 8,805477E-11 | 2,097829E-09 | 0,0000 | 0,0000 | |
| BO2 = 6,874270E-11 | 1,637736E-09 | 0,0000 | 0,0000 | |
| NH2 = 2,628826E-11 | 6,262954E-10 | 0,0000 | 0,0000 | |
| NO = 2,596537E-11 | 6,186026E-10 | 0,0000 | 0,0000 | |
| BO = 1,246514E-11 | 2,969712E-10 | 0,0000 | 0,0000 | |
| B2O2 = 1,592183E-12 | 3,793238E-11 | 0,0000 | 0,0000 | |
| C2H4 = 1,231580E-12 | 2,934135E-11 | 0,0000 | 0,0000 | |
| C2H6 = 3,719764E-14 | 8,862019E-13 | 0,0000 | 0,0000 | |
| B4C(l) = 2,744002E-15 | 6,537349E-14 | 0,0000 | 0,0000 | |
| H2O2 = 2,252983E-15 | 5,367539E-14 | 0,0000 | 0,0000 | |
| B4C(s) = 6,343694E-16 | 1,511331E-14 | 0,0000 | 0,0000 | |
| BH2 = 5,874422E-16 | 1,399531E-14 | 0,0000 | 0,0000 | |
| CNO = 5,246610E-16 | 1,249960E-14 | 0,0000 | 0,0000 | |
| B2O3(s) = 2,084436E-16 | 4,965990E-15 | 0,0000 | 0,0000 | |
| N = 2,834685E-17 | 6,753395E-16 | 0,0000 | 0,0000 | |
| BHO2(s) = 5,014031E-18 | 1,194550E-16 | 0,0000 | 0,0000 | |
| C(gr) = 2,505356E-19 | 5,968796E-18 | 0,0000 | 0,0000 | |
| BN(s) = 1,548014E-19 | 3,688010E-18 | 0,0000 | 0,0000 | |
| NO2 = 4,374493E-20 | 1,042185E-18 | 0,0000 | 0,0000 | |
| N2O3 = 3,208890E-22 | 7,644904E-21 | 0,0000 | 0,0000 | |
| BH = 1,454331E-22 | 3,464820E-21 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 8,026241E-23 | 1,912183E-21 | 0,0000 | 0,0000 | |
| B = 3,811263E-23 | 9,080007E-22 | 0,0000 | 0,0000 | |
| B(l) = 2,532197E-23 | 6,032743E-22 | 0,0000 | 0,0000 | |
| BN = 2,819752E-24 | 6,717817E-23 | 0,0000 | 0,0000 | |
| B(s) = 1,073374E-24 | 2,557220E-23 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 1,440855E-31 | 3,432712E-30 | 0,0000 | 0,0000 | |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2H4; N2O; O; O2; O3; OH;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 20

**Combustion conditions (Number 20):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 25 .00 %**
**2. Hydrogen peroxide ($H_2O_2$), 71.25 %**
**3. Water ($H_2O$, liquid), 3.75 %**

C(0,469) H(2,805) N(0,201) O(1,782) B(0,067)

Molecular weight = 40,51
Oxygen balance = -26,07909 %
Enthalpy of formation = -4163,42 kJ/kg
Internal energy of formation = -3974,06 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5183,4 kJ/kg
- Total enthalpy of combustion prod. = -4164,12 kJ/kg
- Entropy of combustion products = 12,3 kJ/K kg
- Isobaric combustion temperature = 2749,02 K
- Mole number of gaseous products = 49,573 mol/kg expl.
- Total mole number of products = 49,573 mol/kg expl.
- Volume of gaseous products (at SATP) = 1228,86 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,172 g
- Mean molecular mass of all products = 20,172 g
- Density of products = 6,178 kg/m3
- Specific gas constant = 412,148 J/kg K
- Specific heat capacity at p=const. (Cp) = 2445,58 J/kgK
- Specific heat capacity at V=const. (Cv) = 2033,44 J/molK
- Specific heat ratio (Cp/Cv) = 1,2027

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,034947E+00 | 2,554694E+01 | | 51,5342 | 46,0236 |
| H2 = | 3,296536E-01 | 8,137272E+00 | 16,4148 | 1,6405 | |
| CO = | 3,269986E-01 | 8,071735E+00 | 16,2826 | 22,6089 | |
| CO2 = | 1,424510E-01 | 3,516305E+00 | | 7,0932 | 15,4753 |
| N2 = | 1,004526E-01 | 2,479603E+00 | 5,0019 | 6,9461 | |
| BHO2 = | 6,339435E-02 | 1,564846E+00 | | 3,1567 | 6,8537 |
| H = | 6,949128E-03 | 1,715344E-01 | 0,3460 | 0,0173 | |
| B(OH)3 = | 1,519044E-03 | 3,749656E-02 | | 0,0756 | 0,2318 |
| BHO = | 5,904800E-04 | 1,457559E-02 | | 0,0294 | 0,0405 |
| B2O3 = | 5,375902E-04 | 1,327004E-02 | | 0,0268 | 0,0924 |
| BO2 = | 3,815136E-04 | 9,417400E-03 | | 0,0190 | 0,0403 |
| NO = | 2,654390E-04 | 6,552178E-03 | | 0,0132 | 0,0197 |
| BO = | 1,011251E-04 | 2,496204E-03 | 0,0050 | 0,0067 | |
| NH3 = | 2,091893E-05 | 5,163694E-04 | | 0,0010 | 0,0009 |
| CH2O = | 2,981051E-06 | 7,358519E-05 | | 0,0001 | 0,0002 |
| HCN = | 1,320686E-06 | 3,260021E-05 | | 0,0001 | 0,0001 |
| NH2 = | 1,293211E-06 | 3,192202E-05 | | 0,0001 | 0,0001 |
| B2O2 = | 1,246993E-06 | 3,078116E-05 | | 0,0001 | 0,0002 |
| HCNO = | 6,652504E-07 | 1,642125E-05 | | 0,0000 | 0,0001 |

| | | | | |
|---|---|---|---|---|
| H2O2 = | 6,375493E-07 | 1,573746E-05 | 0,0000 | 0,0001 |
| N = | 1,236620E-07 | 3,052512E-06 | 0,0000 | 0,0000 |
| CH4 = | 1,895683E-08 | 4,679363E-07 | 0,0000 | 0,0000 |
| NO2 = | 1,868932E-08 | 4,613329E-07 | 0,0000 | 0,0000 |
| BH2 = | 6,948636E-09 | 1,715223E-07 | 0,0000 | 0,0000 |
| CNO = | 5,945107E-09 | 1,467509E-07 | 0,0000 | 0,0000 |
| CH3OH = | 8,651930E-10 | 2,135669E-08 | 0,0000 | 0,0000 |
| BH = | 5,670636E-11 | 1,399757E-09 | 0,0000 | 0,0000 |
| B = | 5,265615E-11 | 1,299781E-09 | 0,0000 | 0,0000 |
| BN = | 2,489751E-11 | 6,145778E-10 | 0,0000 | 0,0000 |
| N2H4 = | 5,102505E-13 | 1,259518E-11 | 0,0000 | 0,0000 |
| C2H4 = | 1,873786E-13 | 4,625311E-12 | 0,0000 | 0,0000 |
| C2H6 = | 1,644780E-16 | 4,060025E-15 | 0,0000 | 0,0000 |
| N2O3 = | 8,154896E-17 | 2,012980E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 2,606929E-17 | 6,435024E-16 | 0,0000 | 0,0000 |
| B4C(l) = | 2,567626E-17 | 6,338006E-16 | 0,0000 | 0,0000 |
| B2O3(l) = | 9,327204E-19 | 2,302356E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,260245E-19 | 3,110827E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 5,432162E-20 | 1,340892E-18 | 0,0000 | 0,0000 |
| C(gr) = | 2,545512E-20 | 6,283420E-19 | 0,0000 | 0,0000 |
| BN(s) = | 4,740421E-21 | 1,170140E-19 | 0,0000 | 0,0000 |
| B(l) = | 2,482492E-21 | 6,127860E-20 | 0,0000 | 0,0000 |
| B(s) = | 1,663727E-21 | 4,106796E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,642528E-23 | 4,054466E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 6,884676E-29 | 1,699435E-27 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -4785,96 kJ/kg
- Entropy of combustion products = 12,3 kJ/K kg
- Temperature at nozzle throat = 2504,71 K
- Pressure at nozzle throat = 3,93874 MPa
- Mole number of gaseous products = 49,517 mol/kg expl.
- Total mole number of products = 49,517 mol/kg expl.
- Volume of gaseous products (at SATP) = 1227,48 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,195 g
- Mean molecular mass of all products = 20,195 g
- Density of products = 3,82 kg/m3
- Specific gas constant = 411,685 J/kg K
- Specific heat capacity at p=const. (Cp) = 2406,42 J/kgK
- Specific heat capacity at V=const. (Cv) = 1994,73 J/molK
- Specific heat ratio (Cp/Cv) = 1,2064

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1115,2 m/s
- Sound velocity at throat ) = 1115,3 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,563
- Pressure ratio (pc/pt) = 1,777

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,027823E+00 | 2,537109E+01 | 51,2371 | 45,7068 |
| H2 = | 3,379309E-01 | 8,341591E+00 | 16,8459 | 1,6817 |
| CO = | 3,203882E-01 | 7,908562E+00 | 15,9714 | 22,1519 |
| CO2 = | 1,490641E-01 | 3,679543E+00 | 7,4309 | 16,1937 |
| N2 = | 1,005498E-01 | 2,482003E+00 | 5,0124 | 6,9528 |
| BHO2 = | 6,378875E-02 | 1,574581E+00 | 3,1799 | 6,8964 |
| H = | 3,530530E-03 | 8,714869E-02 | 0,1760 | 0,0088 |
| B(OH)3 = | 1,842016E-03 | 4,546889E-02 | 0,0918 | 0,2811 |
| B2O3 = | 4,359952E-04 | 1,076224E-02 | 0,0217 | 0,0749 |

| | | | | |
|---|---|---|---|---|
| BHO = | 3,761759E-04 | 9,285643E-03 | 0,0188 | 0,0258 |
| BO2 = | 1,475546E-04 | 3,642283E-03 | 0,0074 | 0,0156 |
| NO = | 7,856750E-05 | 1,939384E-03 | 0,0039 | 0,0058 |
| BO = | 3,731975E-05 | 9,212123E-04 | 0,0019 | 0,0025 |
| NH3 = | 1,529398E-05 | 3,775212E-04 | 0,0008 | 0,0006 |
| CH2O = | 1,735258E-06 | 4,283363E-05 | 0,0001 | 0,0001 |
| HCN = | 7,579807E-07 | 1,871023E-05 | 0,0000 | 0,0001 |
| B2O2 = | 6,079972E-07 | 1,500799E-05 | 0,0000 | 0,0001 |
| NH2 = | 4,532044E-07 | 1,118704E-05 | 0,0000 | 0,0000 |
| HCNO = | 3,478048E-07 | 8,585321E-06 | 0,0000 | 0,0000 |
| H2O2 = | 1,304525E-07 | 3,220130E-06 | 0,0000 | 0,0000 |
| N = | 2,112759E-08 | 5,215200E-07 | 0,0000 | 0,0000 |
| CH4 = | 1,640946E-08 | 4,050563E-07 | 0,0000 | 0,0000 |
| NO2 = | 2,339689E-09 | 5,775360E-08 | 0,0000 | 0,0000 |
| BH2 = | 1,845485E-09 | 4,555453E-08 | 0,0000 | 0,0000 |
| CNO = | 1,309949E-09 | 3,233519E-08 | 0,0000 | 0,0000 |
| CH3OH = | 4,119976E-10 | 1,016988E-08 | 0,0000 | 0,0000 |
| BH = | 7,178726E-12 | 1,772019E-10 | 0,0000 | 0,0000 |
| B = | 5,197408E-12 | 1,282944E-10 | 0,0000 | 0,0000 |
| BN = | 2,679267E-12 | 6,613586E-11 | 0,0000 | 0,0000 |
| N2H4 = | 1,082142E-13 | 2,671192E-12 | 0,0000 | 0,0000 |
| C2H4 = | 9,313630E-14 | 2,299005E-12 | 0,0000 | 0,0000 |
| B4C(l) = | 2,926564E-16 | 7,224021E-15 | 0,0000 | 0,0000 |
| C2H6 = | 8,434792E-17 | 2,082070E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,937643E-18 | 4,782937E-17 | 0,0000 | 0,0000 |
| N2O3 = | 1,916589E-18 | 4,730968E-17 | 0,0000 | 0,0000 |
| B4C(s) = | 1,737187E-18 | 4,288127E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,625301E-19 | 4,011942E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,132426E-19 | 2,795315E-18 | 0,0000 | 0,0000 |
| C(gr) = | 2,303521E-20 | 5,686083E-19 | 0,0000 | 0,0000 |
| BN(s) = | 5,894029E-21 | 1,454900E-19 | 0,0000 | 0,0000 |
| B(l) = | 1,148548E-21 | 2,835111E-20 | 0,0000 | 0,0000 |
| B(s) = | 9,501687E-22 | 2,345426E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 9,533839E-24 | 2,353362E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,721519E-29 | 6,717881E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7607,19 kJ/kg
- Entropy of combustion products = 12,3 kJ/K kg
- Temperature at nozzle exit = 1392,66 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 48,732 mol/kg expl.
- Total mole number of products = 49,162 mol/kg expl.
- Volume of gaseous products (at SATP) = 1208,01 L/kg expl.
- Mass of gaseous products = 970,0 g/kg expl.
- Mass of condensed products = 30,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 19,905 g
- Mean molecular mass of all products = 20,341 g
- Density of products = 0,177 kg/m3
- Specific gas constant = 405,155 J/kg K
- Specific heat capacity at p=const. (Cp) = 2145,78 J/kgK
- Specific heat capacity at V=const. (Cv) = 1740,63 J/molK
- Specific heat ratio (Cp/Cv) = 1,2328

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 267,59 s
- Vacuum-specific impulse (pa=0) = 289,09 s
- Exhaust (or nozzle exit) velocity = 2624,1 m/s
- Characteristic exhaust velocity (c*) = 1643,3 m/s
- Thrust coefficient (Cf) = 1,597
- Nozzle area expansion ratio (Ae/At) = 9,16
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 825,04 m/s
- Mach number at nozzle exit = 3,181

Composition of combustion products at the nozzle exit:

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 9,482996E-01 | 2,340812E+01 | 47,6138 | 42,1704 |
| H2 = | 4,236847E-01 | 1,045836E+01 | 21,2731 | 2,1084 |
| CO = | 2,366603E-01 | 5,841796E+00 | 11,8826 | 16,3629 |
| CO2 = | 2,327945E-01 | 5,746372E+00 | 11,6885 | 25,2898 |
| N2 = | 1,005952E-01 | 2,483123E+00 | 5,0508 | 6,9560 |
| BHO2 = | 1,782418E-02 | 4,399775E-01 | 0,8949 | 1,9270 |
| B2O3(l) = | 1,745388E-02 | 4,308370E-01 | 0,8764 | 2,9990 |
| B(OH)3 = | 1,432131E-02 | 3,535117E-01 | 0,7191 | 2,1858 |
| B2O3 = | 4,979969E-06 | 1,229271E-04 | 0,0003 | 0,0009 |
| NH3 = | 4,652000E-06 | 1,148314E-04 | 0,0002 | 0,0002 |
| H = | 4,215357E-06 | 1,040532E-04 | 0,0002 | 0,0000 |
| BHO = | 1,699245E-06 | 4,194468E-05 | 0,0001 | 0,0001 |
| CH4 = | 1,017610E-07 | 2,511901E-06 | 0,0000 | 0,0000 |
| CH2O = | 6,307869E-08 | 1,557054E-06 | 0,0000 | 0,0000 |
| HCN = | 2,392473E-08 | 5,905653E-07 | 0,0000 | 0,0000 |
| HCNO = | 4,899884E-09 | 1,209502E-07 | 0,0000 | 0,0000 |
| BO2 = | 3,755835E-09 | 9,271018E-08 | 0,0000 | 0,0000 |
| NO = | 6,874030E-10 | 1,696807E-08 | 0,0000 | 0,0000 |
| BO = | 5,074728E-10 | 1,252661E-08 | 0,0000 | 0,0000 |
| NH2 = | 7,944709E-11 | 1,961097E-09 | 0,0000 | 0,0000 |
| B2O2 = | 6,709606E-11 | 1,656220E-09 | 0,0000 | 0,0000 |
| CH3OH = | 1,455185E-11 | 3,592023E-10 | 0,0000 | 0,0000 |
| H2O2 = | 8,896863E-14 | 2,196129E-12 | 0,0000 | 0,0000 |
| C2H4 = | 1,875414E-14 | 4,629330E-13 | 0,0000 | 0,0000 |
| BH2 = | 6,797469E-15 | 1,677908E-13 | 0,0000 | 0,0000 |
| CNO = | 3,725974E-15 | 9,197309E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 1,580391E-15 | 3,901085E-14 | 0,0000 | 0,0000 |
| N = | 1,373190E-15 | 3,389624E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 3,461502E-16 | 8,544477E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,571833E-16 | 3,879960E-15 | 0,0000 | 0,0000 |
| C2H6 = | 1,242530E-16 | 3,067099E-15 | 0,0000 | 0,0000 |
| NO2 = | 9,725613E-18 | 2,400700E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 3,628735E-18 | 8,957281E-17 | 0,0000 | 0,0000 |
| N2H4 = | 3,002902E-18 | 7,412455E-17 | 0,0000 | 0,0000 |
| BN(s) = | 6,120072E-20 | 1,510698E-18 | 0,0000 | 0,0000 |
| C(gr) = | 4,513733E-20 | 1,114184E-18 | 0,0000 | 0,0000 |
| BH = | 1,420235E-20 | 3,505751E-19 | 0,0000 | 0,0000 |
| BN = | 1,236514E-21 | 3,052248E-20 | 0,0000 | 0,0000 |
| B = | 5,465749E-22 | 1,349182E-20 | 0,0000 | 0,0000 |
| N2O3 = | 1,522892E-22 | 3,759154E-21 | 0,0000 | 0,0000 |
| B(l) = | 5,047147E-23 | 1,245853E-21 | 0,0000 | 0,0000 |
| B(s) = | 4,588016E-24 | 1,132520E-22 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,401317E-24 | 5,927486E-23 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,520430E-31 | 6,221506E-30 | 0,0000 | 0,0000 |

Excluded products (11):

C; C(d); C(Liq.1); C(Liq.2); CH2O2; H2O(l);
N2O; O; O2; O3; OH;

NOTES: Running parameters

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 21

**Combustion conditions (Number 21):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 24.39 %**
**2. Hydrogen peroxide ($H_2O_2$), 71.83 %**
**3. Water ($H_2O$, liquid), 3.78 %**

C(0,455) H(2,781) N(0,195) O(1,785) B(0,065)

Molecular weight = 40,27
Oxygen balance = -24,35222 %
Enthalpy of formation = -4209,01 kJ/kg
Internal energy of formation = -4019,70 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5215,34 kJ/kg
- Total enthalpy of combustion prod. = -4209,09 kJ/kg
- Entropy of combustion products = 12,28 kJ/K kg
- Isobaric combustion temperature = 2768,16 K
- Mole number of gaseous products = 49,202 mol/kg expl.
- Total mole number of products = 49,202 mol/kg expl.
- Volume of gaseous products (at SATP) = 1219,67 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,324 g
- Mean molecular mass of all products = 20,324 g
- Density of products = 6,182 kg/m3
- Specific gas constant = 409,065 J/kg K
- Specific heat capacity at p=const. (Cp) = 2443,77 J/kgK
- Specific heat capacity at V=const. (Cv) = 2034,7 J/molK
- Specific heat ratio (Cp/Cv) = 1,201

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,046370E+00 | 2,598251E+01 | | 52,8079 | 46,8083 |
| CO = | 3,087923E-01 | 7,667648E+00 | 15,5840 | 21,4771 | |
| H2 = | 3,040102E-01 | 7,548903E+00 | 15,3427 | 1,5219 | |
| CO2 = | 1,464960E-01 | 3,637656E+00 | | 7,3933 | 16,0093 |
| N2 = | 9,739412E-02 | 2,418402E+00 | 4,9153 | 6,7747 | |
| BHO2 = | 6,152885E-02 | 1,527828E+00 | | 3,1052 | 6,6916 |
| H = | 7,104717E-03 | 1,764178E-01 | 0,3586 | 0,0178 | |
| OH = | 6,193844E-03 | 1,537999E-01 | | 0,3126 | 0,2616 |
| B(OH)3 = | 1,431080E-03 | 3,553527E-02 | | 0,0722 | 0,2197 |
| BHO = | 5,411647E-04 | 1,343771E-02 | | 0,0273 | 0,0374 |
| B2O3 = | 5,091104E-04 | 1,264176E-02 | | 0,0257 | 0,0880 |
| BO2 = | 4,179350E-04 | 1,037778E-02 | | 0,0211 | 0,0444 |
| NO = | 3,159773E-04 | 7,846061E-03 | | 0,0159 | 0,0235 |
| O2 = | 1,461772E-04 | 3,629740E-03 | 0,0074 | 0,0116 | |
| BO = | 1,015841E-04 | 2,522444E-03 | 0,0051 | 0,0068 | |
| O = | 8,632237E-05 | 2,143478E-03 | 0,0044 | 0,0034 | |
| NH3 = | 1,820273E-05 | 4,519936E-04 | | 0,0009 | 0,0008 |
| CH2O = | 2,626603E-06 | 6,522140E-05 | | 0,0001 | 0,0002 |
| NH2 = | 1,250185E-06 | 3,104345E-05 | | 0,0001 | 0,0000 |
| B2O2 = | 1,119175E-06 | 2,779033E-05 | | 0,0001 | 0,0001 |
| HCN = | 1,090939E-06 | 2,708920E-05 | | 0,0001 | 0,0001 |
| H2O2 = | 7,886959E-07 | 1,958418E-05 | | 0,0000 | 0,0001 |

| | | | | |
|---|---|---|---|---|
| HCNO = | 6,051033E-07 | 1,502537E-05 | 0,0000 | 0,0001 |
| N = | 1,399308E-07 | 3,474633E-06 | 0,0000 | 0,0000 |
| NO2 = | 2,587308E-08 | 6,424566E-07 | 0,0000 | 0,0000 |
| CH4 = | 1,334860E-08 | 3,314602E-07 | 0,0000 | 0,0000 |
| CNO = | 6,063538E-09 | 1,505642E-07 | 0,0000 | 0,0000 |
| BH2 = | 5,873347E-09 | 1,458416E-07 | 0,0000 | 0,0000 |
| BH = | 5,326996E-11 | 1,322751E-09 | 0,0000 | 0,0000 |
| B = | 5,310035E-11 | 1,318540E-09 | 0,0000 | 0,0000 |
| BN = | 2,423945E-11 | 6,018920E-10 | 0,0000 | 0,0000 |
| N2H4 = | 4,466270E-13 | 1,109023E-11 | 0,0000 | 0,0000 |
| B4C(s) = | 3,180192E-16 | 7,896762E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 3,093327E-16 | 7,681068E-15 | 0,0000 | 0,0000 |
| N2O3 = | 1,350810E-16 | 3,354209E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 8,048118E-19 | 1,998435E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,170516E-19 | 2,906520E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 4,694625E-20 | 1,165726E-18 | 0,0000 | 0,0000 |
| C(gr) = | 2,151155E-20 | 5,341552E-19 | 0,0000 | 0,0000 |
| BN(s) = | 3,775125E-21 | 9,374045E-20 | 0,0000 | 0,0000 |
| B(l) = | 2,183187E-21 | 5,421092E-20 | 0,0000 | 0,0000 |
| B(s) = | 1,443770E-21 | 3,585038E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,858786E-24 | 1,206489E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,818416E-30 | 1,941398E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -4832,1 kJ/kg
- Entropy of combustion products = 12,28 kJ/K kg
- Temperature at nozzle throat = 2534,65 K
- Pressure at nozzle throat = 3,938458 MPa
- Mole number of gaseous products = 49,1 mol/kg expl.
- Total mole number of products = 49,1 mol/kg expl.
- Volume of gaseous products (at SATP) = 1217,14 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,366 g
- Mean molecular mass of all products = 20,366 g
- Density of products = 3,806 kg/m3
- Specific gas constant = 408,216 J/kg K
- Specific heat capacity at p=const. (Cp) = 2407,02 J/kgK
- Specific heat capacity at V=const. (Cv) = 1998,8 J/molK
- Specific heat ratio (Cp/Cv) = 1,2042

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1116,3 m/s
- Sound velocity at throat ) = 1116,2 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,563
- Pressure ratio (pc/pt) = 1,777

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,043142E+00 | 2,590234E+01 | 52,7545 | 46,6638 |
| H2 = | 3,102361E-01 | 7,703499E+00 | 15,6895 | 1,5530 |
| CO = | 3,019981E-01 | 7,498941E+00 | 15,2729 | 21,0045 |
| CO2 = | 1,532926E-01 | 3,806421E+00 | 7,7524 | 16,7521 |
| N2 = | 9,750400E-02 | 2,421130E+00 | 4,9310 | 6,7823 |
| BHO2 = | 6,197273E-02 | 1,538850E+00 | 3,1341 | 6,7399 |
| H = | 3,820074E-03 | 9,485658E-02 | 0,1932 | 0,0096 |
| OH = | 2,563927E-03 | 6,366509E-02 | 0,1297 | 0,1083 |
| B(OH)3 = | 1,664461E-03 | 4,133039E-02 | 0,0842 | 0,2555 |
| B2O3 = | 4,178788E-04 | 1,037639E-02 | 0,0211 | 0,0722 |
| BHO = | 3,526390E-04 | 8,756411E-03 | 0,0178 | 0,0244 |
| BO2 = | 1,747465E-04 | 4,339145E-03 | 0,0088 | 0,0186 |

| | | | | |
|---|---|---|---|---|
| NO = | 1,031403E-04 | 2,561086E-03 | 0,0052 | 0,0077 |
| BO = | 4,041137E-05 | 1,003458E-03 | 0,0020 | 0,0027 |
| O2 = | 3,269635E-05 | 8,118860E-04 | 0,0017 | 0,0026 |
| O = | 1,946885E-05 | 4,834327E-04 | 0,0010 | 0,0008 |
| NH3 = | 1,304461E-05 | 3,239118E-04 | 0,0007 | 0,0006 |
| CH2O = | 1,516991E-06 | 3,766853E-05 | 0,0001 | 0,0001 |
| HCN = | 6,188286E-07 | 1,536619E-05 | 0,0000 | 0,0000 |
| B2O2 = | 5,661860E-07 | 1,405901E-05 | 0,0000 | 0,0001 |
| NH2 = | 4,577649E-07 | 1,136680E-05 | 0,0000 | 0,0000 |
| HCNO = | 3,164548E-07 | 7,857918E-06 | 0,0000 | 0,0000 |
| H2O2 = | 1,795304E-07 | 4,457935E-06 | 0,0000 | 0,0000 |
| N = | 2,708716E-08 | 6,726037E-07 | 0,0000 | 0,0000 |
| CH4 = | 1,070882E-08 | 2,659118E-07 | 0,0000 | 0,0000 |
| NO2 = | 3,787324E-09 | 9,404337E-08 | 0,0000 | 0,0000 |
| BH2 = | 1,641600E-09 | 4,076272E-08 | 0,0000 | 0,0000 |
| CNO = | 1,435374E-09 | 3,564190E-08 | 0,0000 | 0,0000 |
| BH = | 7,567953E-12 | 1,879205E-10 | 0,0000 | 0,0000 |
| B = | 6,083590E-12 | 1,510622E-10 | 0,0000 | 0,0000 |
| BN = | 2,961086E-12 | 7,352699E-11 | 0,0000 | 0,0000 |
| N2H4 = | 9,653233E-14 | 2,397003E-12 | 0,0000 | 0,0000 |
| B4C(l) = | 1,859401E-15 | 4,617094E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 8,828585E-17 | 2,192234E-15 | 0,0000 | 0,0000 |
| N2O3 = | 4,065873E-18 | 1,009600E-16 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,539887E-18 | 3,823707E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,435302E-19 | 3,564011E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 8,977322E-20 | 2,229167E-18 | 0,0000 | 0,0000 |
| C(gr) = | 1,873593E-20 | 4,652335E-19 | 0,0000 | 0,0000 |
| BN(s) = | 4,431963E-21 | 1,100505E-19 | 0,0000 | 0,0000 |
| B(l) = | 1,030373E-21 | 2,558529E-20 | 0,0000 | 0,0000 |
| B(s) = | 8,288762E-22 | 2,058190E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 8,563327E-24 | 2,126367E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 8,168819E-26 | 2,028406E-24 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7672,78 kJ/kg
- Entropy of combustion products = 12,28 kJ/K kg
- Temperature at nozzle exit = 1412,25 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 48,341 mol/kg expl.
- Total mole number of products = 48,696 mol/kg expl.
- Volume of gaseous products (at SATP) = 1198,32 L/kg expl.
- Mass of gaseous products = 975,2 g/kg expl.
- Mass of condensed products = 24,8 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,174 g
- Mean molecular mass of all products = 20,535 g
- Density of products = 0,176 kg/m3
- Specific gas constant = 401,905 J/kg K
- Specific heat capacity at p=const. (Cp) = 2143,42 J/kgK
- Specific heat capacity at V=const. (Cv) = 1741,52 J/molK
- Specific heat ratio (Cp/Cv) = 1,2308

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 268,39 s
- Vacuum-specific impulse (pa=0) = 289,95 s
- Exhaust (or nozzle exit) velocity = 2632,0 m/s
- Characteristic exhaust velocity (c*) = 1647,5 m/s
- Thrust coefficient (Cf) = 1,598
- Nozzle area expansion ratio (Ae/At) = 9,16
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 826,75 m/s
- Mach number at nozzle exit = 3,184

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 9,668029E-01 | 2,400677E+01 | 49,2989 | 43,2489 |
| H2 = | 3,907309E-01 | 9,702274E+00 | 19,9240 | 1,9560 |
| CO2 = | 2,330499E-01 | 5,786883E+00 | 11,8836 | 25,4681 |
| CO = | 2,222428E-01 | 5,518532E+00 | 11,3325 | 15,4574 |
| N2 = | 9,756086E-02 | 2,422542E+00 | 4,9748 | 6,7863 |
| BHO2 = | 2,185737E-02 | 5,427422E-01 | 1,1145 | 2,3771 |
| B(OH)3 = | 1,451708E-02 | 3,604749E-01 | 0,7402 | 2,2288 |
| B2O3(l) = | 1,432472E-02 | 3,556984E-01 | 0,7304 | 2,4760 |
| B2O3 = | 7,809484E-06 | 1,939180E-04 | 0,0004 | 0,0013 |
| H = | 5,259755E-06 | 1,306054E-04 | 0,0003 | 0,0000 |
| NH3 = | 3,846185E-06 | 9,550496E-05 | 0,0002 | 0,0002 |
| BHO = | 2,166938E-06 | 5,380742E-05 | 0,0001 | 0,0001 |
| OH = | 2,518221E-07 | 6,253016E-06 | 0,0000 | 0,0000 |
| CH4 = | 5,755512E-08 | 1,429156E-06 | 0,0000 | 0,0000 |
| CH2O = | 5,457154E-08 | 1,355071E-06 | 0,0000 | 0,0000 |
| HCN = | 1,941456E-08 | 4,820845E-07 | 0,0000 | 0,0000 |
| BO2 = | 6,710350E-09 | 1,666253E-07 | 0,0000 | 0,0000 |
| HCNO = | 4,458235E-09 | 1,107028E-07 | 0,0000 | 0,0000 |
| NO = | 1,119420E-09 | 2,779642E-08 | 0,0000 | 0,0000 |
| BO = | 8,484216E-10 | 2,106723E-08 | 0,0000 | 0,0000 |
| B2O2 = | 1,113117E-10 | 2,763992E-09 | 0,0000 | 0,0000 |
| NH2 = | 9,059742E-11 | 2,249632E-09 | 0,0000 | 0,0000 |
| O2 = | 4,001222E-12 | 9,935468E-11 | 0,0000 | 0,0000 |
| O = | 2,843361E-12 | 7,060373E-11 | 0,0000 | 0,0000 |
| H2O2 = | 1,539704E-13 | 3,823252E-12 | 0,0000 | 0,0000 |
| BH2 = | 9,071048E-15 | 2,252440E-13 | 0,0000 | 0,0000 |
| CNO = | 4,822278E-15 | 1,197424E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 2,467036E-15 | 6,125919E-14 | 0,0000 | 0,0000 |
| N = | 2,380898E-15 | 5,912028E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 6,292140E-16 | 1,562407E-14 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,510144E-16 | 3,749852E-15 | 0,0000 | 0,0000 |
| NO2 = | 2,198229E-17 | 5,458441E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 3,469654E-18 | 8,615528E-17 | 0,0000 | 0,0000 |
| N2H4 = | 2,835572E-18 | 7,041034E-17 | 0,0000 | 0,0000 |
| BN(s) = | 5,157150E-20 | 1,280576E-18 | 0,0000 | 0,0000 |
| C(gr) = | 3,401767E-20 | 8,446957E-19 | 0,0000 | 0,0000 |
| BH = | 2,621023E-20 | 6,508286E-19 | 0,0000 | 0,0000 |
| BN = | 2,440100E-21 | 6,059034E-20 | 0,0000 | 0,0000 |
| B = | 1,177703E-21 | 2,924364E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,434894E-22 | 3,562999E-21 | 0,0000 | 0,0000 |
| B(s) = | 9,044111E-23 | 2,245751E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 5,603640E-24 | 1,391445E-22 | 0,0000 | 0,0000 |
| N2O3 = | 2,485979E-24 | 6,172957E-23 | 0,0000 | 0,0000 |
| B(l) = | 9,365502E-25 | 2,325556E-23 | 0,0000 | 0,0000 |

Excluded products (11):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 22

**Combustion conditions (Number 22):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 22.22 %**
**2. Hydrogen peroxide ($H_2O_2$), 73.89 %**
**3. Water ($H_2O$, liquid), 3.89 %**

C(0,406) H(2,696) N(0,174) O(1,799) B(0,058)

Molecular weight = 39,44
Oxygen balance = -18,21063 %
Enthalpy of formation = -4371,51 kJ/kg
Internal energy of formation = -4182,42 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5434,75 kJ/kg
- Total enthalpy of combustion prod. = -4372,18 kJ/kg
- Entropy of combustion products = 12,16 kJ/K kg
- Isobaric combustion temperature = 2878,91 K
- Mole number of gaseous products = 47,707 mol/kg expl.
- Total mole number of products = 47,707 mol/kg expl.
- Volume of gaseous products (at SATP) = 1182,6 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 20,961 g
- Mean molecular mass of all products = 20,961 g
- Density of products = 6,13 kg/m3
- Specific gas constant = 396,632 J/kg K
- Specific heat capacity at p=const. (Cp) = 2444,04 J/kgK
- Specific heat capacity at V=const. (Cv) = 2047,41 J/molK
- Specific heat ratio (Cp/Cv) = 1,1937

Composition of combustion products in chamber (44):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,096247E+00 | 2,779435E+01 | | 58,2611 | 50,0724 |
| CO = | 2,408924E-01 | 6,107606E+00 | 12,8025 | 17,1074 | |
| H2 = | 2,123267E-01 | 5,383350E+00 | 11,2843 | 1,0853 | |
| CO2 = | 1,653341E-01 | 4,191894E+00 | | 8,7868 | 18,4485 |
| N2 = | 8,665493E-02 | 2,197057E+00 | 4,6054 | 6,1546 | |
| BHO2 = | 5,492582E-02 | 1,392594E+00 | | 2,9191 | 6,0993 |
| OH = | 1,225060E-02 | 3,106027E-01 | | 0,6511 | 0,5282 |
| H = | 8,489769E-03 | 2,152503E-01 | 0,4512 | 0,0217 | |
| B(OH)3 = | 1,045316E-03 | 2,650303E-02 | | 0,0556 | 0,1639 |
| NO = | 7,761742E-04 | 1,967919E-02 | | 0,0413 | 0,0590 |
| O2 = | 7,269671E-04 | 1,843159E-02 | 0,0386 | 0,0590 | |
| BO2 = | 7,044850E-04 | 1,786157E-02 | | 0,0374 | 0,0765 |
| B2O3 = | 4,237678E-04 | 1,074425E-02 | | 0,0225 | 0,0748 |
| BHO = | 3,898751E-04 | 9,884925E-03 | | 0,0207 | 0,0275 |
| O = | 2,881119E-04 | 7,304813E-03 | 0,0153 | 0,0117 | |
| BO = | 1,174883E-04 | 2,978808E-03 | 0,0062 | 0,0080 | |
| NH3 = | 9,688499E-06 | 2,456430E-04 | | 0,0005 | 0,0004 |
| H2O2 = | 2,274169E-06 | 5,765947E-05 | | 0,0001 | 0,0002 |
| CH2O = | 1,493412E-06 | 3,786409E-05 | | 0,0001 | 0,0001 |
| NH2 = | 1,151227E-06 | 2,918832E-05 | | 0,0001 | 0,0000 |
| B2O2 = | 7,669916E-07 | 1,944637E-05 | | 0,0000 | 0,0001 |
| HCN = | 4,729665E-07 | 1,199163E-05 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| HCNO = | 4,032052E-07 | 1,022290E-05 | 0,0000 | 0,0000 |
| N = | 2,878716E-07 | 7,298722E-06 | 0,0000 | 0,0000 |
| NO2 = | 1,320580E-07 | 3,348210E-06 | 0,0000 | 0,0000 |
| CNO = | 7,358513E-09 | 1,865684E-07 | 0,0000 | 0,0000 |
| BH2 = | 3,098952E-09 | 7,857108E-08 | 0,0000 | 0,0000 |
| CH4 = | 2,604146E-09 | 6,602574E-08 | 0,0000 | 0,0000 |
| B = | 6,953106E-11 | 1,762896E-09 | 0,0000 | 0,0000 |
| BH = | 4,871911E-11 | 1,235228E-09 | 0,0000 | 0,0000 |
| BN = | 2,654656E-11 | 6,730637E-10 | 0,0000 | 0,0000 |
| N2H4 = | 2,581601E-13 | 6,545413E-12 | 0,0000 | 0,0000 |
| N2O3 = | 1,705601E-15 | 4,324396E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 1,153645E-16 | 2,924962E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 1,054777E-16 | 2,674290E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 3,929107E-19 | 9,961892E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 8,030194E-20 | 2,035982E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,321347E-20 | 5,885563E-19 | 0,0000 | 0,0000 |
| C(gr) = | 9,851522E-21 | 2,497763E-19 | 0,0000 | 0,0000 |
| BN(s) = | 1,339092E-21 | 3,395146E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,318399E-21 | 3,342679E-20 | 0,0000 | 0,0000 |
| B(s) = | 8,028774E-22 | 2,035622E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,314546E-23 | 3,332911E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,593123E-29 | 4,039217E-28 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5000,13 kJ/kg
- Entropy of combustion products = 12,16 kJ/K kg
- Temperature at nozzle throat = 2656,17 K
- Pressure at nozzle throat = 3,946689 MPa
- Mole number of gaseous products = 47,552 mol/kg expl.
- Total mole number of products = 47,552 mol/kg expl.
- Volume of gaseous products (at SATP) = 1178,76 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,03 g
- Mean molecular mass of all products = 21,03 g
- Density of products = 3,758 kg/m3
- Specific gas constant = 395,344 J/kg K
- Specific heat capacity at p=const. (Cp) = 2411,64 J/kgK
- Specific heat capacity at V=const. (Cv) = 2016,29 J/molK
- Specific heat ratio (Cp/Cv) = 1,1961

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1120,7 m/s
- Sound velocity at throat ) = 1120,7 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,564
- Pressure ratio (pc/pt) = 1,774

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,097683E+00 | 2,783076E+01 | 58,5275 | 50,1379 |
| CO = | 2,345873E-01 | 5,947747E+00 | 12,5080 | 16,6596 |
| H2 = | 2,154275E-01 | 5,461968E+00 | 11,4864 | 1,1011 |
| CO2 = | 1,716406E-01 | 4,351790E+00 | 9,1517 | 19,1522 |
| N2 = | 8,689331E-02 | 2,203100E+00 | 4,6331 | 6,1715 |
| BHO2 = | 5,553009E-02 | 1,407915E+00 | 2,9608 | 6,1664 |
| OH = | 5,893873E-03 | 1,494337E-01 | 0,3143 | 0,2541 |
| H = | 5,090872E-03 | 1,290744E-01 | 0,2714 | 0,0130 |
| B(OH)3 = | 1,121543E-03 | 2,843569E-02 | 0,0598 | 0,1758 |
| B2O3 = | 3,582028E-04 | 9,081903E-03 | 0,0191 | 0,0632 |
| BO2 = | 3,420717E-04 | 8,672916E-03 | 0,0182 | 0,0371 |
| NO = | 3,038819E-04 | 7,704647E-03 | 0,0162 | 0,0231 |

| | | | | |
|---|---|---|---|---|
| BHO = | 2,674428E-04 | 6,780766E-03 | 0,0143 | 0,0189 |
| O2 = | 2,129321E-04 | 5,398698E-03 | 0,0114 | 0,0173 |
| O = | 8,434886E-05 | 2,138588E-03 | 0,0045 | 0,0034 |
| BO = | 5,435430E-05 | 1,378104E-03 | 0,0029 | 0,0037 |
| NH3 = | 6,717865E-06 | 1,703253E-04 | 0,0004 | 0,0003 |
| CH2O = | 8,517371E-07 | 2,159502E-05 | 0,0000 | 0,0001 |
| H2O2 = | 6,295964E-07 | 1,596284E-05 | 0,0000 | 0,0001 |
| NH2 = | 4,603566E-07 | 1,167192E-05 | 0,0000 | 0,0000 |
| B2O2 = | 4,218111E-07 | 1,069464E-05 | 0,0000 | 0,0001 |
| HCN = | 2,642923E-07 | 6,700890E-06 | 0,0000 | 0,0000 |
| HCNO = | 2,113146E-07 | 5,357688E-06 | 0,0000 | 0,0000 |
| N = | 7,079591E-08 | 1,794965E-06 | 0,0000 | 0,0000 |
| NO2 = | 2,578240E-08 | 6,536891E-07 | 0,0000 | 0,0000 |
| CNO = | 1,998066E-09 | 5,065915E-08 | 0,0000 | 0,0000 |
| CH4 = | 1,827227E-09 | 4,632768E-08 | 0,0000 | 0,0000 |
| BH2 = | 9,708530E-10 | 2,461509E-08 | 0,0000 | 0,0000 |
| B = | 1,073845E-11 | 2,722637E-10 | 0,0000 | 0,0000 |
| BH = | 8,765615E-12 | 2,222441E-10 | 0,0000 | 0,0000 |
| BN = | 4,194730E-12 | 1,063535E-10 | 0,0000 | 0,0000 |
| N2H4 = | 5,826827E-14 | 1,477339E-12 | 0,0000 | 0,0000 |
| B4C(l) = | 2,208163E-16 | 5,598595E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 9,073305E-17 | 2,300454E-15 | 0,0000 | 0,0000 |
| N2O3 = | 8,108043E-17 | 2,055720E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 6,437076E-19 | 1,632062E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 8,928752E-20 | 2,263803E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 3,737823E-20 | 9,476909E-19 | 0,0000 | 0,0000 |
| C(gr) = | 8,013143E-21 | 2,031659E-19 | 0,0000 | 0,0000 |
| BN(s) = | 1,423670E-21 | 3,609586E-20 | 0,0000 | 0,0000 |
| B(l) = | 6,528625E-22 | 1,655273E-20 | 0,0000 | 0,0000 |
| B(s) = | 4,715360E-22 | 1,195536E-20 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 6,233748E-24 | 1,580510E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 8,383084E-31 | 2,125454E-29 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -7912,44 kJ/kg
- Entropy of combustion products = 12,16 kJ/K kg
- Temperature at nozzle exit = 1473,39 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 46,999 mol/kg expl.
- Total mole number of products = 47,04 mol/kg expl.
- Volume of gaseous products (at SATP) = 1165,07 L/kg expl.
- Mass of gaseous products = 997,1 g/kg expl.
- Mass of condensed products = 2,9 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,216 g
- Mean molecular mass of all products = 21,258 g
- Density of products = 0,174 kg/m3
- Specific gas constant = 390,753 J/kg K
- Specific heat capacity at p=const. (Cp) = 2131,5 J/kgK
- Specific heat capacity at V=const. (Cv) = 1740,74 J/molK
- Specific heat ratio (Cp/Cv) = 1,2245

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 271,34 s
- Vacuum-specific impulse (pa=0) = 292,98 s
- Exhaust (or nozzle exit) velocity = 2660,9 m/s
- Characteristic exhaust velocity (c*) = 1662,0 m/s
- Thrust coefficient (Cf) = 1,601
- Nozzle area expansion ratio (Ae/At) = 9,11
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 829,83 m/s
- Mach number at nozzle exit = 3,207

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 1,026092E+00 | 2,601562E+01 | 55,3049 | 46,8679 |
| H2 = | 2,795713E-01 | 7,088274E+00 | 15,0685 | 1,4290 |
| CO2 = | 2,368759E-01 | 6,005773E+00 | 12,7673 | 26,4314 |
| CO = | 1,693533E-01 | 4,293797E+00 | 9,1279 | 12,0269 |
| N2 = | 8,704817E-02 | 2,207027E+00 | 4,6918 | 6,1825 |
| BHO2 = | 3,957554E-02 | 1,003402E+00 | 2,1331 | 4,3947 |
| B(OH)3 = | 1,515710E-02 | 3,842944E-01 | 0,8169 | 2,3761 |
| B2O3(l) = | 1,619124E-03 | 4,105141E-02 | 0,0873 | 0,2858 |
| B2O3 = | 2,891422E-05 | 7,330936E-04 | 0,0016 | 0,0051 |
| H = | 9,599385E-06 | 2,433836E-04 | 0,0005 | 0,0000 |
| BHO = | 3,989329E-06 | 1,011458E-04 | 0,0002 | 0,0003 |
| NH3 = | 1,892769E-06 | 4,798943E-05 | 0,0001 | 0,0001 |
| OH = | 8,517989E-07 | 2,159658E-05 | 0,0000 | 0,0000 |
| BO2 = | 3,855140E-08 | 9,774354E-07 | 0,0000 | 0,0000 |
| CH2O = | 2,990017E-08 | 7,580914E-07 | 0,0000 | 0,0000 |
| HCN = | 8,274171E-09 | 2,097840E-07 | 0,0000 | 0,0000 |
| CH4 = | 7,468135E-09 | 1,893477E-07 | 0,0000 | 0,0000 |
| NO = | 5,126318E-09 | 1,299731E-07 | 0,0000 | 0,0000 |
| BO = | 3,626084E-09 | 9,193604E-08 | 0,0000 | 0,0000 |
| HCNO = | 2,939668E-09 | 7,453259E-08 | 0,0000 | 0,0000 |
| B2O2 = | 4,406424E-10 | 1,117208E-08 | 0,0000 | 0,0000 |
| NH2 = | 1,202463E-10 | 3,048735E-09 | 0,0000 | 0,0000 |
| O2 = | 4,917068E-11 | 1,246678E-09 | 0,0000 | 0,0000 |
| O = | 2,384973E-11 | 6,046882E-10 | 0,0000 | 0,0000 |
| H2O2 = | 8,594896E-13 | 2,179157E-11 | 0,0000 | 0,0000 |
| BH2 = | 1,655021E-14 | 4,196155E-13 | 0,0000 | 0,0000 |
| N = | 1,188595E-14 | 3,013574E-13 | 0,0000 | 0,0000 |
| CNO = | 9,397515E-15 | 2,382654E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 1,405497E-15 | 3,563510E-14 | 0,0000 | 0,0000 |
| NO2 = | 2,922862E-16 | 7,410650E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,342383E-16 | 3,403490E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 9,252356E-18 | 2,345850E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 3,049012E-18 | 7,730491E-17 | 0,0000 | 0,0000 |
| N2H4 = | 1,962801E-18 | 4,976501E-17 | 0,0000 | 0,0000 |
| BH = | 1,299618E-19 | 3,295062E-18 | 0,0000 | 0,0000 |
| BN(s) = | 2,650454E-20 | 6,719983E-19 | 0,0000 | 0,0000 |
| BN = | 1,528654E-20 | 3,875762E-19 | 0,0000 | 0,0000 |
| C(gr) = | 1,220353E-20 | 3,094094E-19 | 0,0000 | 0,0000 |
| B = | 1,034329E-20 | 2,622448E-19 | 0,0000 | 0,0000 |
| B(s) = | 6,411867E-24 | 1,625670E-22 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,326344E-24 | 1,096905E-22 | 0,0000 | 0,0000 |
| B(l) = | 1,484267E-25 | 3,763222E-24 | 0,0000 | 0,0000 |
| N2O3 = | 7,807176E-31 | 1,979438E-29 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 2,094625E-31 | 5,310729E-30 | 0,0000 | 0,0000 |

Excluded products (11):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 23

**Combustion conditions (Number 23):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

Reactant information:

---

**1. [EMIM][$BH_3CN$], 20.00 %**
**2. Hydrogen peroxide ($H_2O_2$), 76.00 %**
**3. Water ($H_2O$, liquid), 4.00 %**

C(0,358) H(2,614) N(0,153) O(1,812) B(0,051)

Molecular weight = 38,63
Oxygen balance = -11,92633 %
Enthalpy of formation = -4537,49 kJ/kg
Internal energy of formation = -4348,63 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5601,76 kJ/kg
- Total enthalpy of combustion prod. = -4537,15 kJ/kg
- Entropy of combustion products = 12,03 kJ/K kg
- Isobaric combustion temperature = 2968,46 K
- Mole number of gaseous products = 46,288 mol/kg expl.
- Total mole number of products = 46,288 mol/kg expl.
- Volume of gaseous products (at SATP) = 1147,42 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,604 g
- Mean molecular mass of all products = 21,604 g
- Density of products = 6,128 kg/m3
- Specific gas constant = 384,835 J/kg K
- Specific heat capacity at p=const. (Cp) = 2440,72 J/kgK
- Specific heat capacity at V=const. (Cv) = 2055,89 J/molK
- Specific heat ratio (Cp/Cv) = 1,1872

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,132158E+00 | 2,930984E+01 | | 63,3212 | 52,8026 |
| CO2 = | 1,872174E-01 | 4,846772E+00 | | 10,4710 | 21,3306 |
| CO = | 1,708765E-01 | 4,423731E+00 | 9,5571 | 12,3909 | |
| H2 = | 1,337686E-01 | 3,463066E+00 | 7,4816 | 0,6982 | |
| N2 = | 7,583438E-02 | 1,963236E+00 | 4,2414 | 5,4996 | |
| BHO2 = | 4,823291E-02 | 1,248676E+00 | | 2,6976 | 5,4690 |
| OH = | 2,234380E-02 | 5,784469E-01 | | 1,2497 | 0,9838 |
| H = | 8,773864E-03 | 2,271420E-01 | 0,4907 | 0,0229 | |
| O2 = | 3,511679E-03 | 9,091202E-02 | 0,1964 | 0,2909 | |
| NO = | 1,793744E-03 | 4,643730E-02 | | 0,1003 | 0,1393 |
| BO2 = | 1,092951E-03 | 2,829482E-02 | | 0,0611 | 0,1211 |
| O = | 8,530243E-04 | 2,208350E-02 | 0,0477 | 0,0353 | |
| B(OH)3 = | 7,969504E-04 | 2,063183E-02 | | 0,0446 | 0,1276 |
| B2O3 = | 3,387328E-04 | 8,769274E-03 | | 0,0189 | 0,0610 |
| BHO = | 2,412109E-04 | 6,244583E-03 | | 0,0135 | 0,0174 |
| BO = | 1,135357E-04 | 2,939265E-03 | 0,0064 | 0,0079 | |
| H2O2 = | 6,084631E-06 | 1,575218E-04 | | 0,0003 | 0,0005 |
| NH3 = | 4,474920E-06 | 1,158489E-04 | | 0,0003 | 0,0002 |
| NH2 = | 8,790026E-07 | 2,275604E-05 | | 0,0000 | 0,0000 |
| CH2O = | 6,981847E-07 | 1,807494E-05 | | 0,0000 | 0,0001 |
| NO2 = | 6,398272E-07 | 1,656415E-05 | | 0,0000 | 0,0001 |
| N = | 4,820964E-07 | 1,248074E-05 | 0,0000 | 0,0000 | |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 4,384343E-07 | 1,135040E-05 | 0,0000 | 0,0001 |
| HCNO = | 2,285493E-07 | 5,916794E-06 | 0,0000 | 0,0000 |
| HCN = | 1,605608E-07 | 4,156674E-06 | 0,0000 | 0,0000 |
| CNO = | 7,169632E-09 | 1,856108E-07 | 0,0000 | 0,0000 |
| BH2 = | 1,147880E-09 | 2,971687E-08 | 0,0000 | 0,0000 |
| B = 6,112628E-11 | 1,582466E-09 | 0,0000 | 0,0000 | |
| BH = 2,987042E-11 | 7,732996E-10 | 0,0000 | 0,0000 | |
| BN = 2,005848E-11 | 5,192835E-10 | 0,0000 | 0,0000 | |
| N2H4 = | 1,142522E-13 | 2,957814E-12 | 0,0000 | 0,0000 |
| N2O3 = | 1,944440E-14 | 5,033858E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 4,666131E-16 | 1,207990E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 4,116214E-16 | 1,065625E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 2,133085E-19 | 5,522231E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,868201E-20 | 1,519188E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,279749E-20 | 3,313075E-19 | 0,0000 | 0,0000 |
| C(gr) = | 3,924020E-21 | 1,015869E-19 | 0,0000 | 0,0000 |
| B(l) = | 6,551383E-22 | 1,696053E-20 | 0,0000 | 0,0000 |
| BN(s) = | 4,380649E-22 | 1,134083E-20 | 0,0000 | 0,0000 |
| B(s) = | 3,755948E-22 | 9,723576E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,063836E-23 | 2,754110E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,610831E-27 | 4,170195E-26 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5166,81 kJ/kg
- Entropy of combustion products = 12,03 kJ/K kg
- Temperature at nozzle throat = 2766,26 K
- Pressure at nozzle throat = 3,951361 MPa
- Mole number of gaseous products = 46,042 mol/kg expl.
- Total mole number of products = 46,042 mol/kg expl.
- Volume of gaseous products (at SATP) = 1141,32 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,719 g
- Mean molecular mass of all products = 21,719 g
- Density of products = 3,732 kg/m3
- Specific gas constant = 382,789 J/kg K
- Specific heat capacity at p=const. (Cp) = 2413,58 J/kgK
- Specific heat capacity at V=const. (Cv) = 2030,79 J/molK
- Specific heat ratio (Cp/Cv) = 1,1885

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1122,2 m/s
- Sound velocity at throat ) = 1121,8 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,564
- Pressure ratio (pc/pt) = 1,772

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,139777E+00 | 2,950708E+01 | 64,0880 | 53,1579 |
| CO2 = | 1,945794E-01 | 5,037363E+00 | 10,9409 | 22,1694 |
| CO = 1,635153E-01 | 4,233161E+00 | 9,1942 | 11,8571 | |
| H2 = 1,320999E-01 | 3,419864E+00 | 7,4278 | 0,6894 | |
| N2 = 7,629507E-02 | 1,975163E+00 | 4,2900 | 5,5330 | |
| BHO2 = | 4,891971E-02 | 1,266457E+00 | 2,7507 | 5,5468 |
| OH = | 1,280117E-02 | 3,314027E-01 | 0,7198 | 0,5636 |
| H = 5,867410E-03 | 1,518983E-01 | 0,3299 | 0,0153 | |
| O2 = 1,440003E-03 | 3,727949E-02 | 0,0810 | 0,1193 | |
| NO = | 8,754346E-04 | 2,266367E-02 | 0,0492 | 0,0680 |
| B(OH)3 = | 7,835295E-04 | 2,028438E-02 | 0,0441 | 0,1254 |
| BO2 = | 6,304838E-04 | 1,632226E-02 | 0,0355 | 0,0699 |
| O = 3,391902E-04 | 8,781117E-03 | 0,0191 | 0,0140 | |

| | | | | |
|---|---|---|---|---|
| B2O3 = | 2,950196E-04 | 7,637608E-03 | 0,0166 | 0,0532 |
| BHO = | 1,710802E-04 | 4,429006E-03 | 0,0096 | 0,0123 |
| BO = | 6,110035E-05 | 1,581795E-03 | 0,0034 | 0,0042 |
| NH3 = | 2,906462E-06 | 7,524388E-05 | 0,0002 | 0,0001 |
| H2O2 = | 2,131760E-06 | 5,518801E-05 | 0,0001 | 0,0002 |
| CH2O = | 3,801567E-07 | 9,841676E-06 | 0,0000 | 0,0000 |
| NH2 = | 3,793154E-07 | 9,819898E-06 | 0,0000 | 0,0000 |
| B2O2 = | 2,578151E-07 | 6,674439E-06 | 0,0000 | 0,0000 |
| NO2 = | 1,787037E-07 | 4,626367E-06 | 0,0000 | 0,0000 |
| N = | 1,540611E-07 | 3,988406E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,175225E-07 | 3,042477E-06 | 0,0000 | 0,0000 |
| HCN = | 8,456205E-08 | 2,189182E-06 | 0,0000 | 0,0000 |
| CNO = | 2,235780E-09 | 5,788093E-08 | 0,0000 | 0,0000 |
| BH2 = | 3,856017E-10 | 9,982639E-09 | 0,0000 | 0,0000 |
| B = | 1,262747E-11 | 3,269058E-10 | 0,0000 | 0,0000 |
| BH = | 6,645276E-12 | 1,720361E-10 | 0,0000 | 0,0000 |
| BN = | 4,055940E-12 | 1,050021E-10 | 0,0000 | 0,0000 |
| N2H4 = | 2,604904E-14 | 6,743698E-13 | 0,0000 | 0,0000 |
| N2O3 = | 1,627029E-15 | 4,212129E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 1,387817E-15 | 3,592846E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 9,043974E-16 | 2,341347E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 2,960506E-19 | 7,664299E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 5,884428E-20 | 1,523389E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,727320E-20 | 4,471768E-19 | 0,0000 | 0,0000 |
| C(gr) = | 2,866429E-21 | 7,420746E-20 | 0,0000 | 0,0000 |
| BN(s) = | 4,054961E-22 | 1,049768E-20 | 0,0000 | 0,0000 |
| B(l) = | 3,313534E-22 | 8,578234E-21 | 0,0000 | 0,0000 |
| B(s) = | 2,191434E-22 | 5,673287E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,668906E-24 | 1,208708E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,936415E-25 | 5,013082E-24 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8150,63 kJ/kg
- Entropy of combustion products = 12,03 kJ/K kg
- Temperature at nozzle exit = 1566,52 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 45,557 mol/kg expl.
- Total mole number of products = 45,557 mol/kg expl.
- Volume of gaseous products (at SATP) = 1129,31 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 21,951 g
- Mean molecular mass of all products = 21,951 g
- Density of products = 0,169 kg/m3
- Specific gas constant = 378,758 J/kg K
- Specific heat capacity at p=const. (Cp) = 2138,06 J/kgK
- Specific heat capacity at V=const. (Cv) = 1759,3 J/molK
- Specific heat ratio (Cp/Cv) = 1,2153

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 274,13 s
- Vacuum-specific impulse (pa=0) = 296,2 s
- Exhaust (or nozzle exit) velocity = 2688,3 m/s
- Characteristic exhaust velocity (c*) = 1671,6 m/s
- Thrust coefficient (Cf) = 1,608
- Nozzle area expansion ratio (Ae/At) = 9,24
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 839,74 m/s
- Mach number at nozzle exit = 3,201

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | |
|---|---|---|---|---|
| H2O = | 1,101113E+00 | 2,850613E+01 | 62,5729 | 51,3546 |
| CO2 = | 2,428096E-01 | 6,285969E+00 | 13,7981 | 27,6645 |
| H2 = | 1,726450E-01 | 4,469515E+00 | 9,8109 | 0,9011 |
| CO = | 1,152854E-01 | 2,984562E+00 | 6,5513 | 8,3598 |
| N2 = | 7,673430E-02 | 1,986534E+00 | 4,3606 | 5,5649 |
| BHO2 = | 4,344330E-02 | 1,124681E+00 | 2,4688 | 4,9259 |
| B(OH)3 = | 7,624684E-03 | 1,973914E-01 | 0,4333 | 1,2205 |
| B2O3 = | 4,168987E-05 | 1,079287E-03 | 0,0024 | 0,0075 |
| H = | 2,188874E-05 | 5,666660E-04 | 0,0012 | 0,0001 |
| OH = | 4,579285E-06 | 1,185507E-04 | 0,0003 | 0,0002 |
| BHO = | 4,427105E-06 | 1,146110E-04 | 0,0003 | 0,0003 |
| NH3 = | 6,912653E-07 | 1,789580E-05 | 0,0000 | 0,0000 |
| BO2 = | 2,108447E-07 | 5,458448E-06 | 0,0000 | 0,0000 |
| NO = | 4,292746E-08 | 1,111327E-06 | 0,0000 | 0,0000 |
| BO = | 1,301645E-08 | 3,369761E-07 | 0,0000 | 0,0000 |
| CH2O = | 1,247194E-08 | 3,228795E-07 | 0,0000 | 0,0000 |
| HCN = | 2,479933E-09 | 6,420169E-08 | 0,0000 | 0,0000 |
| HCNO = | 1,624950E-09 | 4,206748E-08 | 0,0000 | 0,0000 |
| O2 = | 1,604478E-09 | 4,153750E-08 | 0,0000 | 0,0000 |
| B2O2 = | 6,875223E-10 | 1,779890E-08 | 0,0000 | 0,0000 |
| O = | 4,553321E-10 | 1,178785E-08 | 0,0000 | 0,0000 |
| NH2 = | 1,746635E-10 | 4,521773E-09 | 0,0000 | 0,0000 |
| H2O2 = | 9,135608E-12 | 2,365070E-10 | 0,0000 | 0,0000 |
| N = | 1,107625E-13 | 2,867473E-12 | 0,0000 | 0,0000 |
| CNO = | 2,345609E-14 | 6,072424E-13 | 0,0000 | 0,0000 |
| BH2 = | 1,758379E-14 | 4,552174E-13 | 0,0000 | 0,0000 |
| NO2 = | 1,071277E-14 | 2,773372E-13 | 0,0000 | 0,0000 |
| B2O3(l) = | 3,054621E-16 | 7,907949E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 2,371601E-16 | 6,139714E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 9,223698E-17 | 2,387875E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 2,507915E-17 | 6,492611E-16 | 0,0000 | 0,0000 |
| BHO2(s) = | 1,230229E-18 | 3,184875E-17 | 0,0000 | 0,0000 |
| N2H4 = | 1,136280E-18 | 2,941656E-17 | 0,0000 | 0,0000 |
| BH = | 5,548025E-19 | 1,436299E-17 | 0,0000 | 0,0000 |
| B = | 9,871100E-20 | 2,555477E-18 | 0,0000 | 0,0000 |
| BN = | 9,237370E-20 | 2,391414E-18 | 0,0000 | 0,0000 |
| BN(s) = | 5,109196E-21 | 1,322693E-19 | 0,0000 | 0,0000 |
| C(gr) = | 2,892859E-21 | 7,489170E-20 | 0,0000 | 0,0000 |
| B(s) = | 4,060749E-24 | 1,051266E-22 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 2,186483E-24 | 5,660472E-23 | 0,0000 | 0,0000 |
| B(l) = | 1,183270E-24 | 3,063306E-23 | 0,0000 | 0,0000 |
| N2O3 = | 1,612769E-28 | 4,175212E-27 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,280881E-31 | 3,316007E-30 | 0,0000 | 0,0000 |

Excluded products (12):

- ---

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; CH4; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 24

**Combustion conditions (Number 24):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 18.18 %**
**2. Hydrogen peroxide ($H_2O_2$), 77.73 %**
**3. Water ($H_2O$, liquid), 4.09 %**

C(0,320) H(2,549) N(0,137) O(1,822) B(0,046)

Molecular weight = 37,98
Oxygen balance = -6,774266 %
Enthalpy of formation = -4673,54 kJ/kg
Internal energy of formation = -4484,87 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5651,4 kJ/kg
- Total enthalpy of combustion prod. = -4673,05 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Isobaric combustion temperature = 3005,03 K
- Mole number of gaseous products = 45,292 mol/kg expl.
- Total mole number of products = 45,292 mol/kg expl.
- Volume of gaseous products (at SATP) = 1122,75 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,079 g
- Mean molecular mass of all products = 22,079 g
- Density of products = 6,186 kg/m3
- Specific gas constant = 376,56 J/kg K
- Specific heat capacity at p=const. (Cp) = 2432,97 J/kgK
- Specific heat capacity at V=const. (Cv) = 2056,41 J/molK
- Specific heat ratio (Cp/Cv) = 1,1831

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,147549E+00 | 3,021098E+01 | | 66,7023 | 54,4260 |
| CO2 = | 2,034536E-01 | 5,356226E+00 | | 11,8259 | 23,5728 |
| CO = | 1,166381E-01 | 3,070675E+00 | 6,7797 | 8,6010 | |
| H2 = | 8,430096E-02 | 2,219352E+00 | 4,9001 | 0,4474 | |
| N2 = | 6,701113E-02 | 1,764171E+00 | 3,8951 | 4,9420 | |
| BHO2 = | 4,288442E-02 | 1,128998E+00 | | 2,4927 | 4,9448 |
| OH = | 3,225761E-02 | 8,492310E-01 | | 1,8750 | 1,4443 |
| O2 = | 1,121626E-02 | 2,952853E-01 | 0,6520 | 0,9449 | |
| H = | 7,652135E-03 | 2,014542E-01 | 0,4448 | 0,0203 | |
| NO = | 3,154681E-03 | 8,305181E-02 | | 0,1834 | 0,2492 |
| O = | 1,697347E-03 | 4,468527E-02 | 0,0987 | 0,0715 | |
| BO2 = | 1,384688E-03 | 3,645403E-02 | | 0,0805 | 0,1561 |
| B(OH)3 = | 6,836757E-04 | 1,799881E-02 | | 0,0397 | 0,1113 |
| B2O3 = | 2,713296E-04 | 7,143168E-03 | | 0,0158 | 0,0497 |
| BHO = | 1,410687E-04 | 3,713849E-03 | | 0,0082 | 0,0103 |
| BO = | 9,012655E-05 | 2,372719E-03 | 0,0052 | 0,0064 | |
| H2O2 = | 1,186459E-05 | 3,123536E-04 | | 0,0007 | 0,0011 |
| NH3 = | 2,133502E-06 | 5,616772E-05 | | 0,0001 | 0,0001 |
| NO2 = | 1,993198E-06 | 5,247400E-05 | | 0,0001 | 0,0002 |
| NH2 = | 5,816591E-07 | 1,531307E-05 | | 0,0000 | 0,0000 |
| N = | 5,639392E-07 | 1,484656E-05 | 0,0000 | 0,0000 | |
| CH2O = | 3,114654E-07 | 8,199804E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 2,323952E-07 | 6,118160E-06 | 0,0000 | 0,0000 |
| HCNO = | 1,220778E-07 | 3,213884E-06 | 0,0000 | 0,0000 |
| HCN = | 5,293242E-08 | 1,393527E-06 | 0,0000 | 0,0000 |
| CNO = | 5,397282E-09 | 1,420917E-07 | 0,0000 | 0,0000 |
| BH2 = | 3,633757E-10 | 9,566421E-09 | 0,0000 | 0,0000 |
| B = | 3,527397E-11 | 9,286412E-10 | 0,0000 | 0,0000 |
| BH = | 1,312971E-11 | 3,456597E-10 | 0,0000 | 0,0000 |
| BN = | 1,062567E-11 | 2,797371E-10 | 0,0000 | 0,0000 |
| N2O3 = | 1,092951E-13 | 2,877360E-12 | 0,0000 | 0,0000 |
| N2H4 = | 4,577206E-14 | 1,205020E-12 | 0,0000 | 0,0000 |
| B4C(s) = | 6,346011E-17 | 1,670684E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 5,587324E-17 | 1,470948E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,496730E-19 | 3,940370E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,949497E-20 | 1,303031E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 9,049283E-21 | 2,382362E-19 | 0,0000 | 0,0000 |
| C(gr) = | 1,642806E-21 | 4,324937E-20 | 0,0000 | 0,0000 |
| B(l) = | 3,082327E-22 | 8,114697E-21 | 0,0000 | 0,0000 |
| B(s) = | 1,725843E-22 | 4,543545E-21 | 0,0000 | 0,0000 |
| BN(s) = | 1,702110E-22 | 4,481065E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,035467E-23 | 2,726025E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,526928E-26 | 4,019872E-25 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5298,05 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Temperature at nozzle throat = 2825,34 K
- Pressure at nozzle throat = 3,952973 MPa
- Mole number of gaseous products = 44,954 mol/kg expl.
- Total mole number of products = 44,954 mol/kg expl.
- Volume of gaseous products (at SATP) = 1114,36 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,245 g
- Mean molecular mass of all products = 22,245 g
- Density of products = 3,743 kg/m3
- Specific gas constant = 373,747 J/kg K
- Specific heat capacity at p=const. (Cp) = 2410,13 J/kgK
- Specific heat capacity at V=const. (Cv) = 2036,38 J/molK
- Specific heat ratio (Cp/Cv) = 1,1835

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1118,0 m/s
- Sound velocity at throat ) = 1117,9 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,565
- Pressure ratio (pc/pt) = 1,771

Composition of combustion products at nozzle throat:

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,159803E+00 | 3,053359E+01 | 67,9220 | 55,0072 |
| CO2 = | 2,134930E-01 | 5,620531E+00 | 12,5029 | 24,7360 |
| CO = | 1,065991E-01 | 2,806383E+00 | 6,2428 | 7,8607 |
| H2 = | 7,829996E-02 | 2,061366E+00 | 4,5855 | 0,4156 |
| N2 = | 6,764120E-02 | 1,780758E+00 | 3,9613 | 4,9884 |
| BHO2 = | 4,353694E-02 | 1,146177E+00 | 2,5497 | 5,0200 |
| OH = | 2,153812E-02 | 5,670239E-01 | 1,2613 | 0,9643 |
| O2 = | 6,446899E-03 | 1,697245E-01 | 0,3776 | 0,5431 |
| H = | 5,450463E-03 | 1,434918E-01 | 0,3192 | 0,0145 |
| NO = | 1,897443E-03 | 4,995310E-02 | 0,1111 | 0,1499 |
| BO2 = | 9,279376E-04 | 2,442938E-02 | 0,0543 | 0,1046 |
| O = | 8,876577E-04 | 2,336895E-02 | 0,0520 | 0,0374 |
| B(OH)3 = | 6,284072E-04 | 1,654378E-02 | 0,0368 | 0,1023 |

| | | | | |
|---|---|---|---|---|
| B2O3 = | 2,411543E-04 | 6,348757E-03 | 0,0141 | 0,0442 |
| BHO = | 9,840095E-05 | 2,590555E-03 | 0,0058 | 0,0072 |
| BO = | 5,321241E-05 | 1,400898E-03 | 0,0031 | 0,0038 |
| H2O2 = | 5,178952E-06 | 1,363438E-04 | 0,0003 | 0,0005 |
| NH3 = | 1,241969E-06 | 3,269674E-05 | 0,0001 | 0,0001 |
| NO2 = | 7,937007E-07 | 2,089538E-05 | 0,0000 | 0,0001 |
| NH2 = | 2,555995E-07 | 6,729048E-06 | 0,0000 | 0,0000 |
| N = | 2,201777E-07 | 5,796515E-06 | 0,0000 | 0,0000 |
| CH2O = | 1,522896E-07 | 4,009257E-06 | 0,0000 | 0,0000 |
| B2O2 = | 1,376886E-07 | 3,624862E-06 | 0,0000 | 0,0000 |
| HCNO = | 5,876411E-08 | 1,547055E-06 | 0,0000 | 0,0000 |
| HCN = | 2,430656E-08 | 6,399073E-07 | 0,0000 | 0,0000 |
| CNO = | 1,812721E-09 | 4,772265E-08 | 0,0000 | 0,0000 |
| BH2 = | 1,161549E-10 | 3,057955E-09 | 0,0000 | 0,0000 |
| B = | 8,542474E-12 | 2,248937E-10 | 0,0000 | 0,0000 |
| BH = | 3,159981E-12 | 8,319132E-11 | 0,0000 | 0,0000 |
| BN = | 2,435850E-12 | 6,412748E-11 | 0,0000 | 0,0000 |
| N2O3 = | 1,592582E-14 | 4,192716E-13 | 0,0000 | 0,0000 |
| N2H4 = | 9,726899E-15 | 2,560755E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 1,669456E-16 | 4,395099E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 4,684807E-17 | 1,233347E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,833648E-19 | 4,827358E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,595620E-20 | 1,209867E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,075996E-20 | 2,832723E-19 | 0,0000 | 0,0000 |
| C(gr) = | 1,028912E-21 | 2,708769E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,489854E-22 | 3,922270E-21 | 0,0000 | 0,0000 |
| BN(s) = | 1,336030E-22 | 3,517303E-21 | 0,0000 | 0,0000 |
| B(s) = | 9,426365E-23 | 2,481635E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,361388E-24 | 1,148202E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 3,144782E-32 | 8,279119E-31 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8333,37 kJ/kg
- Entropy of combustion products = 11,91 kJ/K kg
- Temperature at nozzle exit = 1660,17 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 44,29 mol/kg expl.
- Total mole number of products = 44,29 mol/kg expl.
- Volume of gaseous products (at SATP) = 1097,89 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,579 g
- Mean molecular mass of all products = 22,579 g
- Density of products = 0,164 kg/m3
- Specific gas constant = 368,224 J/kg K
- Specific heat capacity at p=const. (Cp) = 2150,84 J/kgK
- Specific heat capacity at V=const. (Cv) = 1782,61 J/molK
- Specific heat ratio (Cp/Cv) = 1,2066

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 275,9 s
- Vacuum-specific impulse (pa=0) = 298,5 s
- Exhaust (or nozzle exit) velocity = 2705,7 m/s
- Characteristic exhaust velocity (c*) = 1672,5 m/s
- Thrust coefficient (Cf) = 1,618
- Nozzle area expansion ratio (Ae/At) = 9,46
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 850,6 m/s
- Mach number at nozzle exit = 3,181

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | |
|---|---|---|---|---|
| H2O = | 1,155800E+00 | 3,042821E+01 | 68,7029 | 54,8173 |
| CO2 = | 2,513596E-01 | 6,617426E+00 | 14,9413 | 29,1233 |
| H2 = | 9,208882E-02 | 2,424379E+00 | 5,4739 | 0,4888 |
| CO = | 6,873226E-02 | 1,809482E+00 | 4,0856 | 5,0684 |
| N2 = | 6,859092E-02 | 1,805761E+00 | 4,0772 | 5,0585 |
| BHO2 = | 4,200583E-02 | 1,105868E+00 | 2,4969 | 4,8435 |
| B(OH)3 = | 3,623998E-03 | 9,540730E-02 | 0,2154 | 0,5899 |
| B2O3 = | 4,646400E-05 | 1,223236E-03 | 0,0028 | 0,0085 |
| H = | 4,147299E-05 | 1,091840E-03 | 0,0025 | 0,0001 |
| OH = | 2,239388E-05 | 5,895532E-04 | 0,0013 | 0,0010 |
| BHO = | 3,593669E-06 | 9,460883E-05 | 0,0002 | 0,0003 |
| BO2 = | 9,457062E-07 | 2,489716E-05 | 0,0001 | 0,0001 |
| NO = | 3,446034E-07 | 9,072212E-06 | 0,0000 | 0,0000 |
| NH3 = | 2,087467E-07 | 5,495577E-06 | 0,0000 | 0,0000 |
| O2 = | 5,218752E-08 | 1,373916E-06 | 0,0000 | 0,0000 |
| BO = | 3,323697E-08 | 8,750141E-07 | 0,0000 | 0,0000 |
| O = | 7,638483E-09 | 2,010947E-07 | 0,0000 | 0,0000 |
| CH2O = | 3,937826E-09 | 1,036693E-07 | 0,0000 | 0,0000 |
| HCNO = | 7,290352E-10 | 1,919297E-08 | 0,0000 | 0,0000 |
| B2O2 = | 6,830906E-10 | 1,798340E-08 | 0,0000 | 0,0000 |
| HCN = | 5,356612E-10 | 1,410210E-08 | 0,0000 | 0,0000 |
| NH2 = | 1,996646E-10 | 5,256476E-09 | 0,0000 | 0,0000 |
| H2O2 = | 8,942144E-11 | 2,354156E-09 | 0,0000 | 0,0000 |
| N = | 8,137859E-13 | 2,142416E-11 | 0,0000 | 0,0000 |
| NO2 = | 3,866346E-13 | 1,017875E-11 | 0,0000 | 0,0000 |
| CNO = | 4,468017E-14 | 1,176274E-12 | 0,0000 | 0,0000 |
| BH2 = | 1,033046E-14 | 2,719651E-13 | 0,0000 | 0,0000 |
| B4C(l) = | 2,009810E-15 | 5,291132E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 8,615991E-16 | 2,268291E-14 | 0,0000 | 0,0000 |
| B2O3(l) = | 5,551076E-17 | 1,461406E-15 | 0,0000 | 0,0000 |
| B2O3(s) = | 4,905777E-18 | 1,291521E-16 | 0,0000 | 0,0000 |
| BH = | 1,244411E-18 | 3,276102E-17 | 0,0000 | 0,0000 |
| B = | 5,019964E-19 | 1,321582E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,909698E-19 | 1,292553E-17 | 0,0000 | 0,0000 |
| N2H4 = | 4,699787E-19 | 1,237291E-17 | 0,0000 | 0,0000 |
| BN = | 3,120666E-19 | 8,215631E-18 | 0,0000 | 0,0000 |
| BN(s) = | 7,998459E-22 | 2,105717E-20 | 0,0000 | 0,0000 |
| C(gr) = | 5,597399E-22 | 1,473601E-20 | 0,0000 | 0,0000 |
| B(s) = | 2,054755E-24 | 5,409456E-23 | 0,0000 | 0,0000 |
| B(l) = | 7,276399E-25 | 1,915623E-23 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,577066E-25 | 1,204983E-23 | 0,0000 | 0,0000 |
| N2O3 = | 3,894605E-29 | 1,025314E-27 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 5,709598E-30 | 1,503139E-28 | 0,0000 | 0,0000 |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; CH4; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 25

**Combustion conditions (Number 25):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 16.67 %**
**2. Hydrogen peroxide ($H_2O_2$), 79.17 %**
**3. Water ($H_2O$, liquid), 4.16 %**

C(0,290) H(2,496) N(0,124) O(1,831) B(0,041)

Molecular weight = 37,47
Oxygen balance = -2,497542 %
Enthalpy of formation = -4785,94 kJ/kg
Internal energy of formation = -4597,42 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5603,57 kJ/kg
- Total enthalpy of combustion prod. = -4784,97 kJ/kg
- Entropy of combustion products = 11,8 kJ/K kg
- Isobaric combustion temperature = 2998,54 K
- Mole number of gaseous products = 44,64 mol/kg expl.
- Total mole number of products = 44,64 mol/kg expl.
- Volume of gaseous products (at SATP) = 1106,57 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,402 g
- Mean molecular mass of all products = 22,402 g
- Density of products = 6,29 kg/m3
- Specific gas constant = 371,134 J/kg K
- Specific heat capacity at p=const. (Cp) = 2421,35 J/kgK
- Specific heat capacity at V=const. (Cv) = 2050,22 J/molK
- Specific heat ratio (Cp/Cv) = 1,181

Composition of combustion products in chamber (43):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,150968E+00 | 3,071790E+01 | | 68,8131 | 55,3392 |
| CO2 = | 2,114788E-01 | 5,644107E+00 | | 12,6437 | 24,8397 |
| CO = | 7,804333E-02 | 2,082879E+00 | 4,6660 | 5,8341 | |
| N2 = | 5,982587E-02 | 1,596678E+00 | 3,5768 | 4,4728 | |
| H2 = | 5,452354E-02 | 1,455165E+00 | 3,2598 | 0,2934 | |
| OH = | 3,868824E-02 | 1,032541E+00 | | 2,3131 | 1,7560 |
| BHO2 = | 3,864167E-02 | 1,031298E+00 | | 2,3103 | 4,5169 |
| O2 = | 2,508786E-02 | 6,695638E-01 | 1,4999 | 2,1425 | |
| H = | 5,948241E-03 | 1,587511E-01 | 0,3556 | 0,0160 | |
| NO = | 4,423022E-03 | 1,180449E-01 | | 0,2644 | 0,3542 |
| O = | 2,448387E-03 | 6,534439E-02 | 0,1464 | 0,1045 | |
| BO2 = | 1,491896E-03 | 3,981686E-02 | | 0,0892 | 0,1704 |
| B(OH)3 = | 6,454105E-04 | 1,722520E-02 | | 0,0386 | 0,1065 |
| B2O3 = | 2,186434E-04 | 5,835321E-03 | | 0,0131 | 0,0406 |
| BHO = | 8,116080E-05 | 2,166081E-03 | | 0,0049 | 0,0060 |
| BO = | 6,253216E-05 | 1,668905E-03 | 0,0037 | 0,0045 | |
| H2O2 = | 1,788131E-05 | 4,772299E-04 | | 0,0011 | 0,0016 |
| NO2 = | 4,260619E-06 | 1,137106E-04 | | 0,0003 | 0,0005 |
| NH3 = | 1,083246E-06 | 2,891048E-05 | | 0,0001 | 0,0000 |
| N = | 5,038829E-07 | 1,344801E-05 | 0,0000 | 0,0000 | |
| NH2 = | 3,547511E-07 | 9,467864E-06 | | 0,0000 | 0,0000 |
| CH2O = | 1,386943E-07 | 3,701578E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 1,194330E-07 | 3,187518E-06 | 0,0000 | 0,0000 |
| HCNO = | 6,374305E-08 | 1,701223E-06 | 0,0000 | 0,0000 |
| HCN = | 1,784686E-08 | 4,763105E-07 | 0,0000 | 0,0000 |
| CNO = | 3,376277E-09 | 9,010863E-08 | 0,0000 | 0,0000 |
| BH2 = | 1,085554E-10 | 2,897208E-09 | 0,0000 | 0,0000 |
| B = | 1,535500E-11 | 4,098059E-10 | 0,0000 | 0,0000 |
| BH = | 4,711535E-12 | 1,257450E-10 | 0,0000 | 0,0000 |
| BN = | 4,466000E-12 | 1,191920E-10 | 0,0000 | 0,0000 |
| N2O3 = | 3,376799E-13 | 9,012256E-12 | 0,0000 | 0,0000 |
| N2H4 = | 1,790963E-14 | 4,779857E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 3,864801E-16 | 1,031467E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 3,418836E-16 | 9,124447E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,276520E-19 | 3,406873E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,661343E-20 | 1,244054E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 7,717830E-21 | 2,059793E-19 | 0,0000 | 0,0000 |
| C(gr) = | 7,358018E-22 | 1,963764E-20 | 0,0000 | 0,0000 |
| B(l) = | 1,440194E-22 | 3,843698E-21 | 0,0000 | 0,0000 |
| B(s) = | 8,098738E-23 | 2,161452E-21 | 0,0000 | 0,0000 |
| BN(s) = | 7,834016E-23 | 2,090801E-21 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,868035E-24 | 4,985553E-23 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,381219E-26 | 1,169293E-24 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5399,91 kJ/kg
- Entropy of combustion products = 11,8 kJ/K kg
- Temperature at nozzle throat = 2831,45 K
- Pressure at nozzle throat = 3,954991 MPa
- Mole number of gaseous products = 44,26 mol/kg expl.
- Total mole number of products = 44,26 mol/kg expl.
- Volume of gaseous products (at SATP) = 1097,16 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,594 g
- Mean molecular mass of all products = 22,594 g
- Density of products = 3,796 kg/m3
- Specific gas constant = 367,977 J/kg K
- Specific heat capacity at p=const. (Cp) = 2400,34 J/kgK
- Specific heat capacity at V=const. (Cv) = 2032,36 J/molK
- Specific heat ratio (Cp/Cv) = 1,1811

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1109,0 m/s
- Sound velocity at throat ) = 1109,3 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,565
- Pressure ratio (pc/pt) = 1,77

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,164729E+00 | 3,108515E+01 | 70,2331 | 56,0008 |
| CO2 = | 2,232694E-01 | 5,958782E+00 | 13,4631 | 26,2246 |
| CO = | 6,625301E-02 | 1,768210E+00 | 3,9951 | 4,9528 |
| N2 = | 6,050079E-02 | 1,614691E+00 | 3,6482 | 4,5232 |
| H2 = | 4,663923E-02 | 1,244743E+00 | 2,8123 | 0,2509 |
| BHO2 = | 3,920715E-02 | 1,046390E+00 | 2,3642 | 4,5830 |
| OH = | 2,834799E-02 | 7,565726E-01 | 1,7094 | 1,2867 |
| O2 = | 1,862834E-02 | 4,971673E-01 | 1,1233 | 1,5909 |
| H = | 4,232182E-03 | 1,129517E-01 | 0,2552 | 0,0114 |
| NO = | 3,076321E-03 | 8,210318E-02 | 0,1855 | 0,2464 |
| O = | 1,521849E-03 | 4,061626E-02 | 0,0918 | 0,0650 |
| BO2 = | 1,095240E-03 | 2,923058E-02 | 0,0660 | 0,1251 |
| B(OH)3 = | 5,759918E-04 | 1,537250E-02 | 0,0347 | 0,0950 |

| | | | | |
|---|---|---|---|---|
| B2O3 = | 1,957074E-04 | 5,223186E-03 | 0,0118 | 0,0364 |
| BHO = | 5,311148E-05 | 1,417479E-03 | 0,0032 | 0,0039 |
| BO = | 3,731047E-05 | 9,957701E-04 | 0,0022 | 0,0027 |
| H2O2 = | 9,064050E-06 | 2,419082E-04 | 0,0005 | 0,0008 |
| NO2 = | 2,208497E-06 | 5,894204E-05 | 0,0001 | 0,0003 |
| NH3 = | 5,536771E-07 | 1,477695E-05 | 0,0000 | 0,0000 |
| N = | 2,143859E-07 | 5,721692E-06 | 0,0000 | 0,0000 |
| NH2 = | 1,486310E-07 | 3,966777E-06 | 0,0000 | 0,0000 |
| B2O2 = | 6,704470E-08 | 1,789339E-06 | 0,0000 | 0,0000 |
| CH2O = | 5,805143E-08 | 1,549320E-06 | 0,0000 | 0,0000 |
| HCNO = | 2,750583E-08 | 7,340963E-07 | 0,0000 | 0,0000 |
| HCN = | 6,739199E-09 | 1,798608E-07 | 0,0000 | 0,0000 |
| CNO = | 1,109854E-09 | 2,962063E-08 | 0,0000 | 0,0000 |
| BH2 = | 2,952561E-11 | 7,880019E-10 | 0,0000 | 0,0000 |
| B = | 3,656878E-12 | 9,759753E-11 | 0,0000 | 0,0000 |
| BH = | 1,047839E-12 | 2,796552E-11 | 0,0000 | 0,0000 |
| BN = | 9,929878E-13 | 2,650161E-11 | 0,0000 | 0,0000 |
| N2O3 = | 7,383438E-14 | 1,970548E-12 | 0,0000 | 0,0000 |
| N2H4 = | 3,308838E-15 | 8,830878E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 4,569682E-17 | 1,219591E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 9,603867E-18 | 2,563153E-16 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,484808E-19 | 3,962768E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,190861E-20 | 1,118489E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 8,719304E-21 | 2,327074E-19 | 0,0000 | 0,0000 |
| C(gr) = | 3,869509E-22 | 1,032724E-20 | 0,0000 | 0,0000 |
| B(l) = | 6,279547E-23 | 1,675933E-21 | 0,0000 | 0,0000 |
| BN(s) = | 5,260851E-23 | 1,404056E-21 | 0,0000 | 0,0000 |
| B(s) = | 3,938833E-23 | 1,051225E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,359098E-24 | 1,163389E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 8,138164E-33 | 2,171975E-31 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8461,81 kJ/kg
- Entropy of combustion products = 11,8 kJ/K kg
- Temperature at nozzle exit = 1753,19 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 43,201 mol/kg expl.
- Total mole number of products = 43,201 mol/kg expl.
- Volume of gaseous products (at SATP) = 1070,91 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23,147 g
- Mean molecular mass of all products = 23,147 g
- Density of products = 0,159 kg/m3
- Specific gas constant = 359,173 J/kg K
- Specific heat capacity at p=const. (Cp) = 2166,62 J/kgK
- Specific heat capacity at V=const. (Cv) = 1807,44 J/molK
- Specific heat ratio (Cp/Cv) = 1,1987

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 276,52 s
- Vacuum-specific impulse (pa=0) = 299,74 s
- Exhaust (or nozzle exit) velocity = 2711,8 m/s
- Characteristic exhaust velocity (c*) = 1662,8 m/s
- Thrust coefficient (Cf) = 1,631
- Nozzle area expansion ratio (Ae/At) = 9,78
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 862,39 m/s
- Mach number at nozzle exit = 3,144

Composition of combustion products at the nozzle exit:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|

---

| | | | | |
|---|---|---|---|---|
| H2O = | 1,193871E+00 | 3,186293E+01 | 73,7550 | 57,4020 |
| CO2 = | 2,627631E-01 | 7,012820E+00 | 16,2330 | 30,8634 |
| N2 = | 6,203869E-02 | 1,655736E+00 | 3,8326 | 4,6382 |
| BHO2 = | 3,946217E-02 | 1,053196E+00 | 2,4379 | 4,6128 |
| H2 = | 3,177451E-02 | 8,480220E-01 | 1,9630 | 0,1710 |
| CO = | 2,675869E-02 | 7,141562E-01 | 1,6531 | 2,0004 |
| B(OH)3 = | 1,794518E-03 | 4,789346E-02 | 0,1109 | 0,2961 |
| OH = | 1,168823E-04 | 3,119443E-03 | 0,0072 | 0,0053 |
| H = | 5,689516E-05 | 1,518461E-03 | 0,0035 | 0,0002 |
| B2O3 = | 4,847508E-05 | 1,293739E-03 | 0,0030 | 0,0090 |
| BO2 = | 4,474694E-06 | 1,194240E-04 | 0,0003 | 0,0005 |
| NO = | 3,598574E-06 | 9,604147E-05 | 0,0002 | 0,0003 |
| O2 = | 3,102392E-06 | 8,279898E-05 | 0,0002 | 0,0003 |
| BHO = | 1,759568E-06 | 4,696068E-05 | 0,0001 | 0,0001 |
| O = | 1,536707E-07 | 4,101280E-06 | 0,0000 | 0,0000 |
| BO = | 5,791178E-08 | 1,545593E-06 | 0,0000 | 0,0000 |
| NH3 = | 3,370589E-08 | 8,995682E-07 | 0,0000 | 0,0000 |
| H2O2 = | 1,101847E-09 | 2,940692E-08 | 0,0000 | 0,0000 |
| CH2O = | 5,254839E-10 | 1,402451E-08 | 0,0000 | 0,0000 |
| B2O2 = | 3,915073E-10 | 1,044884E-08 | 0,0000 | 0,0000 |
| HCNO = | 1,712171E-10 | 4,569570E-09 | 0,0000 | 0,0000 |
| NH2 = | 1,353031E-10 | 3,611072E-09 | 0,0000 | 0,0000 |
| HCN = | 4,000395E-11 | 1,067656E-09 | 0,0000 | 0,0000 |
| NO2 = | 2,519090E-11 | 6,723139E-10 | 0,0000 | 0,0000 |
| N = | 4,783484E-12 | 1,276652E-10 | 0,0000 | 0,0000 |
| CNO = | 4,882167E-14 | 1,302990E-12 | 0,0000 | 0,0000 |
| BH2 = | 1,792564E-15 | 4,784129E-14 | 0,0000 | 0,0000 |
| B4C(l) = | 9,075286E-17 | 2,422081E-15 | 0,0000 | 0,0000 |
| B4C(s) = | 5,040445E-17 | 1,345232E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,349591E-17 | 3,601890E-16 | 0,0000 | 0,0000 |
| B2O3(s) = | 1,122437E-18 | 2,995645E-17 | 0,0000 | 0,0000 |
| B = | 9,820128E-19 | 2,620870E-17 | 0,0000 | 0,0000 |
| BH = | 9,128776E-19 | 2,436357E-17 | 0,0000 | 0,0000 |
| BN = | 4,239991E-19 | 1,131601E-17 | 0,0000 | 0,0000 |
| BHO2(s) = | 2,117813E-19 | 5,652180E-18 | 0,0000 | 0,0000 |
| N2H4 = | 7,802368E-20 | 2,082355E-18 | 0,0000 | 0,0000 |
| N2O3 = | 5,469681E-23 | 1,459790E-21 | 0,0000 | 0,0000 |
| BN(s) = | 5,306084E-23 | 1,416128E-21 | 0,0000 | 0,0000 |
| C(gr) = | 4,883793E-23 | 1,303423E-21 | 0,0000 | 0,0000 |
| B(s) = | 6,321675E-26 | 1,687176E-24 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 1,093498E-26 | 2,918409E-25 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 1,774558E-27 | 4,736074E-26 | 0,0000 | 0,0000 |
| B(l) = | 1,009726E-28 | 2,694834E-27 | 0,0000 | 0,0000 |

Excluded products (12):

- ----------

C; C(d); C(Liq.1); C(Liq.2); C2H4; C2H6;
CH2O2; CH3OH; CH4; H2O(l); N2O; O3;

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculation Number 26

**Combustion conditions (Number 26):**

---

Isobaric combustion (p = const.)
Chamber pressure = 7,000 MPa
Ambient pressure = 0,100 MPa
Pressure ratio (pc/pe) = 70,000
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

**1. [EMIM][$BH_3CN$], 15.39 %**
**2. Hydrogen peroxide ($H_2O_2$), 80,38 %**
**3. Water ($H_2O$, liquid), 4.23 %**

C(0,264) H(2,453) N(0,113) O(1,838) B(0,038)

Molecular weight = 37,04
Oxygen balance = 1,122742 %
Enthalpy of formation = -4882,32 kJ/kg
Internal energy of formation = -4693,93 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -5495,1 kJ/kg
- Total enthalpy of combustion prod. = -4882,48 kJ/kg
- Entropy of combustion products = 11,7 kJ/K kg
- Isobaric combustion temperature = 2964,01 K
- Mole number of gaseous products = 44,221 mol/kg expl.
- Total mole number of products = 44,221 mol/kg expl.
- Volume of gaseous products (at SATP) = 1096,2 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,614 g
- Mean molecular mass of all products = 22,614 g
- Density of products = 6,424 kg/m3
- Specific gas constant = 367,654 J/kg K
- Specific heat capacity at p=const. (Cp) = 2407,23 J/kgK
- Specific heat capacity at V=const. (Cv) = 2039,58 J/molK
- Specific heat ratio (Cp/Cv) = 1,1803

Composition of combustion products in chamber (39):

---

| Products | mol/mol EM | mol/kg EM | | Mol % | Mass % |
|---|---|---|---|---|---|
| H2O = | 1,148892E+00 | 3,101845E+01 | | 70,1441 | 55,8807 |
| CO2 = | 2,123972E-01 | 5,734423E+00 | | 12,9676 | 25,2372 |
| N2 = | 5,396682E-02 | 1,457028E+00 | 3,2949 | 4,0816 | |
| CO = | 5,182695E-02 | 1,399254E+00 | 3,1642 | 3,9193 | |
| O2 = | 4,352286E-02 | 1,175056E+00 | 2,6572 | 3,7601 | |
| OH = | 4,091339E-02 | 1,104604E+00 | | 2,4979 | 1,8786 |
| H2 = | 3,634023E-02 | 9,811349E-01 | 2,2187 | 0,1978 | |
| BHO2 = | 3,521314E-02 | 9,507048E-01 | | 2,1499 | 4,1639 |
| NO = | 5,297138E-03 | 1,430152E-01 | | 0,3234 | 0,4291 |
| H = | 4,316370E-03 | 1,165359E-01 | 0,2635 | 0,0117 | |
| O = | 2,829803E-03 | 7,640067E-02 | 0,1728 | 0,1222 | |
| BO2 = | 1,440022E-03 | 3,887856E-02 | | 0,0879 | 0,1664 |
| B(OH)3 = | 6,515225E-04 | 1,759019E-02 | | 0,0398 | 0,1088 |
| B2O3 = | 1,773433E-04 | 4,788017E-03 | | 0,0108 | 0,0333 |
| BHO = | 4,680918E-05 | 1,263782E-03 | | 0,0029 | 0,0035 |
| BO = | 3,999889E-05 | 1,079913E-03 | 0,0024 | 0,0029 | |
| H2O2 = | 2,255965E-05 | 6,090786E-04 | | 0,0014 | 0,0021 |
| NO2 = | 6,974803E-06 | 1,883098E-04 | | 0,0004 | 0,0009 |
| NH3 = | 5,850619E-07 | 1,579584E-05 | | 0,0000 | 0,0000 |
| N = | 3,780236E-07 | 1,020610E-05 | 0,0000 | 0,0000 | |
| NH2 = | 2,080997E-07 | 5,618396E-06 | | 0,0000 | 0,0000 |
| CH2O = | 6,275550E-08 | 1,694310E-06 | | 0,0000 | 0,0000 |

| | | | | |
|---|---|---|---|---|
| B2O2 = | 6,097054E-08 | 1,646118E-06 | 0,0000 | 0,0000 |
| HCNO = | 3,321507E-08 | 8,967598E-07 | 0,0000 | 0,0000 |
| HCN = | 6,248646E-09 | 1,687046E-07 | 0,0000 | 0,0000 |
| CNO = | 1,883908E-09 | 5,086286E-08 | 0,0000 | 0,0000 |
| BH2 = | 3,218785E-11 | 8,690265E-10 | 0,0000 | 0,0000 |
| BN = 1,642706E-12 | | 4,435074E-11 | 0,0000 | 0,0000 |
| BH = 1,513662E-12 | | 4,086674E-11 | 0,0000 | 0,0000 |
| N2O3 = | 6,843520E-13 | 1,847654E-11 | 0,0000 | 0,0000 |
| N2H4 = | 7,101700E-15 | 1,917358E-13 | 0,0000 | 0,0000 |
| B4C(s) = | 2,303794E-16 | 6,219918E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 2,043359E-16 | 5,516781E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,244769E-19 | 3,360700E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,729483E-20 | 1,276894E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 7,461914E-21 | 2,014611E-19 | 0,0000 | 0,0000 |
| BN(s) = | 4,091864E-23 | 1,104745E-21 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,972416E-24 | 1,342482E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,693445E-27 | 2,077121E-25 | 0,0000 | 0,0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -5484,84 kJ/kg
- Entropy of combustion products = 11,7 kJ/K kg
- Temperature at nozzle throat = 2798,4 K
- Pressure at nozzle throat = 3,954926 MPa
- Mole number of gaseous products = 43,854 mol/kg expl.
- Total mole number of products = 43,854 mol/kg expl.
- Volume of gaseous products (at SATP) = 1087,1 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22,803 g
- Mean molecular mass of all products = 22,803 g
- Density of products = 3,876 kg/m3
- Specific gas constant = 364,603 J/kg K
- Specific heat capacity at p=const. (Cp) = 2385,68 J/kgK
- Specific heat capacity at V=const. (Cv) = 2021,08 J/molK
- Specific heat ratio (Cp/Cv) = 1,1804

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 1097,6 m/s
- Sound velocity at throat ) = 1097,4 m/s
- Mach number at nozzle throat = 1,0
- Critical pressure ratio (pt/pc) = 0,565
- Pressure ratio (pc/pt) = 1,77

Composition of combustion products at nozzle throat:

---

| Products | mol/mol EM | mol/kg EM | Mol % | Mol % |
|---|---|---|---|---|
| H2O = | 1,162151E+00 | 3,137644E+01 | 71,5474 | 56,5256 |
| CO2 = | 2,237826E-01 | 6,041813E+00 | 13,7771 | 26,5900 |
| N2 = 5,464077E-02 | | 1,475223E+00 | 3,3639 | 4,1325 |
| CO = 4,044162E-02 | | 1,091866E+00 | 2,4898 | 3,0583 |
| O2 = 3,736860E-02 | | 1,008899E+00 | 2,3006 | 3,2284 |
| BHO2 = | 3,570445E-02 | 9,639696E-01 | 2,1981 | 4,2220 |
| OH = | 3,091362E-02 | 8,346239E-01 | 1,9032 | 1,4194 |
| H2 = 2,865096E-02 | | 7,735353E-01 | 1,7639 | 0,1559 |
| NO = | 3,952736E-03 | 1,067183E-01 | 0,2433 | 0,3202 |
| H = 2,926551E-03 | | 7,901274E-02 | 0,1802 | 0,0080 |
| O = 1,875917E-03 | | 5,064709E-02 | 0,1155 | 0,0810 |
| BO2 = | 1,089957E-03 | 2,942730E-02 | 0,0671 | 0,1260 |
| B(OH)3 = | 5,844181E-04 | 1,577846E-02 | 0,0360 | 0,0976 |
| B2O3 = | 1,583268E-04 | 4,274598E-03 | 0,0097 | 0,0298 |
| BHO = | 2,811999E-05 | 7,592000E-04 | 0,0017 | 0,0021 |
| BO = 2,266423E-05 | | 6,119022E-04 | 0,0014 | 0,0016 |
| H2O2 = | 1,224709E-05 | 3,306542E-04 | 0,0008 | 0,0011 |

| | | | | |
|---|---|---|---|---|
| NO2 = | 4,180367E-06 | 1,128640E-04 | 0,0003 | 0,0005 |
| NH3 = | 2,653767E-07 | 7,164796E-06 | 0,0000 | 0,0000 |
| N = | 1,583871E-07 | 4,276228E-06 | 0,0000 | 0,0000 |
| NH2 = | 7,992121E-08 | 2,157760E-06 | 0,0000 | 0,0000 |
| B2O2 = | 3,134610E-08 | 8,463004E-07 | 0,0000 | 0,0000 |
| CH2O = | 2,228501E-08 | 6,016638E-07 | 0,0000 | 0,0000 |
| HCNO = | 1,265974E-08 | 3,417950E-07 | 0,0000 | 0,0000 |
| HCN = | 1,923641E-09 | 5,193557E-08 | 0,0000 | 0,0000 |
| CNO = | 5,643275E-10 | 1,523604E-08 | 0,0000 | 0,0000 |
| BH2 = | 7,076910E-12 | 1,910666E-10 | 0,0000 | 0,0000 |
| BN = | 3,178855E-13 | 8,582459E-12 | 0,0000 | 0,0000 |
| BH = | 2,816027E-13 | 7,602875E-12 | 0,0000 | 0,0000 |
| N2O3 = | 1,858138E-13 | 5,016709E-12 | 0,0000 | 0,0000 |
| N2H4 = | 1,112786E-15 | 3,004364E-14 | 0,0000 | 0,0000 |
| B4C(s) = | 1,809668E-16 | 4,885849E-15 | 0,0000 | 0,0000 |
| B4C(l) = | 8,966357E-17 | 2,420789E-15 | 0,0000 | 0,0000 |
| B2O3(l) = | 1,461378E-19 | 3,945514E-18 | 0,0000 | 0,0000 |
| BHO2(s) = | 4,282424E-20 | 1,156194E-18 | 0,0000 | 0,0000 |
| B2O3(s) = | 8,551589E-21 | 2,308808E-19 | 0,0000 | 0,0000 |
| BN(s) = | 2,188044E-23 | 5,907410E-22 | 0,0000 | 0,0000 |
| B(OH)3(s) = | 4,044192E-24 | 1,091875E-22 | 0,0000 | 0,0000 |
| B3H3O3(s) = | 7,973270E-32 | 2,152670E-30 | 0,0000 | 0,0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8500,53 kJ/kg
- Entropy of combustion products = 11,7 kJ/K kg
- Temperature at nozzle exit = 1777,49 K
- Pressure at nozzle exit = 0,1 MPa
- Mole number of gaseous products = 42,621 mol/kg expl.
- Total mole number of products = 42,621 mol/kg expl.
- Volume of gaseous products (at SATP) = 1056,52 L/kg expl.
- Mass of gaseous products = 1000,0 g/kg expl.
- Mass of condensed products = 0,0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23,463 g
- Mean molecular mass of all products = 23,463 g
- Density of products = 0,159 kg/m3
- Specific gas constant = 354,348 J/kg K
- Specific heat capacity at p=const. (Cp) = 2163,4 J/kgK
- Specific heat capacity at V=const. (Cv) = 1809,06 J/molK
- Specific heat ratio (Cp/Cv) = 1,1959

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 274,3 s
- Vacuum-specific impulse (pa=0) = 297,72 s
- Exhaust (or nozzle exit) velocity = 2690,0 m/s
- Characteristic exhaust velocity (c*) = 1645,3 m/s
- Thrust coefficient (Cf) = 1,635
- Nozzle area expansion ratio (Ae/At) = 9,96
- Pressure ratio (pc/pe) = 70,0
- Sound velocity at nozzle exit = 862,25 m/s
- Mach number at nozzle exit = 3,12

Composition of combustion products at the nozzle exit:

| Products | mol/mol EM | mol/kg EM | Mol % | Mass % |
|---|---|---|---|---|
| H2O = | 1,205068E+00 | 3,253513E+01 | 76,3367 | 58,6130 |
| CO2 = | 2,637023E-01 | 7,119589E+00 | 16,7046 | 31,3333 |
| N2 = | 5,649756E-02 | 1,525354E+00 | 3,5789 | 4,2730 |
| BHO2 = | 3,619054E-02 | 9,770934E-01 | 2,2925 | 4,2795 |
| O2 = | 1,315366E-02 | 3,551302E-01 | 0,8332 | 1,1364 |
| B(OH)3 = | 1,432770E-03 | 3,868277E-02 | 0,0908 | 0,2392 |
| OH = | 1,096778E-03 | 2,961145E-02 | 0,0695 | 0,0504 |
| H2 = | 6,121796E-04 | 1,652798E-02 | 0,0388 | 0,0033 |

| | | | | |
|---|---|---|---|---|
| CO = 5,219672E-04 | 1,409238E-02 | 0,0331 | 0,0395 | |
| NO = 2,437488E-04 | 6,580873E-03 | 0,0154 | 0,0197 | |
| B2O3 = 4,242395E-05 | 1,145387E-03 | 0,0027 | 0,0080 | |
| BO2 = 3,811592E-05 | 1,029076E-03 | 0,0024 | 0,0044 | |
| O = 1,254644E-05 | 3,387362E-04 | 0,0008 | 0,0005 | |
| H = 9,609209E-06 | 2,594350E-04 | 0,0006 | 0,0000 | |
| NO2 = 1,063648E-07 | 2,871700E-06 | 0,0000 | 0,0000 | |
| H2O2 = 8,120720E-08 | 2,192479E-06 | 0,0000 | 0,0000 | |
| BHO = 3,448485E-08 | 9,310421E-07 | 0,0000 | 0,0000 | |
| BO = 9,628686E-09 | 2,599609E-07 | 0,0000 | 0,0000 | |
| NH3 = 8,438254E-11 | 2,278209E-09 | 0,0000 | 0,0000 | |
| B2O2 = 7,421277E-12 | 2,003640E-10 | 0,0000 | 0,0000 | |
| N = 7,065069E-12 | 1,907469E-10 | 0,0000 | 0,0000 | |
| NH2 = 3,007598E-12 | 8,120088E-11 | 0,0000 | 0,0000 | |
| HCNO = 4,655763E-13 | 1,256990E-11 | 0,0000 | 0,0000 | |
| CH2O = 2,042892E-13 | 5,515520E-12 | 0,0000 | 0,0000 | |
| HCN = 2,063773E-15 | 5,571895E-14 | 0,0000 | 0,0000 | |
| CNO = 1,209570E-15 | 3,265667E-14 | 0,0000 | 0,0000 | |
| B4C(l) = 1,822482E-16 | 4,920443E-15 | 0,0000 | 0,0000 | |
| B4C(s) = 1,044768E-16 | 2,820725E-15 | 0,0000 | 0,0000 | |
| N2O3 = 1,602083E-17 | 4,325397E-16 | 0,0000 | 0,0000 | |
| B2O3(l) = 8,461091E-18 | 2,284375E-16 | 0,0000 | 0,0000 | |
| B2O3(s) = 6,908022E-19 | 1,865068E-17 | 0,0000 | 0,0000 | |
| BHO2(s) = 1,633554E-19 | 4,410366E-18 | 0,0000 | 0,0000 | |
| BH2 = 1,094365E-19 | 2,954630E-18 | 0,0000 | 0,0000 | |
| BN = 1,631428E-21 | 4,404625E-20 | 0,0000 | 0,0000 | |
| BH = 4,958332E-22 | 1,338679E-20 | 0,0000 | 0,0000 | |
| N2H4 = 5,057784E-24 | 1,365530E-22 | 0,0000 | 0,0000 | |
| BN(s) = 1,434960E-25 | 3,874189E-24 | 0,0000 | 0,0000 | |
| B(OH)3(s) = 8,023696E-27 | 2,166284E-25 | 0,0000 | 0,0000 | |
| B3H3O3(s) = 8,373177E-30 | 2,260639E-28 | 0,0000 | 0,0000 | |

Excluded products (16):

| | | | | | |
|---|---|---|---|---|---|
| B; | B(l); | B(s); | C; | C(d); | C(gr); |
| C(Liq.1); | C(Liq.2); | C2H4; | C2H6; | CH2O2; | CH3OH; |
| CH4; | H2O(l); | N2O; | O3; | | |

NOTES: Running parameters

---

DataBase: F:\+DB_V6.05_48_17July18.xlsx
Activity: Model 1: Condensed products form pure phase (Default)

Products concentration threshold (mol) = 1E-45
Sum of amounts of negligible products (mol) = 1E-15
Correction parameter for condensed products (mol) = 1E-15
Products convergence tolerance (mol) = 9,99999974737875E-06

# Calculations Number 27-37 Were Conducted for [EMIM][$BH_3CN$] and Hydrogen Peroxide (conc. 95%) Bipropellant System with Promoter 4 (8 wt.% in fuel)

(The enthalpy of formation value for [EMIM][$BH_3CN$] fuel was obtained from bomb calorimetry experiments)

# Calculation Number 27

**Combustion conditions (Number 27):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 36.80 %**
2. **AKC-266, 3.20 %**
3. **Hydrogen peroxide ($H_2O_2$), 57.00 %**
4. **Water ($H_2O$, liquid), 3.00 %**

C(0.823) H(3.417) N(0.355) O(1.685) B(0.126) Cu(0.001) I(0.010)

Molecular weight = 47.9
Oxygen balance = -62.1371 %
Enthalpy of formation = -8023.98 kJ/kg
Internal energy of formation = -7882.80 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -1032.36 kJ/kg
- Total enthalpy of combustion prod. = -8025.61 kJ/kg
- Entropy of combustion products = 8.50 kJ/K kg
- Isobaric combustion temperature = 895.0 K
- Mole number of gaseous products = 37.895 mol/kg expl.
- Total mole number of products = 37.913 mol/kg expl.
- Volume of gaseous products (at SATP) = 939.39 L/kg expl.
- Mass of gaseous products = 998.9 g/kg expl.
- Mass of condensed products = 1.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 26.359 g
- Mean molecular mass of all products = 26.377 g
- Specific gas constant = 315.062 J/kg K
- Specific heat capacity at p=const. (Cp) = 1963.31 J/kgK
- Specific heat capacity at V=const. (Cv) = 1648.25 J/molK
- Specific heat ratio (Cp/Cv) = 1.1911

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 5.388607 E-01 | 1.124958 E01 | 29.6722 |
| CH4 = | 4.172499 E-01 | 8.710755 E00 | 22.9758 |
| CO2 = | 3.612722 E-01 | 7.542133 E00 | 19.8934 |
| N2 = | 1.768503 E-01 | 3.692032 E00 | 9.7382 |
| H2 = | 1.389518 E-01 | 2.900841 E00 | 7.6513 |
| B(OH)3 = | 1.262405 E-01 | 2.635472 E00 | 6.9514 |
| CO = | 4.494693 E-02 | 9.383387 E-01 | 2.4750 |
| IH = | 9.528649 E-03 | 1.989257 E-01 | 0.5247 |
| NH3 = | 1.269215 E-03 | 2.649689 E-02 | 0.0699 |
| Cu(s) = | 7.990106 E-04 | 1.668062 E-02 | 0.0440 |
| B2O3(s) = | 3.566218 E-05 | 7.445049 E-04 | 0.0020 |
| I2 = | 2.167103 E-05 | 4.524172 E-04 | 0.0012 |
| I = | 1.599760 E-05 | 3.339754 E-04 | 0.0009 |
| B2O3(l) = | 5.240844 E-07 | 1.094110 E-05 | 0.0000 |
| BHO2 = | 4.276258 E-07 | 8.927370 E-06 | 0.0000 |
| CH3OH = | 2.577720 E-07 | 5.381401 E-06 | 0.0000 |

| | | | |
|---|---|---|---|
| HCN = | 1.823857 E-07 | 3.807593 E-06 | 0.0000 |
| CHNO = | 3.560677 E-08 | 7.433482 E-07 | 0.0000 |
| Cu(l) = | 1.072733 E-09 | 2.239500 E-08 | 0.0000 |
| Cu2O(s) = | 3.905313 E-11 | 8.152963 E-10 | 0.0000 |
| BHO2(s) = | 1.194350 E-11 | 2.493395 E-10 | 0.0000 |
| H = | 5.481230 E-12 | 1.144294 E-10 | 0.0000 |
| Cu2O(l) = | 4.288169 E-12 | 8.952236 E-11 | 0.0000 |
| BN(s) = | 1.122369 E-12 | 2.343125 E-11 | 0.0000 |
| BN = | 5.410238 E-13 | 1.129473 E-11 | 0.0000 |
| N = | 2.833184 E-13 | 5.914724 E-12 | 0.0000 |
| CuO = | 2.825581 E-13 | 5.898850 E-12 | 0.0000 |
| BH2 = | 2.450589 E-13 | 5.115994 E-12 | 0.0000 |
| BO = | 1.835130 E-13 | 3.831126 E-12 | 0.0000 |
| INO = | 1.684129 E-13 | 3.515888 E-12 | 0.0000 |
| CNO = | 1.459078 E-13 | 3.046057 E-12 | 0.0000 |
| BO2 = | 1.432811 E-13 | 2.991222 E-12 | 0.0000 |
| Cu(OH)2(s) = | 1.123825 E-13 | 2.346163 E-12 | 0.0000 |
| CuO(s) = | 7.971090 E-14 | 1.664092 E-12 | 0.0000 |
| NO = | 7.888009 E-14 | 1.646747 E-12 | 0.0000 |
| ICN = | 6.636096 E-14 | 1.385391 E-12 | 0.0000 |
| B2O3 = | 3.851776 E-14 | 8.041196 E-13 | 0.0000 |
| Cu = | 2.896483 E-14 | 6.046870 E-13 | 0.0000 |
| NH2 = | 1.654509 E-14 | 3.454051 E-13 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -8182.32 kJ/kg
- Temperature at nozzle throat = 834.6 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 37.795 mol/kg expl.
- Total mole number of products = 38.047 mol/kg expl.
- Volume of gaseous products (at SATP) = 936.90 L/kg expl.
- Mass of gaseous products = 982.6 g/kg expl.
- Mass of condensed products = 17.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 25.998 g
- Mean molecular mass of all products = 26.284 g
- Specific gas constant = 314.228 J/kg K
- Specific heat capacity at p=const. (Cp) = 1930.95 J/kgK
- Specific heat capacity at V=const. (Cv) = 1616.72 J/molK
- Specific heat ratio (Cp/Cv) = 1.1944

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 559.8 m/s
- Sound velocity at throat) = 559.7 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.563
- Pressure ratio (pc/pt) = 1.777

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 5.709687 E-01 | 1.191988 E01 | 31.3295 |
| CH4 = | 4.254001 E-01 | 8.880905 E00 | 23.3420 |
| CO2 = | 3.709946 E-01 | 7.745104 E00 | 20.3568 |
| N2 = | 1.769864 E-01 | 3.694873 E00 | 9.7114 |
| H2 = | 1.246197 E-01 | 2.601635 E00 | 6.8380 |
| B(OH)3 = | 1.037871 E-01 | 2.166722 E00 | 5.6949 |

| | | | |
|---|---|---|---|
| CO = | 2.707454 E-02 | 5.652242 E-01 | 1.4856 |
| B2O3(l) = | 1.126308 E-02 | 2.351348 E-01 | 0.6180 |
| IH = | 9.553059 E-03 | 1.994353 E-01 | 0.5242 |
| NH3 = | 9.972552 E-04 | 2.081929 E-02 | 0.0547 |
| Cu(s) = | 7.989988 E-04 | 1.668037 E-02 | 0.0438 |
| I2 = | 1.361378 E-05 | 2.842093 E-04 | 0.0007 |
| I = | 7.702160 E-06 | 1.607949 E-04 | 0.0004 |
| CH3OH = | 1.111516 E-07 | 2.320467 E-06 | 0.0000 |
| BHO2 = | 8.810305 E-08 | 1.839291 E-06 | 0.0000 |
| HCN = | 4.745889 E-08 | 9.907800 E-07 | 0.0000 |
| CHNO = | 1.106704 E-08 | 2.310422 E-07 | 0.0000 |
| BN = | 4.827365 E-09 | 1.007789 E-07 | 0.0000 |
| Cu(l) = | 2.002415 E-10 | 4.180360 E-09 | 0.0000 |
| B2O3(s) = | 1.957600 E-10 | 4.086801 E-09 | 0.0000 |
| BHO2(s) = | 7.138191 E-11 | 1.490211 E-09 | 0.0000 |
| H = | 6.984295 E-13 | 1.458083 E-11 | 0.0000 |
| ICN = | 4.270090 E-14 | 8.914493 E-13 | 0.0000 |
| BN(s) = | 2.434921 E-14 | 5.083285 E-13 | 0.0000 |
| NH2 = | 3.717295 E-15 | 7.760445 E-14 | 0.0000 |
| Cu2O(s) = | 6.903269 E-16 | 1.441167 E-14 | 0.0000 |
| Cu = | 8.439516 E-17 | 1.761883 E-15 | 0.0000 |
| Cu2O(l) = | 1.881274 E-17 | 3.927458 E-16 | 0.0000 |
| CuO(s) = | 1.400370 E-17 | 2.923496 E-16 | 0.0000 |
| B2O3 = | 9.406517 E-18 | 1.963760 E-16 | 0.0000 |
| Cu(OH)2(s) = | 4.595905 E-19 | 9.594685 E-18 | 0.0000 |
| NO = | 2.485168 E-20 | 5.188183 E-19 | 0.0000 |
| CNO = | 4.345513 E-22 | 9.071950 E-21 | 0.0000 |
| BO2 = | 2.202355 E-22 | 4.597768 E-21 | 0.0000 |
| INO = | 4.251680 E-23 | 8.876060 E-22 | 0.0000 |
| BO = | 2.321383 E-24 | 4.846257 E-23 | 0.0000 |
| BH2 = | 4.706297 E-25 | 9.825145 E-24 | 0.0000 |
| N = | 4.320828 E-26 | 9.020416 E-25 | 0.0000 |
| CuO = | 2.490611 E-28 | 5.199548 E-27 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8954.33 kJ/kg
- Temperature at nozzle exit = 553.9 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 36.295 mol/kg expl.
- Total mole number of products = 38.802 mol/kg expl.
- Volume of gaseous products (at SATP) = 899.72 L/kg expl.
- Mass of gaseous products = 889.9 g/kg expl.
- Mass of condensed products = 110.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 24.517 g
- Mean molecular mass of all products = 25.771 g
- Specific gas constant = 301.759 J/kg K
- Specific heat capacity at p=const. (Cp) = 1754.41 J/kgK
- Specific heat capacity at V=const. (Cv) = 1452.65 J/molK
- Specific heat ratio (Cp/Cv) = 1.2077

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 138.93 s
- Exhaust (or nozzle exit) velocity = 1362.9 m/s
- Characteristic exhaust velocity (c*) = 799.5 m/s
- Thrust coefficient (Cf) = 1.705
- Nozzle area expansion ratio (Ae/At) = 8.92
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 446.79 m/s
- Mach number at nozzle exit = 3.050

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 6.911479 E-01 | 1.442881 E01 | 37.1859 |
| CH4 = | 4.561103 E-01 | 9.522029 E00 | 24.5402 |
| CO2 = | 3.670046 E-01 | 7.661806 E00 | 19.7460 |
| N2 = | 1.774086 E-01 | 3.703686 E00 | 9.5451 |
| BHO2(s) = | 1.192683 E-01 | 2.489916 E00 | 6.4170 |
| H2 = | 2.978424 E-02 | 6.217934 E-01 | 1.6025 |
| IH = | 9.516510 E-03 | 1.986723 E-01 | 0.5120 |
| B(OH)3 = | 7.045015 E-03 | 1.470759 E-01 | 0.3790 |
| Cu(s) = | 7.990376 E-04 | 1.668118 E-02 | 0.0430 |
| CO = | 3.545086 E-04 | 7.400932 E-03 | 0.0191 |
| NH3 = | 1.529011 E-04 | 3.192053 E-03 | 0.0082 |
| I2 = | 3.554460 E-05 | 7.420501 E-04 | 0.0019 |
| I = | 3.889679 E-07 | 8.120323 E-06 | 0.0000 |
| Cu(l) = | 3.554470 E-09 | 7.420523 E-08 | 0.0000 |
| Cu2O(s) = | 1.428694 E-10 | 2.982627 E-09 | 0.0000 |
| CH3OH = | 1.069804 E-10 | 2.233385 E-09 | 0.0000 |
| B2O3(l) = | 1.544941 E-11 | 3.225311 E-10 | 0.0000 |
| Cu2O(l) = | 1.146258 E-11 | 2.392996 E-10 | 0.0000 |
| B2O3(s) = | 9.857297 E-12 | 2.057868 E-10 | 0.0000 |
| BN(s) = | 4.284174 E-12 | 8.943896 E-11 | 0.0000 |
| HCN = | 1.656458 E-12 | 3.458119 E-11 | 0.0000 |
| CHNO = | 1.237761 E-12 | 2.584024 E-11 | 0.0000 |
| BN = | 1.172075 E-12 | 2.446893 E-11 | 0.0000 |
| BH2 = | 6.827720 E-13 | 1.425395 E-11 | 0.0000 |
| CuO = | 6.791162 E-13 | 1.417763 E-11 | 0.0000 |
| N = | 6.558658 E-13 | 1.369224 E-11 | 0.0000 |
| BO = | 5.838279 E-13 | 1.218834 E-11 | 0.0000 |
| BO2 = | 4.949183 E-13 | 1.033221 E-11 | 0.0000 |
| CNO = | 4.388907 E-13 | 9.162542 E-12 | 0.0000 |
| INO = | 4.150381 E-13 | 8.664582 E-12 | 0.0000 |
| B2O3 = | 3.752184 E-13 | 7.833283 E-12 | 0.0000 |
| NO = | 3.190088 E-13 | 6.659817 E-12 | 0.0000 |
| Cu = | 2.662040 E-13 | 5.557433 E-12 | 0.0000 |
| NH2 = | 1.895872 E-13 | 3.957935 E-12 | 0.0000 |
| Cu(OH)2(s) = | 1.754516 E-13 | 3.662833 E-12 | 0.0000 |
| BHO2 = | 1.588558 E-13 | 3.316368 E-12 | 0.0000 |
| CuO(s) = | 1.399029 E-13 | 2.920696 E-12 | 0.0000 |
| ICN = | 1.291966 E-13 | 2.697185 E-12 | 0.0000 |
| H = | 1.183000 E-13 | 2.469701 E-12 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 28

**Combustion conditions (Number 28):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 30.73 %**
2. **AKC-266, 2.67 %**
3. **Hydrogen peroxide ($H_2O_2$), 63.27 %**
4. **Water ($H_2O$, liquid), 3.33 %**

C(0.638) H(3.098) N(0.275) O(1.736) B(0.098) Cu(0.001) I(0.007)

Molecular weight = 44.45
Oxygen balance = -44.51551 %
Enthalpy of formation = -7695.54 kJ/kg
Internal energy of formation = -7553.10 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -1435.47 kJ/kg
- Total enthalpy of combustion prod. = -7695.94 kJ/kg
- Entropy of combustion products = 9.62 kJ/K kg
- Isobaric combustion temperature = 1083.3 K
- Mole number of gaseous products = 44.303 mol/kg expl.
- Total mole number of products = 44.317 mol/kg expl.
- Volume of gaseous products (at SATP) = 1098.22 L/kg expl.
- Mass of gaseous products = 999.1 g/kg expl.
- Mass of condensed products = 0.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.551 g
- Mean molecular mass of all products = 22.565 g
- Specific gas constant = 368.333 J/kg K
- Specific heat capacity at p=const. (Cp) = 2046.10 J/kgK
- Specific heat capacity at V=const. (Cv) = 1677.76 J/molK
- Specific heat ratio (Cp/Cv) = 1.2195

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 6.646003 E-01 | 1.495246 E01 | 33.7396 |
| H2 = | 4.229948 E-01 | 9.516716 E00 | 21.4741 |
| CO2 = | 2.938851 E-01 | 6.611951 E00 | 14.9196 |
| CO = | 1.898322 E-01 | 4.270926 E00 | 9.6372 |
| CH4 = | 1.543474 E-01 | 3.472574 E00 | 7.8357 |
| N2 = | 1.367975 E-01 | 3.077729 E00 | 6.9448 |
| B(OH)3 = | 9.779505 E-02 | 2.200235 E00 | 4.9647 |
| IH = | 7.371390 E-03 | 1.658447 E-01 | 0.3742 |
| NH3 = | 1.450820 E-03 | 3.264116 E-02 | 0.0737 |
| Cu(l) = | 6.106663 E-04 | 1.373903 E-02 | 0.0310 |
| I = | 4.139543 E-05 | 9.313319 E-04 | 0.0021 |
| BHO2 = | 2.505915 E-05 | 5.637914 E-04 | 0.0013 |
| B2O3(l) = | 2.438918 E-05 | 5.487180 E-04 | 0.0012 |
| Cu(s) = | 8.040149 E-06 | 1.808907 E-04 | 0.0004 |
| I2 = | 5.250775 E-06 | 1.181342 E-04 | 0.0003 |
| HCN = | 2.309123 E-06 | 5.195164 E-05 | 0.0001 |

| | | | |
|---|---|---|---|
| CH3OH = | 7.649998 E-07 | 1.721129 E-05 | 0.0000 |
| CHNO = | 2.491772 E-07 | 5.606095 E-06 | 0.0000 |
| Cu2O(s) = | 4.489721 E-09 | 1.010117 E-07 | 0.0000 |
| H = | 1.819905 E-09 | 4.094499 E-08 | 0.0000 |
| Cu2O(l) = | 4.461464 E-10 | 1.003759 E-08 | 0.0000 |
| B2O3(s) = | 2.558085 E-10 | 5.755288 E-09 | 0.0000 |
| BN(s) = | 1.606457 E-10 | 3.614275 E-09 | 0.0000 |
| BN = | 4.087811 E-11 | 9.196932 E-10 | 0.0000 |
| BHO2(s) = | 2.702550 E-11 | 6.080311 E-10 | 0.0000 |
| N = | 2.189667 E-11 | 4.926405 E-10 | 0.0000 |
| CuO = | 2.089544 E-11 | 4.701146 E-10 | 0.0000 |
| BH2 = | 1.662739 E-11 | 3.740901 E-10 | 0.0000 |
| INO = | 1.546988 E-11 | 3.480480 E-10 | 0.0000 |
| Cu(OH)2(s) = | 1.516425 E-11 | 3.411717 E-10 | 0.0000 |
| CNO = | 1.157026 E-11 | 2.603125 E-10 | 0.0000 |
| BO = | 1.119366 E-11 | 2.518397 E-10 | 0.0000 |
| CuO(s) = | 1.116821 E-11 | 2.512671 E-10 | 0.0000 |
| BO2 = | 8.788421 E-12 | 1.977256 E-10 | 0.0000 |
| NH2 = | 7.985921 E-12 | 1.796706 E-10 | 0.0000 |
| NO = | 5.493950 E-12 | 1.236052 E-10 | 0.0000 |
| ICN = | 5.135070 E-12 | 1.155310 E-10 | 0.0000 |
| B2O3 = | 4.981245 E-12 | 1.120702 E-10 | 0.0000 |
| Cu = | 2.515870 E-12 | 5.660310 E-11 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7921.37 kJ/kg
- Temperature at nozzle throat = 1017.3 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 43.699 mol/kg expl.
- Total mole number of products = 43.795 mol/kg expl.
- Volume of gaseous products (at SATP) = 1083.25 L/kg expl.
- Mass of gaseous products = 993.4 g/kg expl.
- Mass of condensed products = 6.6 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.733 g
- Mean molecular mass of all products = 22.834 g
- Specific gas constant = 363.313 J/kg K
- Specific heat capacity at p=const. (Cp) = 2017.58 J/kgK
- Specific heat capacity at V=const. (Cv) = 1654.27 J/molK
- Specific heat ratio (Cp/Cv) = 1.2196

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 671.5 m/s
- Sound velocity at throat) = 671.4 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.555
- Pressure ratio (pc/pt) = 1.800

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 6.699140 E-01 | 1.507201 E01 | 34.4149 |
| H2 = | 3.982524 E-01 | 8.960052 E00 | 20.4591 |
| CO2 = | 3.148198 E-01 | 7.082949 E00 | 16.1730 |
| CH4 = | 1.697306 E-01 | 3.818671 E00 | 8.7194 |
| CO = | 1.535161 E-01 | 3.453871 E00 | 7.8865 |
| N2 = | 1.369573 E-01 | 3.081323 E00 | 7.0358 |

| | | | |
|---|---|---|---|
| B(OH)3 = | 9.055556 E-02 | 2.037357 E00 | 4.6520 |
| IH = | 7.386167 E-03 | 1.661771 E-01 | 0.3794 |
| B2O3(l) = | 3.651539 E-03 | 8.215386 E-02 | 0.1876 |
| NH3 = | 1.132803 E-03 | 2.548629 E-02 | 0.0582 |
| Cu(s) = | 6.186050 E-04 | 1.391764 E-02 | 0.0318 |
| I = | 3.011640 E-05 | 6.775715 E-04 | 0.0015 |
| BHO2 = | 1.029775 E-05 | 2.316832 E-04 | 0.0005 |
| I2 = | 3.501847 E-06 | 7.878605 E-05 | 0.0002 |
| HCN = | 1.027866 E-06 | 2.312536 E-05 | 0.0001 |
| CH3OH = | 3.687057 E-07 | 8.295297 E-06 | 0.0000 |
| CHNO = | 1.104407 E-07 | 2.484742 E-06 | 0.0000 |
| BN = | 5.203979 E-09 | 1.170813 E-07 | 0.0000 |
| Cu(l) = | 2.267075 E-09 | 5.100561 E-08 | 0.0000 |
| H = | 5.271028 E-10 | 1.185898 E-08 | 0.0000 |
| B2O3(s) = | 4.936445 E-11 | 1.110622 E-09 | 0.0000 |
| BHO2(s) = | 1.165430 E-11 | 2.622034 E-10 | 0.0000 |
| Cu = | 1.992389 E-12 | 4.482562 E-11 | 0.0000 |
| NH2 = | 1.488096 E-12 | 3.347982 E-11 | 0.0000 |
| ICN = | 1.386252 E-12 | 3.118849 E-11 | 0.0000 |
| B2O3 = | 4.597341 E-13 | 1.034329 E-11 | 0.0000 |
| BN(s) = | 8.752003 E-14 | 1.969063 E-12 | 0.0000 |
| Cu2O(s) = | 2.013554 E-15 | 4.530179 E-14 | 0.0000 |
| NO = | 1.780539 E-15 | 4.005932 E-14 | 0.0000 |
| Cu2O(l) = | 2.826319 E-16 | 6.358773 E-15 | 0.0000 |
| CuO(s) = | 6.372165 E-17 | 1.433637 E-15 | 0.0000 |
| BO2 = | 3.212597 E-17 | 7.227837 E-16 | 0.0000 |
| CNO = | 2.793636 E-18 | 6.285241 E-17 | 0.0000 |
| BO = | 1.833849 E-18 | 4.125871 E-17 | 0.0000 |
| Cu(OH)2(s) = | 8.331142 E-19 | 1.874376 E-17 | 0.0000 |
| INO = | 5.441188 E-20 | 1.224182 E-18 | 0.0000 |
| BH2 = | 8.390881 E-21 | 1.887816 E-19 | 0.0000 |
| CuO = | 2.480421 E-22 | 5.580555 E-21 | 0.0000 |
| N = | 4.103381 E-23 | 9.231960 E-22 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9007.93 kJ/kg
- Temperature at nozzle exit = 695.1 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 40.729 mol/kg expl.
- Total mole number of products = 41.562 mol/kg expl.
- Volume of gaseous products (at SATP) = 1009.64 L/kg expl.
- Mass of gaseous products = 942.1 g/kg expl.
- Mass of condensed products = 57.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.132 g
- Mean molecular mass of all products = 24.061 g
- Specific gas constant = 338.623 J/kg K
- Specific heat capacity at p=const. (Cp) = 1832.71 J/kgK
- Specific heat capacity at V=const. (Cv) = 1494.08 J/molK
- Specific heat ratio (Cp/Cv) = 1.2266

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 165.12 s
- Exhaust (or nozzle exit) velocity = 1619.9 m/s
- Characteristic exhaust velocity (c*) = 926.6 m/s
- Thrust coefficient (Cf) = 1.748
- Nozzle area expansion ratio (Ae/At) = 8.60
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 535.79 m/s
- Mach number at nozzle exit = 3.023

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 7.920657 E-01 | 1.782023 E01 | 42.8764 |
| CO2 = | 3.736764 E-01 | 8.407130 E00 | 20.2280 |
| CH4 = | 2.525376 E-01 | 5.681699 E00 | 13.6705 |
| H2 = | 2.100308 E-01 | 4.725362 E00 | 11.3695 |
| N2 = | 1.374100 E-01 | 3.091508 E00 | 7.4383 |
| B2O3(s) = | 3.638830 E-02 | 8.186795 E-01 | 1.9698 |
| B(OH)3 = | 2.509084 E-02 | 5.645044 E-01 | 1.3582 |
| CO = | 1.185398 E-02 | 2.666959 E-01 | 0.6417 |
| IH = | 7.417948 E-03 | 1.668921 E-01 | 0.4016 |
| Cu(s) = | 6.186184 E-04 | 1.391794 E-02 | 0.0335 |
| NH3 = | 2.284774 E-04 | 5.140380 E-03 | 0.0124 |
| I = | 2.762545 E-06 | 6.215291 E-05 | 0.0001 |
| I2 = | 1.288585 E-06 | 2.899113 E-05 | 0.0001 |
| B2O3(l) = | 7.143793 E-07 | 1.607241 E-05 | 0.0000 |
| BHO2 = | 2.389912 E-09 | 5.376927 E-08 | 0.0000 |
| CH3OH = | 1.677993 E-09 | 3.775220 E-08 | 0.0000 |
| Cu(l) = | 1.104248 E-09 | 2.484385 E-08 | 0.0000 |
| HCN = | 8.123158 E-10 | 1.827583 E-08 | 0.0000 |
| CHNO = | 1.192419 E-10 | 2.682754 E-09 | 0.0000 |
| BHO2(s) = | 3.192050 E-11 | 7.181609 E-10 | 0.0000 |
| Cu2O(s) = | 6.830329 E-12 | 1.536716 E-10 | 0.0000 |
| Cu2O(l) = | 6.413103 E-13 | 1.442847 E-11 | 0.0000 |
| BN(s) = | 1.221303 E-13 | 2.747738 E-12 | 0.0000 |
| BN = | 7.843305 E-14 | 1.764620 E-12 | 0.0000 |
| CuO = | 4.305092 E-14 | 9.685778 E-13 | 0.0000 |
| N = | 4.241325 E-14 | 9.542314 E-13 | 0.0000 |
| BH2 = | 3.971855 E-14 | 8.936047 E-13 | 0.0000 |
| BO = | 3.150582 E-14 | 7.088313 E-13 | 0.0000 |
| INO = | 2.792519 E-14 | 6.282727 E-13 | 0.0000 |
| CNO = | 2.634475 E-14 | 5.927153 E-13 | 0.0000 |
| BO2 = | 2.611579 E-14 | 5.875641 E-13 | 0.0000 |
| NO = | 1.666213 E-14 | 3.748716 E-13 | 0.0000 |
| Cu(OH)2(s) = | 1.496182 E-14 | 3.366175 E-13 | 0.0000 |
| B2O3 = | 1.401629 E-14 | 3.153445 E-13 | 0.0000 |
| H = | 1.210634 E-14 | 2.723736 E-13 | 0.0000 |
| CuO(s) = | 9.424664 E-15 | 2.120401 E-13 | 0.0000 |
| Cu = | 9.367671 E-15 | 2.107578 E-13 | 0.0000 |
| NH2 = | 6.614961 E-15 | 1.488262 E-13 | 0.0000 |
| ICN = | 3.965815 E-15 | 8.922458 E-14 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 29

**Combustion conditions (Number 29):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 26.86 %**
2. **AKC-266, 2.34 %**
3. **Hydrogen peroxide ($H_2O_2$), 67.26 %**
4. **Water ($H_2O$, liquid), 3.54 %**

C(0.533) H(2.917) N(0.230) O(1.764) B(0.082) Cu(0.001) I(0.006)

Molecular weight = 42.5
Oxygen balance = -33.2872 %
Enthalpy of formation = -7486.73 kJ/kg
Internal energy of formation = -7343.50 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -1741.12 kJ/kg
- Total enthalpy of combustion prod. = -7487.00 kJ/kg
- Entropy of combustion products = 10.22 kJ/K kg
- Isobaric combustion temperature = 1228.3 K
- Mole number of gaseous products = 47.847 mol/kg expl.
- Total mole number of products = 47.915 mol/kg expl.
- Volume of gaseous products (at SATP) = 1186.07 L/kg expl.
- Mass of gaseous products = 995.3 g/kg expl.
- Mass of condensed products = 4.7 g/kg expl.
- Mean molecular mass of gaseous prod. = 20.802 g
- Mean molecular mass of all products = 20.870 g
- Specific gas constant = 397.797 J/kg K
- Specific heat capacity at p=const. (Cp) = 2078.59 J/kgK
- Specific heat capacity at V=const. (Cv) = 1680.80 J/molK
- Specific heat ratio (Cp/Cv) = 1.2367

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 7.677385 E-01 | 1.806493 E01 | 37.7018 |
| H2 = | 5.338004 E-01 | 1.256035 E01 | 26.2137 |
| CO = | 2.705783 E-01 | 6.366723 E00 | 13.2875 |
| CO2 = | 2.439641 E-01 | 5.740489 E00 | 11.9805 |
| N2 = | 1.144861 E-01 | 2.693865 E00 | 5.6221 |
| B(OH)3 = | 7.680812 E-02 | 1.807299 E00 | 3.7719 |
| CH4 = | 1.872498 E-02 | 4.405997 E-01 | 0.9195 |
| IH = | 6.123905 E-03 | 1.440958 E-01 | 0.3007 |
| B2O3(l) = | 2.399987 E-03 | 5.647182 E-02 | 0.1179 |
| NH3 = | 9.018551 E-04 | 2.122070 E-02 | 0.0443 |
| Cu(l) = | 5.184603 E-04 | 1.219940 E-02 | 0.0255 |
| BHO2 = | 2.017513 E-04 | 4.747220 E-03 | 0.0099 |
| I = | 9.074542 E-05 | 2.135245 E-03 | 0.0045 |
| HCN = | 3.583528 E-06 | 8.432061 E-05 | 0.0002 |
| I2 = | 2.958321 E-06 | 6.960946 E-05 | 0.0001 |
| CHNO = | 4.079132 E-07 | 9.598221 E-06 | 0.0000 |

| | | | |
|---|---|---|---|
| CH3OH = | 4.049396 E-07 | 9.528252 E-06 | 0.0000 |
| H = | 4.155450 E-08 | 9.777798 E-07 | 0.0000 |
| Cu2O(s) = | 3.251162 E-09 | 7.650004 E-08 | 0.0000 |
| Cu(s) = | 7.522618 E-10 | 1.770076 E-08 | 0.0000 |
| B2O3 = | 6.593925 E-10 | 1.551554 E-08 | 0.0000 |
| B2O3(s) = | 5.916184 E-10 | 1.392081 E-08 | 0.0000 |
| Cu2O(l) = | 3.512207 E-10 | 8.264242 E-09 | 0.0000 |
| Cu = | 2.554035 E-10 | 6.009658 E-09 | 0.0000 |
| BN(s) = | 1.560000 E-10 | 3.670690 E-09 | 0.0000 |
| NH2 = | 1.043924 E-10 | 2.456360 E-09 | 0.0000 |
| BHO2(s) = | 3.824021 E-11 | 8.997944 E-10 | 0.0000 |
| BN = | 3.161395 E-11 | 7.438780 E-10 | 0.0000 |
| N = | 1.572187 E-11 | 3.699364 E-10 | 0.0000 |
| Cu(OH)2(s) = | 1.446842 E-11 | 3.404427 E-10 | 0.0000 |
| ICN = | 1.391170 E-11 | 3.273432 E-10 | 0.0000 |
| CuO = | 1.388359 E-11 | 3.266818 E-10 | 0.0000 |
| INO = | 1.160815 E-11 | 2.731405 E-10 | 0.0000 |
| BH2 = | 1.070067 E-11 | 2.517875 E-10 | 0.0000 |
| CuO(s) = | 1.011191 E-11 | 2.379339 E-10 | 0.0000 |
| CNO = | 7.745182 E-12 | 1.822446 E-10 | 0.0000 |
| BO = | 4.949693 E-12 | 1.164666 E-10 | 0.0000 |
| BO2 = | 3.066100 E-12 | 7.214550 E-11 | 0.0000 |
| NO = | 1.220564 E-12 | 2.871993 E-11 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7763.25 kJ/kg
- Temperature at nozzle throat = 1135.3 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 47.236 mol/kg expl.
- Total mole number of products = 47.248 mol/kg expl.
- Volume of gaseous products (at SATP) = 1170.92 L/kg expl.
- Mass of gaseous products = 999.2 g/kg expl.
- Mass of condensed products = 0.8 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.154 g
- Mean molecular mass of all products = 21.165 g
- Specific gas constant = 392.717 J/kg K
- Specific heat capacity at p=const. (Cp) = 2044.60 J/kgK
- Specific heat capacity at V=const. (Cv) = 1651.88 J/molK
- Specific heat ratio (Cp/Cv) = 1.2377

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 743.3 m/s
- Sound velocity at throat) = 742.9 m/s
- Mach number at nozzle throat = 1.001
- Critical pressure ratio (pt/pc) = 0.554
- Pressure ratio (pc/pt) = 1.804

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 7.466922 E-01 | 1.756971 E01 | 37.1860 |
| H2 = | 5.241708 E-01 | 1.233377 E01 | 26.1042 |
| CO2 = | 2.695242 E-01 | 6.341919 E00 | 13.4226 |
| CO = | 2.332273 E-01 | 5.487851 E00 | 11.6150 |
| N2 = | 1.145543 E-01 | 2.695469 E00 | 5.7049 |
| B(OH)3 = | 8.169790 E-02 | 1.922356 E00 | 4.0686 |

| | | | |
|---|---|---|---|
| CH4 = | 3.051809 E-02 | 7.180923 E-01 | 1.5198 |
| IH = | 6.153986 E-03 | 1.448036 E-01 | 0.3065 |
| NH3 = | 7.675121 E-04 | 1.805960 E-02 | 0.0382 |
| Cu(l) = | 4.657188 E-04 | 1.095839 E-02 | 0.0232 |
| BHO2 = | 8.715974 E-05 | 2.050874 E-03 | 0.0043 |
| I = | 6.226644 E-05 | 1.465133 E-03 | 0.0031 |
| Cu(s) = | 5.266168 E-05 | 1.239132 E-03 | 0.0026 |
| B2O3(l) = | 1.239996 E-05 | 2.917716 E-04 | 0.0006 |
| I2 = | 2.157389 E-06 | 5.076347 E-05 | 0.0001 |
| HCN = | 1.803724 E-06 | 4.244172 E-05 | 0.0001 |
| CH3OH = | 2.498095 E-07 | 5.878031 E-06 | 0.0000 |
| CHNO = | 1.863379 E-07 | 4.384542 E-06 | 0.0000 |
| H = | 9.475431 E-09 | 2.229574 E-07 | 0.0000 |
| BN = | 2.734166 E-09 | 6.433508 E-08 | 0.0000 |
| Cu = | 1.106141 E-10 | 2.602755 E-09 | 0.0000 |
| B2O3 = | 8.321589 E-11 | 1.958074 E-09 | 0.0000 |
| B2O3(s) = | 2.588248 E-11 | 6.090161 E-10 | 0.0000 |
| NH2 = | 1.715478 E-11 | 4.036529 E-10 | 0.0000 |
| BHO2(s) = | 5.543589 E-12 | 1.304409 E-10 | 0.0000 |
| ICN = | 3.651221 E-12 | 8.591343 E-11 | 0.0000 |
| NO = | 9.134067 E-14 | 2.149251 E-12 | 0.0000 |
| BN(s) = | 8.860634 E-14 | 2.084912 E-12 | 0.0000 |
| BO2 = | 9.792428 E-15 | 2.304164 E-13 | 0.0000 |
| Cu2O(s) = | 3.718206 E-15 | 8.748959 E-14 | 0.0000 |
| BO = | 1.168288 E-15 | 2.748987 E-14 | 0.0000 |
| Cu2O(l) = | 1.144063 E-15 | 2.691987 E-14 | 0.0000 |
| CuO(s) = | 1.629350 E-16 | 3.833870 E-15 | 0.0000 |
| CNO = | 1.122983 E-16 | 2.642385 E-15 | 0.0000 |
| BH2 = | 3.065526 E-18 | 7.213201 E-17 | 0.0000 |
| INO = | 1.908721 E-18 | 4.491231 E-17 | 0.0000 |
| Cu(OH)2(s) = | 1.485045 E-18 | 3.494319 E-17 | 0.0000 |
| CuO = | 1.953891 E-19 | 4.597516 E-18 | 0.0000 |
| N = | 1.534572 E-20 | 3.610856 E-19 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9050.31 kJ/kg
- Temperature at nozzle exit = 761.4 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 43.627 mol/kg expl.
- Total mole number of products = 44.310 mol/kg expl.
- Volume of gaseous products (at SATP) = 1081.48 L/kg expl.
- Mass of gaseous products = 952.6 g/kg expl.
- Mass of condensed products = 47.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.835 g
- Mean molecular mass of all products = 22.569 g
- Specific gas constant = 362.717 J/kg K
- Specific heat capacity at p=const. (Cp) = 1887.07 J/kgK
- Specific heat capacity at V=const. (Cv) = 1524.36 J/molK
- Specific heat ratio (Cp/Cv) = 1.2379

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 180.25 s
- Exhaust (or nozzle exit) velocity = 1768.2 m/s
- Characteristic exhaust velocity (c*) = 1017.8 m/s
- Thrust coefficient (Cf) = 1.737
- Nozzle area expansion ratio (Ae/At) = 8.42
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 584.66 m/s
- Mach number at nozzle exit = 3.024

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 8.153092 E-01 | 1.918427 E01 | 43.2960 |
| CO2 = | 3.773534 E-01 | 8.879147 E00 | 20.0389 |
| H2 = | 3.594185 E-01 | 8.457136 E00 | 19.0865 |
| CH4 = | 1.216516 E-01 | 2.862468 E00 | 6.4602 |
| N2 = | 1.148357 E-01 | 2.702091 E00 | 6.0982 |
| CO = | 3.426680 E-02 | 8.062998 E-01 | 1.8197 |
| B2O3(l) = | 2.840215 E-02 | 6.683043 E-01 | 1.5083 |
| B(OH)3 = | 2.485066 E-02 | 5.847375 E-01 | 1.3197 |
| IH = | 6.205268 E-03 | 1.460103 E-01 | 0.3295 |
| Cu(s) = | 5.184503 E-04 | 1.219916 E-02 | 0.0275 |
| NH3 = | 2.066367 E-04 | 4.862172 E-03 | 0.0110 |
| B2O3(s) = | 7.740668 E-05 | 1.821383 E-03 | 0.0041 |
| I = | 7.569031 E-06 | 1.780997 E-04 | 0.0004 |
| I2 = | 3.865144 E-06 | 9.094705 E-05 | 0.0002 |
| BHO2 = | 4.366423 E-08 | 1.027422 E-06 | 0.0000 |
| Cu(l) = | 6.835900 E-09 | 1.608491 E-07 | 0.0000 |
| HCN = | 4.203228 E-09 | 9.890219 E-08 | 0.0000 |
| CH3OH = | 2.615958 E-09 | 6.155364 E-08 | 0.0000 |
| CHNO = | 3.953722 E-10 | 9.303129 E-09 | 0.0000 |
| Cu2O(s) = | 6.065287 E-11 | 1.427165 E-09 | 0.0000 |
| Cu2O(l) = | 6.143239 E-12 | 1.445507 E-10 | 0.0000 |
| BHO2(s) = | 5.992875 E-12 | 1.410127 E-10 | 0.0000 |
| BN(s) = | 2.167000 E-12 | 5.098963 E-11 | 0.0000 |
| BN = | 6.895685 E-13 | 1.622559 E-11 | 0.0000 |
| N = | 3.762971 E-13 | 8.854291 E-12 | 0.0000 |
| CuO = | 3.751665 E-13 | 8.827689 E-12 | 0.0000 |
| BH2 = | 3.381860 E-13 | 7.957536 E-12 | 0.0000 |
| INO = | 2.621180 E-13 | 6.167650 E-12 | 0.0000 |
| BO = | 2.592891 E-13 | 6.101086 E-12 | 0.0000 |
| CNO = | 2.360262 E-13 | 5.553709 E-12 | 0.0000 |
| BO2 = | 2.159199 E-13 | 5.080608 E-12 | 0.0000 |
| H = | 2.109317 E-13 | 4.963236 E-12 | 0.0000 |
| Cu(OH)2(s) = | 1.696771 E-13 | 3.992511 E-12 | 0.0000 |
| NO = | 1.445966 E-13 | 3.402366 E-12 | 0.0000 |
| CuO(s) = | 1.079327 E-13 | 2.539664 E-12 | 0.0000 |
| B2O3 = | 9.945375 E-14 | 2.340152 E-12 | 0.0000 |
| Cu = | 6.563002 E-14 | 1.544278 E-12 | 0.0000 |
| NH2 = | 5.662653 E-14 | 1.332425 E-12 | 0.0000 |
| ICN = | 4.210532 E-14 | 9.907405 E-13 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 30

**Combustion conditions (Number 30):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
Expansion conditions: Equilibrium expansion

**Reactant information:**

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1. **[EMIM][BH3CN], 23.00 %**
2. **AKC-266, 2.00 %**
3. **Hydrogen peroxide (H2O2), 71.25 %**
4. **Water (H2O, liqid), 3.75 %**

C(0.437) H(2.753) N(0.189) O(1.790) B(0.067) Cu(0.000) I(0.005)

Molecular weight = 40.71
Oxygen balance = -22.07894 %
Enthalpy of formation = -7277.64 kJ/kg
Internal energy of formation = -7133.61 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -2539.59 kJ/kg
- Total enthalpy of combustion prod. = -7277.66 kJ/kg
- Entropy of combustion products = 10.64 kJ/K kg
- Isobaric combustion temperature = 1633.3 K
- Mole number of gaseous products = 46.363 mol/kg expl.
- Total mole number of products = 46.373 mol/kg expl.
- Volume of gaseous products (at SATP) = 1149.29 L/kg expl.
- Mass of gaseous products = 999.3 g/kg expl.
- Mass of condensed products = 0.7 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.555 g
- Mean molecular mass of all products = 21.564 g
- Specific gas constant = 385.461 J/kg K
- Specific heat capacity at p=const. (Cp) = 2166.31 J/kgK
- Specific heat capacity at V=const. (Cv) = 1780.85 J/molK
- Specific heat ratio (Cp/Cv) = 1.2164

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 9.577479 E-01 | 2.352449 E01 | 50.7286 |
| H2 = | 3.258442 E-01 | 8.003484 E00 | 17.2588 |
| CO = | 2.331274 E-01 | 5.726145 E00 | 12.3479 |
| CO2 = | 2.042972 E-01 | 5.018009 E00 | 10.8209 |
| N2 = | 9.422822 E-02 | 2.314462 E00 | 4.9909 |
| B(OH)3 = | 5.672544 E-02 | 1.393307 E00 | 3.0045 |
| BHO2 = | 1.036462 E-02 | 2.545788 E-01 | 0.5490 |
| IH = | 4.451839 E-03 | 1.093474 E-01 | 0.2358 |
| I = | 6.343496 E-04 | 1.558109 E-02 | 0.0336 |
| Cu(l) = | 4.234877 E-04 | 1.040183 E-02 | 0.0224 |
| NH3 = | 1.076806 E-04 | 2.644883 E-03 | 0.0057 |
| CH4 = | 1.362076 E-05 | 3.345573 E-04 | 0.0007 |
| H = | 7.536628 E-06 | 1.851169 E-04 | 0.0004 |
| B2O3 = | 4.759939 E-06 | 1.169150 E-04 | 0.0003 |
| I2 = | 3.548711 E-06 | 8.716452 E-05 | 0.0002 |
| HCN = | 1.091935 E-06 | 2.682042 E-05 | 0.0001 |

| | | | |
|---|---|---|---|
| Cu = | 9.528010 E-07 | 2.340298 E-05 | 0.0001 |
| OH = | 8.716896 E-07 | 2.141070 E-05 | 0.0000 |
| CHNO = | 3.248044 E-07 | 7.977944 E-06 | 0.0000 |
| CH3OH = | 1.221448 E-08 | 3.000158 E-07 | 0.0000 |
| BO2 = | 1.128240 E-08 | 2.771217 E-07 | 0.0000 |
| NO = | 7.777005 E-09 | 1.910211 E-07 | 0.0000 |
| NH2 = | 5.026336 E-09 | 1.234584 E-07 | 0.0000 |
| BO = | 1.610800 E-09 | 3.956495 E-08 | 0.0000 |
| B2O3(l) = | 6.776139 E-11 | 1.664376 E-09 | 0.0000 |
| Cu(s) = | 6.057409 E-11 | 1.487839 E-09 | 0.0000 |
| ICN = | 2.058942 E-11 | 5.057235 E-10 | 0.0000 |
| O2 = | 1.626812 E-11 | 3.995823 E-10 | 0.0000 |
| O = | 1.419011 E-11 | 3.485417 E-10 | 0.0000 |
| B2O3(s) = | 2.852367 E-12 | 7.006069 E-11 | 0.0000 |
| CNO = | 1.012828 E-12 | 2.487737 E-11 | 0.0000 |
| BHO2(s) = | 9.689862 E-13 | 2.380053 E-11 | 0.0000 |
| CuO = | 7.322177 E-13 | 1.798495 E-11 | 0.0000 |
| BH2 = | 3.572009 E-13 | 8.773674 E-12 | 0.0000 |
| INO = | 1.748892 E-13 | 4.295681 E-12 | 0.0000 |
| Cu2O(l) = | 3.661658 E-14 | 8.993874 E-13 | 0.0000 |
| N = | 3.500300 E-14 | 8.597542 E-13 | 0.0000 |
| Cu2O(s) = | 1.682422 E-14 | 4.132415 E-13 | 0.0000 |
| BN(s) = | 1.570908 E-14 | 3.858513 E-13 | 0.0000 |
| CuO(s) = | 2.229970 E-15 | 5.477319 E-14 | 0.0000 |
| Cu(OH)2(s) = | 2.214851 E-17 | 5.440183 E-16 | 0.0000 |
| BN = | 3.597003 E-19 | 8.835066 E-18 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7626.76 kJ/kg
- Temperature at nozzle throat = 1486.8 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 46.237 mol/kg expl.
- Total mole number of products = 46.247 mol/kg expl.
- Volume of gaseous products (at SATP) = 1146.16 L/kg expl.
- Mass of gaseous products = 999.4 g/kg expl.
- Mass of condensed products = 0.7 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.614 g
- Mean molecular mass of all products = 21.623 g
- Specific gas constant = 384.411 J/kg K
- Specific heat capacity at p=const. (Cp) = 2123.62 J/kgK
- Specific heat capacity at V=const. (Cv) = 1739.21 J/molK
- Specific heat ratio (Cp/Cv) = 1.2210

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 835.6 m/s
- Sound velocity at throat) = 835.4 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.559
- Pressure ratio (pc/pt) = 1.789

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 9.369102 E-01 | 2.301267 E01 | 49.7603 |
| H2 = | 3.415503 E-01 | 8.389260 E00 | 18.1401 |
| CO2 = | 2.201044 E-01 | 5.406270 E00 | 11.6900 |

| | | | |
|---|---|---|---|
| CO = | 2.173100 E-01 | 5.337633 E00 | 11.5416 |
| N2 = | 9.423368 E-02 | 2.314596 E00 | 5.0049 |
| B(OH)3 = | 6.176316 E-02 | 1.517045 E00 | 3.2803 |
| BHO2 = | 5.334641 E-03 | 1.310311 E-01 | 0.2833 |
| IH = | 4.626293 E-03 | 1.136324 E-01 | 0.2457 |
| I = | 4.617572 E-04 | 1.134182 E-02 | 0.0245 |
| Cu(l) = | 4.241521 E-04 | 1.041815 E-02 | 0.0225 |
| NH3 = | 9.737727 E-05 | 2.391810 E-03 | 0.0052 |
| CH4 = | 2.446230 E-05 | 6.008504 E-04 | 0.0013 |
| I2 = | 2.617740 E-06 | 6.429772 E-05 | 0.0001 |
| H = | 2.016266 E-06 | 4.952413 E-05 | 0.0001 |
| B2O3 = | 8.977718 E-07 | 2.205134 E-05 | 0.0000 |
| HCN = | 6.343254 E-07 | 1.558049 E-05 | 0.0000 |
| Cu = | 2.882425 E-07 | 7.079900 E-06 | 0.0000 |
| CHNO = | 1.674850 E-07 | 4.113818 E-06 | 0.0000 |
| OH = | 1.379926 E-07 | 3.389415 E-06 | 0.0000 |
| CH3OH = | 8.321338 E-09 | 2.043912 E-07 | 0.0000 |
| NH2 = | 1.076087 E-09 | 2.643118 E-08 | 0.0000 |
| BO2 = | 9.338419 E-10 | 2.293730 E-08 | 0.0000 |
| NO = | 8.060886 E-10 | 1.979939 E-08 | 0.0000 |
| Cu(s) = | 1.675813 E-10 | 4.116182 E-09 | 0.0000 |
| B2O3(l) = | 1.459908 E-10 | 3.585870 E-09 | 0.0000 |
| BO = | 1.216654 E-10 | 2.988382 E-09 | 0.0000 |
| ICN = | 8.775298 E-12 | 2.155415 E-10 | 0.0000 |
| B2O3(s) = | 7.064207 E-12 | 1.735132 E-10 | 0.0000 |
| BHO2(s) = | 1.363248 E-12 | 3.348451 E-11 | 0.0000 |
| O2 = | 7.686671 E-13 | 1.888023 E-11 | 0.0000 |
| O = | 6.493163 E-13 | 1.594870 E-11 | 0.0000 |
| CuO = | 2.278833 E-13 | 5.597339 E-12 | 0.0000 |
| CNO = | 9.488598 E-14 | 2.330618 E-12 | 0.0000 |
| Cu2O(l) = | 4.490133 E-14 | 1.102880 E-12 | 0.0000 |
| BH2 = | 3.425627 E-14 | 8.414128 E-13 | 0.0000 |
| Cu2O(s) = | 2.880747 E-14 | 7.075776 E-13 | 0.0000 |
| BN(s) = | 2.031541 E-14 | 4.989933 E-13 | 0.0000 |
| INO = | 1.500345 E-14 | 3.685191 E-13 | 0.0000 |
| CuO(s) = | 2.808539 E-15 | 6.898417 E-14 | 0.0000 |
| N = | 2.149359 E-15 | 5.279320 E-14 | 0.0000 |
| Cu(OH)2(s) = | 1.572963 E-17 | 3.863558 E-16 | 0.0000 |
| BN = | 5.795982 E-21 | 1.423627 E-19 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9188.42 kJ/kg
- Temperature at nozzle exit = 826.2 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 45.710 mol/kg expl.
- Total mole number of products = 46.256 mol/kg expl.
- Volume of gaseous products (at SATP) = 1133.12 L/kg expl.
- Mass of gaseous products = 962.1 g/kg expl.
- Mass of condensed products = 37.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.048 g
- Mean molecular mass of all products = 21.619 g
- Specific gas constant = 380.037 J/kg K
- Specific heat capacity at p=const. (Cp) = 1905.68 J/kgK
- Specific heat capacity at V=const. (Cv) = 1525.64 J/molK
- Specific heat ratio (Cp/Cv) = 1.2491

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 199.27 s
- Exhaust (or nozzle exit) velocity = 1954.9 m/s
- Characteristic exhaust velocity (c*) = 1197.5 m/s
- Thrust coefficient (Cf) = 1.632
- Nozzle area expansion ratio (Ae/At) = 8.25
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 619.20 m/s
- Mach number at nozzle exit = 3.157

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 8.738141 E-01 | 2.146288 E01 | 46.4004 |
| H2 = | 4.267735 E-01 | 1.048254 E01 | 22.6621 |
| CO2 = | 3.620154 E-01 | 8.891931 E00 | 19.2234 |
| N2 = | 9.422047 E-02 | 2.314271 E00 | 5.0032 |
| CO = | 5.658988 E-02 | 1.389978 E00 | 3.0050 |
| B(OH)3 = | 2.353759 E-02 | 5.781375 E-01 | 1.2499 |
| B2O3(l) = | 2.178080 E-02 | 5.349866 E-01 | 1.1566 |
| CH4 = | 1.883434 E-02 | 4.626148 E-01 | 1.0001 |
| IH = | 5.064751 E-03 | 1.244019 E-01 | 0.2689 |
| Cu(s) = | 4.244783 E-04 | 1.042616 E-02 | 0.0225 |
| NH3 = | 1.246117 E-04 | 3.060750 E-03 | 0.0066 |
| I = | 2.186919 E-05 | 5.371576 E-04 | 0.0012 |
| I2 = | 3.333108 E-06 | 8.186881 E-05 | 0.0002 |
| BHO2 = | 3.712850 E-07 | 9.119613 E-06 | 0.0000 |
| B2O3(s) = | 8.682834 E-09 | 2.132704 E-07 | 0.0000 |
| HCN = | 8.016747 E-09 | 1.969098 E-07 | 0.0000 |
| Cu(l) = | 3.677190 E-09 | 9.032024 E-08 | 0.0000 |
| CH3OH = | 1.781658 E-09 | 4.376162 E-08 | 0.0000 |
| CHNO = | 8.063331 E-10 | 1.980540 E-08 | 0.0000 |
| Cu2O(s) = | 4.747975 E-11 | 1.166212 E-09 | 0.0000 |
| H = | 7.403932 E-12 | 1.818576 E-10 | 0.0000 |
| BHO2(s) = | 5.314910 E-12 | 1.305464 E-10 | 0.0000 |
| Cu2O(l) = | 4.992049 E-12 | 1.226162 E-10 | 0.0000 |
| BN(s) = | 1.650505 E-12 | 4.054019 E-11 | 0.0000 |
| BN = | 5.986586 E-13 | 1.470443 E-11 | 0.0000 |
| N = | 3.180612 E-13 | 7.812314 E-12 | 0.0000 |
| CuO = | 3.074929 E-13 | 7.552733 E-12 | 0.0000 |
| BH2 = | 2.793021 E-13 | 6.860303 E-12 | 0.0000 |
| O = | 2.619209 E-13 | 6.433380 E-12 | 0.0000 |
| O2 = | 2.601258 E-13 | 6.389287 E-12 | 0.0000 |
| INO = | 2.238393 E-13 | 5.498009 E-12 | 0.0000 |
| CNO = | 1.981865 E-13 | 4.867917 E-12 | 0.0000 |
| BO = | 1.972661 E-13 | 4.845309 E-12 | 0.0000 |
| Cu(OH)2(s) = | 1.632970 E-13 | 4.010950 E-12 | 0.0000 |
| BO2 = | 1.592987 E-13 | 3.912743 E-12 | 0.0000 |
| NO = | 1.044143 E-13 | 2.564656 E-12 | 0.0000 |
| CuO(s) = | 9.706653 E-14 | 2.384177 E-12 | 0.0000 |
| B2O3 = | 4.927622 E-14 | 1.210337 E-12 | 0.0000 |
| NH2 = | 3.259086 E-14 | 8.005065 E-13 | 0.0000 |
| ICN = | 2.995127 E-14 | 7.356720 E-13 | 0.0000 |
| Cu = | 2.364799 E-14 | 5.808491 E-13 | 0.0000 |
| OH = | 1.737912 E-14 | 4.268710 E-13 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 31

**Combustion conditions (Number 31):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 20.70 %**
2. **AKC-266, 1.80 %**
3. **Hydrogen peroxide ($H_2O_2$), 73.63 %**
4. **Water ($H_2O$, liquid), 3.87 %**

C(0.384) H(2.661) N(0.166) O(1.805) B(0.059) Cu(0.000) I(0.004)

Molecular weight = 39.72
Oxygen balance = -15.40022 %
Enthalpy of formation = -7152.73 kJ/kg
Internal energy of formation = -7008.23 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3035.87 kJ/kg
- Total enthalpy of combustion prod. = -7152.74 kJ/kg
- Entropy of combustion products = 10.79 kJ/K kg
- Isobaric combustion temperature = 1879.5 K
- Mole number of gaseous products = 45.296 mol/kg expl.
- Total mole number of products = 45.304 mol/kg expl.
- Volume of gaseous products (at SATP) = 1122.83 L/kg expl.
- Mass of gaseous products = 999.4 g/kg expl.
- Mass of condensed products = 0.6 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.065 g
- Mean molecular mass of all products = 22.073 g
- Specific gas constant = 376.587 J/kg K
- Specific heat capacity at p=const. (Cp) = 2213.39 J/kgK
- Specific heat capacity at V=const. (Cv) = 1836.80 J/molK
- Specific heat ratio (Cp/Cv) = 1.2050

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.064553 E00 | 2.680043 E01 | 59.1563 |
| CO2 = | 2.081078 E-01 | 5.239173 E00 | 11.5644 |
| H2 = | 2.043141 E-01 | 5.143665 E00 | 11.3536 |
| CO = | 1.760011 E-01 | 4.430877 E00 | 9.7802 |
| N2 = | 8.277262 E-02 | 2.083824 E00 | 4.5996 |
| B(OH)3 = | 3.045559 E-02 | 7.667279 E-01 | 1.6924 |
| BHO2 = | 2.835613 E-02 | 7.138733 E-01 | 1.5757 |
| IH = | 3.193823 E-03 | 8.040538 E-02 | 0.1775 |
| I = | 1.272693 E-03 | 3.204041 E-02 | 0.0707 |
| Cu(l) = | 3.538534 E-04 | 8.908357 E-03 | 0.0197 |
| B2O3 = | 5.343022 E-05 | 1.345120 E-03 | 0.0030 |
| H = | 5.159184 E-05 | 1.298839 E-03 | 0.0029 |
| NH3 = | 3.069077 E-05 | 7.726486 E-04 | 0.0017 |
| OH = | 1.921999 E-05 | 4.838686 E-04 | 0.0011 |
| Cu = | 1.884078 E-05 | 4.743218 E-04 | 0.0010 |
| I2 = | 2.914299 E-06 | 7.336830 E-05 | 0.0002 |

| | | | |
|---|---|---|---|
| BO2 = | 6.022038 E-07 | 1.516065 E-05 | 0.0000 |
| HCN = | 3.472215 E-07 | 8.741398 E-06 | 0.0000 |
| NO = | 3.382731 E-07 | 8.516119 E-06 | 0.0000 |
| CH4 = | 2.753768 E-07 | 6.932687 E-06 | 0.0000 |
| CHNO = | 2.161662 E-07 | 5.442044 E-06 | 0.0000 |
| BO = | 6.388362 E-08 | 1.608288 E-06 | 0.0000 |
| NH2 = | 1.836937 E-08 | 4.624541 E-07 | 0.0000 |
| O2 = | 7.075097 E-09 | 1.781175 E-07 | 0.0000 |
| O = | 3.145336 E-09 | 7.918470 E-08 | 0.0000 |
| CH3OH = | 1.493690 E-09 | 3.760406 E-08 | 0.0000 |
| CuO = | 1.180466 E-09 | 2.971856 E-08 | 0.0000 |
| Cu(s) = | 5.410623 E-11 | 1.362139 E-09 | 0.0000 |
| ICN = | 1.871046 E-11 | 4.710411 E-10 | 0.0000 |
| CNO = | 1.055996 E-11 | 2.658500 E-10 | 0.0000 |
| B2O3(l) = | 1.016297 E-11 | 2.558556 E-10 | 0.0000 |
| INO = | 7.811538 E-12 | 1.966576 E-10 | 0.0000 |
| N = | 4.351567 E-12 | 1.095519 E-10 | 0.0000 |
| BH2 = | 4.230195 E-12 | 1.064963 E-10 | 0.0000 |
| B2O3(s) = | 5.484714 E-13 | 1.380792 E-11 | 0.0000 |
| Cu2O(l) = | 2.665278 E-13 | 6.709912 E-12 | 0.0000 |
| BHO2(s) = | 2.642529 E-13 | 6.652642 E-12 | 0.0000 |
| Cu2O(s) = | 3.852444 E-14 | 9.698634 E-13 | 0.0000 |
| CuO(s) = | 1.511548 E-14 | 3.805365 E-13 | 0.0000 |
| BN(s) = | 8.934731 E-16 | 2.249343 E-14 | 0.0000 |
| Cu(OH)2(s) = | 1.205710 E-16 | 3.035409 E-15 | 0.0000 |
| BN = | 9.956390 E-17 | 2.506549 E-15 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7542.50 kJ/kg
- Temperature at nozzle throat = 1720.6 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 45.111 mol/kg expl.
- Total mole number of products = 45.120 mol/kg expl.
- Volume of gaseous products (at SATP) = 1118.25 L/kg expl.
- Mass of gaseous products = 999.4 g/kg expl.
- Mass of condensed products = 0.6 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.155 g
- Mean molecular mass of all products = 22.163 g
- Specific gas constant = 375.051 J/kg K
- Specific heat capacity at p=const. (Cp) = 2171.60 J/kgK
- Specific heat capacity at V=const. (Cv) = 1796.55 J/molK
- Specific heat ratio (Cp/Cv) = 1.2088

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 882.9 m/s
- Sound velocity at throat) = 883.2 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.562
- Pressure ratio (pc/pt) = 1.781

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.047585 E00 | 2.637323 E01 | 58.4514 |
| CO2 = | 2.178565 E-01 | 5.484599 E00 | 12.1556 |
| H2 = | 2.139737 E-01 | 5.386847 E00 | 11.9390 |

| | | | |
|---|---|---|---|
| CO = | 1.662526 E-01 | 4.185454 E00 | 9.2763 |
| N2 = | 8.277532 E-02 | 2.083892 E00 | 4.6186 |
| B(OH)3 = | 3.765955 E-02 | 9.480897 E-01 | 2.1013 |
| BHO2 = | 2.121467 E-02 | 5.340852 E-01 | 1.1837 |
| IH = | 3.404067 E-03 | 8.569832 E-02 | 0.1899 |
| I = | 1.062969 E-03 | 2.676054 E-02 | 0.0593 |
| Cu(l) = | 3.640998 E-04 | 9.166313 E-03 | 0.0203 |
| NH3 = | 2.580988 E-05 | 6.497709 E-04 | 0.0014 |
| B2O3 = | 2.245091 E-05 | 5.652080 E-04 | 0.0013 |
| H = | 1.846783 E-05 | 4.649328 E-04 | 0.0010 |
| Cu = | 8.595396 E-06 | 2.163915 E-04 | 0.0005 |
| OH = | 4.489682 E-06 | 1.130290 E-04 | 0.0003 |
| I2 = | 2.654732 E-06 | 6.683362 E-05 | 0.0001 |
| CH4 = | 3.752352 E-07 | 9.446650 E-06 | 0.0000 |
| HCN = | 2.060515 E-07 | 5.187404 E-06 | 0.0000 |
| CHNO = | 1.112859 E-07 | 2.801655 E-06 | 0.0000 |
| BO2 = | 1.070111 E-07 | 2.694035 E-06 | 0.0000 |
| NO = | 5.686524 E-08 | 1.431598 E-06 | 0.0000 |
| BO = | 1.044600 E-08 | 2.629810 E-07 | 0.0000 |
| NH2 = | 4.905369 E-09 | 1.234940 E-07 | 0.0000 |
| CH3OH = | 8.985493 E-10 | 2.262123 E-08 | 0.0000 |
| O2 = | 5.716019 E-10 | 1.439024 E-08 | 0.0000 |
| O = | 2.828970 E-10 | 7.122010 E-09 | 0.0000 |
| CuO = | 1.348953 E-10 | 3.396027 E-09 | 0.0000 |
| Cu(s) = | 1.225720 E-10 | 3.085784 E-09 | 0.0000 |
| B2O3(l) = | 2.982298 E-11 | 7.508018 E-10 | 0.0000 |
| ICN = | 7.358433 E-12 | 1.852506 E-10 | 0.0000 |
| B2O3(s) = | 2.002012 E-12 | 5.040121 E-11 | 0.0000 |
| CNO = | 1.450357 E-12 | 3.651314 E-11 | 0.0000 |
| INO = | 9.797741 E-13 | 2.466609 E-11 | 0.0000 |
| BH2 = | 6.415264 E-13 | 1.615061 E-11 | 0.0000 |
| BHO2(s) = | 5.351123 E-13 | 1.347160 E-11 | 0.0000 |
| N = | 3.776656 E-13 | 9.507835 E-12 | 0.0000 |
| Cu2O(l) = | 3.240205 E-13 | 8.157306 E-12 | 0.0000 |
| Cu2O(s) = | 1.019396 E-13 | 2.566359 E-12 | 0.0000 |
| CuO(s) = | 1.376404 E-14 | 3.465135 E-13 | 0.0000 |
| BN(s) = | 4.505197 E-15 | 1.134196 E-13 | 0.0000 |
| Cu(OH)2(s) = | 6.779061 E-17 | 1.706647 E-15 | 0.0000 |
| BN = | 3.334112 E-18 | 8.393721 E-17 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9324.88 kJ/kg
- Temperature at nozzle exit = 936.0 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 45.005 mol/kg expl.
- Total mole number of products = 45.466 mol/kg expl.
- Volume of gaseous products (at SATP) = 1115.63 L/kg expl.
- Mass of gaseous products = 968.0 g/kg expl.
- Mass of condensed products = 32.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.508 g
- Mean molecular mass of all products = 21.995 g
- Specific gas constant = 374.171 J/kg K
- Specific heat capacity at p=const. (Cp) = 1921.47 J/kgK
- Specific heat capacity at V=const. (Cv) = 1547.30 J/molK
- Specific heat ratio (Cp/Cv) = 1.2418

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 212.47 s
- Exhaust (or nozzle exit) velocity = 2084.3 m/s
- Characteristic exhaust velocity (c*) = 1277.3 m/s
- Thrust coefficient (Cf) = 1.632
- Nozzle area expansion ratio (Ae/At) = 8.36
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 650.64 m/s
- Mach number at nozzle exit = 3.203

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 9.752641 E-01 | 2.455254 E01 | 54.0016 |
| CO2 = | 3.229561 E-01 | 8.130510 E00 | 17.8825 |
| H2 = | 3.180030 E-01 | 8.005814 E00 | 17.6082 |
| N2 = | 8.277244 E-02 | 2.083819 E00 | 4.5832 |
| CO = | 6.096569 E-02 | 1.534828 E00 | 3.3757 |
| B(OH)3 = | 2.300340 E-02 | 5.791169 E-01 | 1.2737 |
| B2O3(l) = | 1.795330 E-02 | 4.519792 E-01 | 0.9941 |
| IH = | 4.414957 E-03 | 1.111478 E-01 | 0.2445 |
| Cu(s) = | 3.727266 E-04 | 9.383496 E-03 | 0.0206 |
| CH4 = | 1.879883 E-04 | 4.732657 E-03 | 0.0104 |
| I = | 5.300685 E-05 | 1.334462 E-03 | 0.0029 |
| NH3 = | 3.196256 E-05 | 8.046663 E-04 | 0.0018 |
| BHO2 = | 9.251751 E-06 | 2.329154 E-04 | 0.0005 |
| I2 = | 2.190682 E-06 | 5.515104 E-05 | 0.0001 |
| HCN = | 4.154618 E-09 | 1.045937 E-07 | 0.0000 |
| Cu(l) = | 2.360145 E-09 | 5.941731 E-08 | 0.0000 |
| CHNO = | 8.278873 E-10 | 2.084229 E-08 | 0.0000 |
| Cu2O(s) = | 3.363133 E-10 | 8.466780 E-09 | 0.0000 |
| H = | 2.054641 E-10 | 5.172615 E-09 | 0.0000 |
| CH3OH = | 1.780047 E-10 | 4.481318 E-09 | 0.0000 |
| Cu2O(l) = | 4.144360 E-11 | 1.043354 E-09 | 0.0000 |
| BN(s) = | 2.269285 E-11 | 5.712987 E-10 | 0.0000 |
| B2O3(s) = | 1.628344 E-11 | 4.099401 E-10 | 0.0000 |
| BN = | 5.048635 E-12 | 1.271008 E-10 | 0.0000 |
| BHO2(s) = | 2.761328 E-12 | 6.951720 E-11 | 0.0000 |
| N = | 2.607004 E-12 | 6.563204 E-11 | 0.0000 |
| BH2 = | 2.350805 E-12 | 5.918217 E-11 | 0.0000 |
| CuO = | 2.321259 E-12 | 5.843834 E-11 | 0.0000 |
| O = | 1.960877 E-12 | 4.936562 E-11 | 0.0000 |
| O2 = | 1.911287 E-12 | 4.811718 E-11 | 0.0000 |
| INO = | 1.887163 E-12 | 4.750986 E-11 | 0.0000 |
| CNO = | 1.745554 E-12 | 4.394480 E-11 | 0.0000 |
| Cu(OH)2(s) = | 1.702277 E-12 | 4.285529 E-11 | 0.0000 |
| BO = | 1.383930 E-12 | 3.484081 E-11 | 0.0000 |
| Cu = | 1.082055 E-12 | 2.724103 E-11 | 0.0000 |
| OH = | 1.067891 E-12 | 2.688445 E-11 | 0.0000 |
| BO2 = | 1.022332 E-12 | 2.573750 E-11 | 0.0000 |
| CuO(s) = | 9.877138 E-13 | 2.486597 E-11 | 0.0000 |
| NO = | 6.640539 E-13 | 1.671774 E-11 | 0.0000 |
| ICN = | 4.747695 E-13 | 1.195245 E-11 | 0.0000 |
| NH2 = | 2.723863 E-13 | 6.857400 E-12 | 0.0000 |
| B2O3 = | 4.024534 E-14 | 1.013188 E-12 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity : Model 1: Condensed products form pure phase (Default)

# Calculation Number 32

**Combustion conditions (Number 32):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 18.40 %**
2. **AKC-266, 1.60 %**
3. **Hydrogen peroxide ($H_2O_2$), 76.00 %**
4. **Water ($H_2O$, liquid), 4.00 %**

C(0.333) H(2.573) N(0.144) O(1.819) B(0.051) Cu(0.000) I(0.004)

Molecular weight = 38.77
Oxygen balance = -8.726208 %
Enthalpy of formation = -7028.86 kJ/kg
Internal energy of formation = -6883.88 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3571.42 kJ/kg
- Total enthalpy of combustion prod. = -7028.86 kJ/kg
- Entropy of combustion products = 10.87 kJ/K kg
- Isobaric combustion temperature = 2138.0 K
- Mole number of gaseous products = 44.080 mol/kg expl.
- Total mole number of products = 44.084 mol/kg expl.
- Volume of gaseous products (at SATP) = 1092.71 L/kg expl.
- Mass of gaseous products = 999.8 g/kg expl.
- Mass of condensed products = 0.2 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.680 g
- Mean molecular mass of all products = 22.684 g
- Specific gas constant = 366.485 J/kg K
- Specific heat capacity at p=const. (Cp) = 2259.23 J/kgK
- Specific heat capacity at V=const. (Cv) = 1892.74 J/molK
- Specific heat ratio (Cp/Cv) = 1.1936

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.146587 E00 | 2.957148 E01 | 67.0795 |
| CO2 = | 2.249712 E-01 | 5.802201 E00 | 13.1616 |
| CO = | 1.083102 E-01 | 2.793413 E00 | 6.3365 |
| H2 = | 1.019444 E-01 | 2.629234 E00 | 5.9641 |
| N2 = | 7.182478 E-02 | 1.852423 E00 | 4.2020 |
| BHO2 = | 3.926094 E-02 | 1.012574 E00 | 2.2969 |
| B(OH)3 = | 1.156872 E-02 | 2.983673 E-01 | 0.6768 |
| I = | 2.012413 E-03 | 5.190186 E-02 | 0.1177 |
| IH = | 1.862837 E-03 | 4.804417 E-02 | 0.1090 |
| OH = | 2.519606 E-04 | 6.498283 E-03 | 0.0147 |
| H = | 2.056160 E-04 | 5.303015 E-03 | 0.0120 |
| Cu = | 1.745179 E-04 | 4.500967 E-03 | 0.0102 |
| Cu(l) = | 1.487264 E-04 | 3.835782 E-03 | 0.0087 |
| B2O3 = | 1.407453 E-04 | 3.629942 E-03 | 0.0082 |

| | | | |
|---|---|---|---|
| BO2 = | 1.081880 E-05 | 2.790263 E-04 | 0.0006 |
| NO = | 9.737617 E-06 | 2.511416 E-04 | 0.0006 |
| NH3 = | 6.975814 E-06 | 1.799123 E-04 | 0.0004 |
| I2 = | 2.641005 E-06 | 6.811381 E-05 | 0.0002 |
| O2 = | 1.516891 E-06 | 3.912194 E-05 | 0.0001 |
| BO = | 6.305092 E-07 | 1.626138 E-05 | 0.0000 |
| O = | 3.224462 E-07 | 8.316166 E-06 | 0.0000 |
| CuO = | 1.333253 E-07 | 3.438575 E-06 | 0.0000 |
| CHNO = | 1.026684 E-07 | 2.647907 E-06 | 0.0000 |
| HCN = | 6.858356 E-08 | 1.768829 E-06 | 0.0000 |
| NH2 = | 3.481058 E-08 | 8.977950 E-07 | 0.0000 |
| CH4 = | 3.516211 E-09 | 9.068611 E-08 | 0.0000 |
| INO = | 1.803274 E-10 | 4.650800 E-09 | 0.0000 |
| N = | 1.667486 E-10 | 4.300590 E-09 | 0.0000 |
| CH3OH = | 1.198498 E-10 | 3.091031 E-09 | 0.0000 |
| CNO = | 4.641345 E-11 | 1.197043 E-09 | 0.0000 |
| Cu(s) = | 3.314114 E-11 | 8.547386 E-10 | 0.0000 |
| ICN = | 8.508069 E-12 | 2.194305 E-10 | 0.0000 |
| BH2 = | 7.807885 E-12 | 2.013721 E-10 | 0.0000 |
| B2O3(l) = | 1.723147 E-12 | 4.444146 E-11 | 0.0000 |
| Cu2O(l) = | 1.512821 E-12 | 3.901697 E-11 | 0.0000 |
| Cu2O(s) = | 1.933088 E-13 | 4.985600 E-12 | 0.0000 |
| BHO2(s) = | 1.064239 E-13 | 2.744763 E-12 | 0.0000 |
| B2O3(s) = | 1.050187 E-13 | 2.708523 E-12 | 0.0000 |
| CuO(s) = | 5.913632 E-14 | 1.525177 E-12 | 0.0000 |
| BN = | 1.950690 E-15 | 5.030999 E-14 | 0.0000 |
| Cu(OH)2(s) = | 2.810333 E-16 | 7.248091 E-15 | 0.0000 |
| BN(s) = | 2.281841 E-16 | 5.885065 E-15 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7457.27 kJ/kg
- Temperature at nozzle throat = 1957.5 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 43.977 mol/kg expl.
- Total mole number of products = 43.982 mol/kg expl.
- Volume of gaseous products (at SATP) = 1090.15 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.731 g
- Mean molecular mass of all products = 22.736 g
- Specific gas constant = 365.626 J/kg K
- Specific heat capacity at p=const. (Cp) = 2216.57 J/kgK
- Specific heat capacity at V=const. (Cv) = 1850.95 J/molK
- Specific heat ratio (Cp/Cv) = 1.1975

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 925.7 m/s
- Sound velocity at throat) = 925.8 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.564
- Pressure ratio (pc/pt) = 1.772

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.137477 E00 | 2.933651 E01 | 66.7005 |

| | | | |
|---|---|---|---|
| CO2 = | 2.305236 E-01 | 5.945402 E00 | 13.5177 |
| H2 = | 1.073590 E-01 | 2.768882 E00 | 6.2954 |
| CO = | 1.027578 E-01 | 2.650214 E00 | 6.0256 |
| N2 = | 7.182935 E-02 | 1.852541 E00 | 4.2120 |
| BHO2 = | 3.567459 E-02 | 9.200785 E-01 | 2.0919 |
| B(OH)3 = | 1.526288 E-02 | 3.936428 E-01 | 0.8950 |
| IH = | 2.057575 E-03 | 5.306665 E-02 | 0.1207 |
| I = | 1.818548 E-03 | 4.690192 E-02 | 0.1066 |
| Cu(l) = | 2.080719 E-04 | 5.366354 E-03 | 0.0122 |
| Cu = | 1.152805 E-04 | 2.973185 E-03 | 0.0068 |
| B2O3 = | 9.108279 E-05 | 2.349104 E-03 | 0.0053 |
| H = | 8.628860 E-05 | 2.225458 E-03 | 0.0051 |
| OH = | 7.667626 E-05 | 1.977547 E-03 | 0.0045 |
| NH3 = | 5.634452 E-06 | 1.453174 E-04 | 0.0003 |
| BO2 = | 2.815501 E-06 | 7.261422 E-05 | 0.0002 |
| I2 = | 2.204288 E-06 | 5.685048 E-05 | 0.0001 |
| NO = | 2.041687 E-06 | 5.265688 E-05 | 0.0001 |
| O2 = | 1.775463 E-07 | 4.579074 E-06 | 0.0000 |
| BO = | 1.560318 E-07 | 4.024195 E-06 | 0.0000 |
| CHNO = | 5.246061 E-08 | 1.353004 E-06 | 0.0000 |
| O = | 4.198143 E-08 | 1.082737 E-06 | 0.0000 |
| HCN = | 4.018731 E-08 | 1.036466 E-06 | 0.0000 |
| CuO = | 2.504439 E-08 | 6.459165 E-07 | 0.0000 |
| NH2 = | 1.114797 E-08 | 2.875158 E-07 | 0.0000 |
| CH4 = | 4.406280 E-09 | 1.136418 E-07 | 0.0000 |
| Cu(s) = | 1.050238 E-10 | 2.708656 E-09 | 0.0000 |
| CH3OH = | 6.664290 E-11 | 1.718778 E-09 | 0.0000 |
| INO = | 3.015340 E-11 | 7.776822 E-10 | 0.0000 |
| N = | 1.974173 E-11 | 5.091562 E-10 | 0.0000 |
| CNO = | 8.968599 E-12 | 2.313079 E-10 | 0.0000 |
| B2O3(l) = | 4.315364 E-12 | 1.112970 E-10 | 0.0000 |
| ICN = | 3.175660 E-12 | 8.190302 E-11 | 0.0000 |
| Cu2O(l) = | 2.249554 E-12 | 5.801796 E-11 | 0.0000 |
| BH2 = | 1.568261 E-12 | 4.044680 E-11 | 0.0000 |
| Cu2O(s) = | 4.084641 E-13 | 1.053464 E-11 | 0.0000 |
| B2O3(s) = | 2.898474 E-13 | 7.475414 E-12 | 0.0000 |
| BHO2(s) = | 1.606563 E-13 | 4.143465 E-12 | 0.0000 |
| CuO(s) = | 6.781077 E-14 | 1.748898 E-12 | 0.0000 |
| BN(s) = | 5.044309 E-16 | 1.300971 E-14 | 0.0000 |
| Cu(OH)2(s) = | 3.126456 E-16 | 8.063400 E-15 | 0.0000 |
| BN = | 1.525511 E-16 | 3.934425 E-15 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9453.03 kJ/kg
- Temperature at nozzle exit = 1102.7 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 43.406 mol/kg expl.
- Total mole number of products = 43.786 mol/kg expl.
- Volume of gaseous products (at SATP) = 1076.00 L/kg expl.
- Mass of gaseous products = 973.6 g/kg expl.
- Mass of condensed products = 26.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.431 g
- Mean molecular mass of all products = 22.839 g
- Specific gas constant = 360.880 J/kg K
- Specific heat capacity at p=const. (Cp) = 1954.75 J/kgK
- Specific heat capacity at V=const. (Cv) = 1593.88 J/molK
- Specific heat ratio (Cp/Cv) = 1.2264

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 224.45 s
- Exhaust (or nozzle exit) velocity = 2201.9 m/s
- Characteristic exhaust velocity (c*) = 1343.9 m/s
- Thrust coefficient (Cf) = 1.638
- Nozzle area expansion ratio (Ae/At) = 8.61
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 690.33 m/s
- Mach number at nozzle exit = 3.190

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.089588 E00 | 2.810142 E01 | 64.1791 |
| CO2 = | 2.860219 E-01 | 7.376751 E00 | 16.8473 |
| H2 = | 1.620990 E-01 | 4.180674 E00 | 9.5480 |
| N2 = | 7.183129 E-02 | 1.852591 E00 | 4.2310 |
| CO = | 4.725941 E-02 | 1.218861 E00 | 2.7837 |
| B(OH)3 = | 2.203897 E-02 | 5.684042 E-01 | 1.2981 |
| B2O3(l) = | 1.439757 E-02 | 3.713259 E-01 | 0.8480 |
| IH = | 3.580187 E-03 | 9.233611 E-02 | 0.2109 |
| I = | 2.938691 E-04 | 7.579137 E-03 | 0.0173 |
| BHO2 = | 2.884927 E-04 | 7.440476 E-03 | 0.0170 |
| Cu(s) = | 2.631375 E-04 | 6.786543 E-03 | 0.0155 |
| Cu(l) = | 6.025188 E-05 | 1.553948 E-03 | 0.0035 |
| NH3 = | 3.895173 E-06 | 1.004599 E-04 | 0.0002 |
| I2 = | 3.237921 E-06 | 8.350877 E-05 | 0.0002 |
| CH4 = | 2.397693 E-07 | 6.183857 E-06 | 0.0000 |
| H = | 1.478843 E-08 | 3.814065 E-07 | 0.0000 |
| HCN = | 1.127256 E-09 | 2.907291 E-08 | 0.0000 |
| Cu = | 5.293651 E-10 | 1.365278 E-08 | 0.0000 |
| B2O3 = | 5.073515 E-10 | 1.308504 E-08 | 0.0000 |
| CHNO = | 4.825234 E-10 | 1.244470 E-08 | 0.0000 |
| B2O3(s) = | 4.646168 E-10 | 1.198287 E-08 | 0.0000 |
| OH = | 3.595117 E-10 | 9.272118 E-09 | 0.0000 |
| Cu2O(l) = | 2.994370 E-10 | 7.722739 E-09 | 0.0000 |
| Cu2O(s) = | 2.936278 E-10 | 7.572914 E-09 | 0.0000 |
| BN(s) = | 2.439704 E-10 | 6.292208 E-09 | 0.0000 |
| BHO2(s) = | 6.088659 E-11 | 1.570318 E-09 | 0.0000 |
| BN = | 4.004335 E-11 | 1.032753 E-09 | 0.0000 |
| N = | 1.923386 E-11 | 4.960578 E-10 | 0.0000 |
| BH2 = | 1.902002 E-11 | 4.905428 E-10 | 0.0000 |
| Cu(OH)2(s) = | 1.724479 E-11 | 4.447581 E-10 | 0.0000 |
| CNO = | 1.476752 E-11 | 3.808670 E-10 | 0.0000 |
| CuO = | 1.426936 E-11 | 3.680191 E-10 | 0.0000 |
| INO = | 1.392428 E-11 | 3.591193 E-10 | 0.0000 |
| O = | 1.147082 E-11 | 2.958425 E-10 | 0.0000 |
| O2 = | 1.028984 E-11 | 2.653839 E-10 | 0.0000 |
| CuO(s) = | 9.566041 E-12 | 2.467165 E-10 | 0.0000 |
| BO = | 7.041103 E-12 | 1.815961 E-10 | 0.0000 |
| ICN = | 6.766146 E-12 | 1.745048 E-10 | 0.0000 |
| CH3OH = | 6.027285 E-12 | 1.554489 E-10 | 0.0000 |
| BO2 = | 3.279416 E-12 | 8.457897 E-11 | 0.0000 |
| NH2 = | 2.141925 E-12 | 5.524210 E-11 | 0.0000 |
| NO = | 1.679721 E-12 | 4.332145 E-11 | 0.0000 |

Notes:

- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 33

**Combustion conditions (Number 33):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 16.87 %**
2. **AKC-266, 1.47 %**
3. **Hydrogen peroxide ($H_2O_2$), 77.58 %**
4. **Water ($H_2O$, liquid), 4.08 %**

C(0.301) H(2.518) N(0.130) O(1.828) B(0.046) Cu(0.000) I(0.004)

Molecular weight = 38.17
Oxygen balance = -4.286098 %
Enthalpy of formation = -6946.03 kJ/kg
Internal energy of formation = -6800.74 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3957.66 kJ/kg
- Total enthalpy of combustion prod. = -6946.74 kJ/kg
- Entropy of combustion products = 10.88 kJ/K kg
- Isobaric combustion temperature = 2319.0 K
- Mole number of gaseous products = 43.125 mol/kg expl.
- Total mole number of products = 43.125 mol/kg expl.
- Volume of gaseous products (at SATP) = 1069.03 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.188 g
- Mean molecular mass of all products = 23.188 g
- Specific gas constant = 358.542 J/kg K
- Specific heat capacity at p=const. (Cp) = 2289.35 J/kgK
- Specific heat capacity at V=const. (Cv) = 1930.80 J/molK
- Specific heat ratio (Cp/Cv) = 1.1857

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.183305 E00 | 3.099999 E01 | 71.8838 |
| CO2 = | 2.440843 E-01 | 6.394472 E00 | 14.8277 |
| N2 = | 6.479085 E-02 | 1.697378 E00 | 3.9359 |
| CO = | 5.674250 E-02 | 1.486529 E00 | 3.4470 |
| H2 = | 4.548153 E-02 | 1.191516 E00 | 2.7629 |
| BHO2 = | 4.003869 E-02 | 1.048926 E00 | 2.4323 |
| B(OH)3 = | 5.687869 E-03 | 1.490096 E-01 | 0.3455 |
| I = | 2.439216 E-03 | 6.390207 E-02 | 0.1482 |
| OH = | 1.427373 E-03 | 3.739404 E-02 | 0.0867 |
| IH = | 1.067450 E-03 | 2.796484 E-02 | 0.0648 |
| H = | 3.657154 E-04 | 9.580938 E-03 | 0.0222 |
| Cu = | 2.912198 E-04 | 7.629317 E-03 | 0.0177 |
| B2O3 = | 1.830767 E-04 | 4.796207 E-03 | 0.0111 |
| NO = | 9.452954 E-05 | 2.476466 E-03 | 0.0057 |

| | | | |
|---|---|---|---|
| O2 = | 6.586618 E-05 | 1.725549 E-03 | 0.0040 |
| BO2 = | 5.656974 E-05 | 1.482003 E-03 | 0.0034 |
| O = | 7.245222 E-06 | 1.898089 E-04 | 0.0004 |
| NH3 = | 1.602389 E-06 | 4.197907 E-05 | 0.0001 |
| I2 = | 1.595825 E-06 | 4.180711 E-05 | 0.0001 |
| BO = | 1.574919 E-06 | 4.125940 E-05 | 0.0001 |
| CuO = | 1.268373 E-06 | 3.322859 E-05 | 0.0001 |
| CHNO = | 3.704807 E-08 | 9.705778 E-07 | 0.0000 |
| NH2 = | 3.529359 E-08 | 9.246144 E-07 | 0.0000 |
| HCN = | 1.010709 E-08 | 2.647834 E-07 | 0.0000 |
| INO = | 1.476902 E-09 | 3.869158 E-08 | 0.0000 |
| N = | 1.376345 E-09 | 3.605722 E-08 | 0.0000 |
| CNO = | 9.253495 E-11 | 2.424212 E-09 | 0.0000 |
| CH4 = | 6.879678 E-11 | 1.802324 E-09 | 0.0000 |
| Cu(l) = | 3.052769 E-11 | 7.997582 E-10 | 0.0000 |
| Cu(s) = | 1.360701 E-11 | 3.564736 E-10 | 0.0000 |
| CH3OH = | 8.807679 E-12 | 2.307418 E-10 | 0.0000 |
| BH2 = | 3.056399 E-12 | 8.007092 E-11 | 0.0000 |
| ICN = | 1.953273 E-12 | 5.117146 E-11 | 0.0000 |
| Cu2O(l) = | 1.183919 E-12 | 3.101607 E-11 | 0.0000 |
| B2O3(l) = | 4.361773 E-13 | 1.142688 E-11 | 0.0000 |
| Cu2O(s) = | 1.234374 E-13 | 3.233788 E-12 | 0.0000 |
| CuO(s) = | 1.044587 E-13 | 2.736588 E-12 | 0.0000 |
| BHO2(s) = | 4.013967 E-14 | 1.051571 E-12 | 0.0000 |
| B2O3(s) = | 2.563193 E-14 | 6.715001 E-13 | 0.0000 |
| BN = | 7.217918 E-15 | 1.890936 E-13 | 0.0000 |
| Cu(OH)2(s) = | 7.507520 E-16 | 1.966805 E-14 | 0.0000 |
| BN(s) = | 4.280868 E-17 | 1.121493 E-15 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7399.45 kJ/kg
- Temperature at nozzle throat = 2127.9 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 43.067 mol/kg expl.
- Total mole number of products = 43.067 mol/kg expl.
- Volume of gaseous products (at SATP) = 1067.60 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.219 g
- Mean molecular mass of all products = 23.219 g
- Specific gas constant = 358.062 J/kg K
- Specific heat capacity at p=const. (Cp) = 2247.96 J/kgK
- Specific heat capacity at V=const. (Cv) = 1889.90 J/molK
- Specific heat ratio (Cp/Cv) = 1.1895

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 951.5 m/s
- Sound velocity at throat) = 952.0 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.566
- Pressure ratio (pc/pt) = 1.767

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.180001 E00 | 3.091342 E01 | 71.7792 |

| | | | |
|---|---|---|---|
| CO2 = | 2.469851 E-01 | 6.470467 E00 | 15.0241 |
| N2 = | 6.482600 E-02 | 1.698299 E00 | 3.9434 |
| CO = | 5.384172 E-02 | 1.410534 E00 | 3.2752 |
| H2 = | 4.775446 E-02 | 1.251062 E00 | 2.9049 |
| BHO2 = | 3.869901 E-02 | 1.013829 E00 | 2.3541 |
| B(OH)3 = | 7.163664 E-03 | 1.876722 E-01 | 0.4358 |
| I = | 2.335106 E-03 | 6.117465 E-02 | 0.1420 |
| IH = | 1.171267 E-03 | 3.068461 E-02 | 0.0712 |
| OH = | 4.917813 E-04 | 1.288359 E-02 | 0.0299 |
| Cu = | 2.920462 E-04 | 7.650968 E-03 | 0.0178 |
| H = | 1.748854 E-04 | 4.581612 E-03 | 0.0106 |
| B2O3 = | 1.344185 E-04 | 3.521468 E-03 | 0.0082 |
| NO = | 2.462274 E-05 | 6.450616 E-04 | 0.0015 |
| BO2 = | 1.884012 E-05 | 4.935696 E-04 | 0.0011 |
| O2 = | 1.135987 E-05 | 2.976036 E-04 | 0.0007 |
| I2 = | 1.742657 E-06 | 4.565378 E-05 | 0.0001 |
| NH3 = | 1.255265 E-06 | 3.288518 E-05 | 0.0001 |
| O = | 1.174417 E-06 | 3.076715 E-05 | 0.0001 |
| BO = | 5.011375 E-07 | 1.312870 E-05 | 0.0000 |
| CuO = | 4.418144 E-07 | 1.157457 E-05 | 0.0000 |
| CHNO = | 1.923005 E-08 | 5.037851 E-07 | 0.0000 |
| NH2 = | 1.200257 E-08 | 3.144409 E-07 | 0.0000 |
| HCN = | 5.904202 E-09 | 1.546771 E-07 | 0.0000 |
| INO = | 3.127578 E-10 | 8.193566 E-09 | 0.0000 |
| N = | 2.005348 E-10 | 5.253570 E-09 | 0.0000 |
| Cu(l) = | 1.304018 E-10 | 3.416240 E-09 | 0.0000 |
| CH4 = | 6.861210 E-11 | 1.797486 E-09 | 0.0000 |
| Cu(s) = | 3.791800 E-11 | 9.933682 E-10 | 0.0000 |
| CNO = | 1.826003 E-11 | 4.783726 E-10 | 0.0000 |
| CH3OH = | 4.592226 E-12 | 1.203062 E-10 | 0.0000 |
| Cu2O(l) = | 3.267663 E-12 | 8.560559 E-11 | 0.0000 |
| B2O3(l) = | 1.014598 E-12 | 2.658024 E-11 | 0.0000 |
| ICN = | 8.547979 E-13 | 2.239382 E-11 | 0.0000 |
| BH2 = | 7.916768 E-13 | 2.074019 E-11 | 0.0000 |
| Cu2O(s) = | 4.353072 E-13 | 1.140409 E-11 | 0.0000 |
| CuO(s) = | 1.453941 E-13 | 3.809006 E-12 | 0.0000 |
| BHO2(s) = | 6.506346 E-14 | 1.704519 E-12 | 0.0000 |
| B2O3(s) = | 6.374519 E-14 | 1.669983 E-12 | 0.0000 |
| Cu(OH)2(s) = | 6.480361 E-16 | 1.697712 E-14 | 0.0000 |
| BN = | 6.345837 E-16 | 1.662470 E-14 | 0.0000 |
| BN(s) = | 6.207301 E-17 | 1.626176 E-15 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9530.91 kJ/kg
- Temperature at nozzle exit = 1219.0 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 42.367 mol/kg expl.
- Total mole number of products = 42.687 mol/kg expl.
- Volume of gaseous products (at SATP) = 1050.23 L/kg expl.
- Mass of gaseous products = 977.8 g/kg expl.
- Mass of condensed products = 22.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.078 g
- Mean molecular mass of all products = 23.427 g
- Specific gas constant = 352.237 J/kg K
- Specific heat capacity at p=const. (Cp) = 1980.61 J/kgK
- Specific heat capacity at V=const. (Cv) = 1628.37 J/molK
- Specific heat ratio (Cp/Cv) = 1.2163

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 231.74 s
- Exhaust (or nozzle exit) velocity = 2273.4 m/s
- Characteristic exhaust velocity (c*) = 1386.8 m/s
- Thrust coefficient (Cf) = 1.639
- Nozzle area expansion ratio (Ae/At) = 8.78
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 714.66 m/s
- Mach number at nozzle exit = 3.181

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.152285 E00 | 3.018734 E01 | 70.7177 |
| CO2 = | 2.736643 E-01 | 7.169401 E00 | 16.7953 |
| H2 = | 7.345009 E-02 | 1.924231 E00 | 4.5078 |
| N2 = | 6.483863 E-02 | 1.698629 E00 | 3.9793 |
| CO = | 2.716261 E-02 | 7.116006 E-01 | 1.6670 |
| B(OH)3 = | 2.054319 E-02 | 5.381863 E-01 | 1.2608 |
| B2O3(l) = | 1.193753 E-02 | 3.127369 E-01 | 0.7326 |
| IH = | 2.706880 E-03 | 7.091428 E-02 | 0.1661 |
| BHO2 = | 1.732578 E-03 | 4.538973 E-02 | 0.1063 |
| I = | 7.978418 E-04 | 2.090170 E-02 | 0.0490 |
| Cu(l) = | 1.470828 E-04 | 3.853245 E-03 | 0.0090 |
| Cu(s) = | 1.453975 E-04 | 3.809095 E-03 | 0.0089 |
| I2 = | 2.568924 E-06 | 6.730014 E-05 | 0.0002 |
| NH3 = | 6.574083 E-07 | 1.722265 E-05 | 0.0000 |
| H = | 1.017996 E-07 | 2.666926 E-06 | 0.0000 |
| B2O3 = | 2.834492 E-08 | 7.425746 E-07 | 0.0000 |
| Cu = | 1.674447 E-08 | 4.386682 E-07 | 0.0000 |
| OH = | 1.257237 E-08 | 3.293684 E-07 | 0.0000 |
| CH4 = | 1.355434 E-09 | 3.550938 E-08 | 0.0000 |
| B2O3(s) = | 5.536177 E-10 | 1.450356 E-08 | 0.0000 |
| BN(s) = | 2.513612 E-10 | 6.585110 E-09 | 0.0000 |
| Cu2O(l) = | 2.150561 E-10 | 5.633995 E-09 | 0.0000 |
| Cu2O(s) = | 2.106344 E-10 | 5.518157 E-09 | 0.0000 |
| CHNO = | 1.958228 E-10 | 5.130126 E-09 | 0.0000 |
| HCN = | 1.719009 E-10 | 4.503425 E-09 | 0.0000 |
| BHO2(s) = | 5.476394 E-11 | 1.434695 E-09 | 0.0000 |
| NO = | 4.206068 E-11 | 1.101897 E-09 | 0.0000 |
| BN = | 3.389770 E-11 | 8.880451 E-10 | 0.0000 |
| BO2 = | 1.843872 E-11 | 4.830540 E-10 | 0.0000 |
| BH2 = | 1.647082 E-11 | 4.314993 E-10 | 0.0000 |
| Cu(OH)2(s) = | 1.563639 E-11 | 4.096391 E-10 | 0.0000 |
| N = | 1.434178 E-11 | 3.757231 E-10 | 0.0000 |
| CNO = | 1.249411 E-11 | 3.273181 E-10 | 0.0000 |
| INO = | 9.519675 E-12 | 2.493945 E-10 | 0.0000 |
| CuO = | 7.765156 E-12 | 2.034300 E-10 | 0.0000 |
| CuO(s) = | 7.700695 E-12 | 2.017412 E-10 | 0.0000 |
| ICN = | 7.326529 E-12 | 1.919389 E-10 | 0.0000 |
| O = | 5.456942 E-12 | 1.429599 E-10 | 0.0000 |
| O2 = | 3.493969 E-12 | 9.153429 E-11 | 0.0000 |
| CH3OH = | 2.493946 E-12 | 6.533590 E-11 | 0.0000 |
| BO = | 2.425610 E-12 | 6.354564 E-11 | 0.0000 |
| NH2 = | 1.022881 E-12 | 2.679723 E-11 | 0.0000 |

Notes:

- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 34

**Combustion conditions (Number 34):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 15.35 %**
2. **AKC-266, 1.33 %**
3. **Hydrogen peroxide ($H_2O_2$), 79.16 %**
4. **Water ($H_2O$, liquid), 4.16 %**

C(0.270) H(2.464) N(0.116) O(1.836) B(0.041) Cu(0.000) I(0.003)

Molecular weight = 37.59
Oxygen balance = 0.1340216 %
Enthalpy of formation = -6862.93 kJ/kg
Internal energy of formation = -6717.32 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -4206.00 kJ/kg
- Total enthalpy of combustion prod. = -6862.90 kJ/kg
- Entropy of combustion products = 10.86 kJ/K kg
- Isobaric combustion temperature = 2436.8 K
- Mole number of gaseous products = 42.376 mol/kg expl.
- Total mole number of products = 42.379 mol/kg expl.
- Volume of gaseous products (at SATP) = 1050.47 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.590 g
- Mean molecular mass of all products = 23.597 g
- Specific gas constant = 352.317 J/kg K
- Specific heat capacity at p=const. (Cp) = 2304.65 J/kgK
- Specific heat capacity at V=const. (Cv) = 1952.33 J/molK
- Specific heat ratio (Cp/Cv) = 1.1805

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.196277 E00 | 3.182735 E01 | 75.1022 |
| CO2 = | 2.586539 E-01 | 6.881574 E00 | 16.2383 |
| N2 = | 5.747332 E-02 | 1.529097 E00 | 3.6082 |
| BHO2 = | 3.721040 E-02 | 9.899954 E-01 | 2.3361 |
| CO = | 1.086358 E-02 | 2.890291 E-01 | 0.6820 |
| O2 = | 8.602297 E-03 | 2.288670 E-01 | 0.5401 |
| H2 = | 7.818459 E-03 | 2.080127 E-01 | 0.4908 |
| OH = | 7.083449 E-03 | 1.884575 E-01 | 0.4447 |
| B(OH)3 = | 3.505109 E-03 | 9.325463 E-02 | 0.2201 |
| I = | 2.719997 E-03 | 7.236644 E-02 | 0.1708 |
| NO = | 1.230766 E-03 | 3.274494 E-02 | 0.0773 |
| IH = | 4.040612 E-04 | 1.075019 E-02 | 0.0254 |
| H = | 2.637673 E-04 | 7.017618 E-03 | 0.0166 |
| BO2 = | 2.571129 E-04 | 6.840575 E-03 | 0.0161 |
| B2O3 = | 1.788630 E-04 | 4.758710 E-03 | 0.0112 |
| O = | 1.475553 E-04 | 3.925759 E-03 | 0.0093 |

| | | | |
|---|---|---|---|
| Cu2O(l) = | 8.786887 E-05 | 2.337781 E-03 | 0.0055 |
| CuO = | 8.484082 E-05 | 2.257219 E-03 | 0.0053 |
| I2 = | 1.433529 E-06 | 3.813953 E-05 | 0.0001 |
| BO = | 1.281136 E-06 | 3.408505 E-05 | 0.0001 |
| NH3 = | 9.636383 E-08 | 2.563792 E-06 | 0.0000 |
| INO = | 1.766618 E-08 | 4.700148 E-07 | 0.0000 |
| NH2 = | 9.135970 E-09 | 2.430656 E-07 | 0.0000 |
| N = | 4.262305 E-09 | 1.134001 E-07 | 0.0000 |
| CHNO = | 2.966112 E-09 | 7.891440 E-08 | 0.0000 |
| HCN = | 1.332620 E-10 | 3.545480 E-09 | 0.0000 |
| CNO = | 3.425600 E-11 | 9.113925 E-10 | 0.0000 |
| Cu2O(s) = | 9.192268 E-12 | 2.445634 E-10 | 0.0000 |
| CuO(s) = | 2.552377 E-12 | 6.790687 E-11 | 0.0000 |
| B2O3(l) = | 1.853979 E-13 | 4.932574 E-12 | 0.0000 |
| BH2 = | 6.992358 E-14 | 1.860340 E-12 | 0.0000 |
| ICN = | 6.771969 E-14 | 1.801705 E-12 | 0.0000 |
| CH3OH = | 4.190581 E-14 | 1.114918 E-12 | 0.0000 |
| CH4 = | 4.035434 E-14 | 1.073641 E-12 | 0.0000 |
| BHO2(s) = | 2.756854 E-14 | 7.334703 E-13 | 0.0000 |
| Cu(OH)2(s) = | 1.788868 E-14 | 4.759343 E-13 | 0.0000 |
| B2O3(s) = | 1.069878 E-14 | 2.846446 E-13 | 0.0000 |
| BN = | 1.697336 E-15 | 4.515820 E-14 | 0.0000 |
| BN(s) = | 1.919486 E-18 | 5.106857 E-17 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7332.95 kJ/kg
- Temperature at nozzle throat = 2263.5 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 42.238 mol/kg expl.
- Total mole number of products = 42.241 mol/kg expl.
- Volume of gaseous products (at SATP) = 1047.04 L/kg expl.
- Mass of gaseous products = 999.6 g/kg expl.
- Mass of condensed products = 0.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.665 g
- Mean molecular mass of all products = 23.674 g
- Specific gas constant = 351.169 J/kg K
- Specific heat capacity at p=const. (Cp) = 2270.04 J/kgK
- Specific heat capacity at V=const. (Cv) = 1918.87 J/molK
- Specific heat ratio (Cp/Cv) = 1.1830

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 969.6 m/s
- Sound velocity at throat) = 969.7 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.566
- Pressure ratio (pc/pt) = 1.766

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.200347 E00 | 3.193564 E01 | 75.6030 |
| CO2 = | 2.632713 E-01 | 7.004421 E00 | 16.5820 |
| N2 = | 5.772979 E-02 | 1.535921 E00 | 3.6361 |
| BHO2 = | 3.696013 E-02 | 9.833369 E-01 | 2.3279 |
| CO = | 6.246177 E-03 | 1.661817 E-01 | 0.3934 |
| O2 = | 5.867218 E-03 | 1.560993 E-01 | 0.3695 |

| | | | |
|---|---|---|---|
| H2 = | 4.859458 E-03 | 1.292875 E-01 | 0.3061 |
| OH = | 4.020279 E-03 | 1.069609 E-01 | 0.2532 |
| B(OH)3 = | 3.939013 E-03 | 1.047988 E-01 | 0.2481 |
| I = | 2.783279 E-03 | 7.405009 E-02 | 0.1753 |
| NO = | 7.179052 E-04 | 1.910011 E-02 | 0.0452 |
| IH = | 3.405903 E-04 | 9.061519 E-03 | 0.0215 |
| BO2 = | 1.445217 E-04 | 3.845049 E-03 | 0.0091 |
| B2O3 = | 1.437762 E-04 | 3.825214 E-03 | 0.0091 |
| H = | 1.167646 E-04 | 3.106562 E-03 | 0.0074 |
| Cu2O(l) = | 1.130228 E-04 | 3.007011 E-03 | 0.0071 |
| O = | 6.144151 E-05 | 1.634672 E-03 | 0.0039 |
| CuO = | 3.453290 E-05 | 9.187596 E-04 | 0.0022 |
| I2 = | 1.532486 E-06 | 4.077230 E-05 | 0.0001 |
| BO = | 4.129264 E-07 | 1.098605 E-05 | 0.0000 |
| NH3 = | 3.325551 E-08 | 8.847741 E-07 | 0.0000 |
| INO = | 8.383398 E-09 | 2.230431 E-07 | 0.0000 |
| NH2 = | 2.160175 E-09 | 5.747219 E-08 | 0.0000 |
| N = | 9.199956 E-10 | 2.447679 E-08 | 0.0000 |
| CHNO = | 7.262817 E-10 | 1.932297 E-08 | 0.0000 |
| HCN = | 2.130276 E-11 | 5.667671 E-10 | 0.0000 |
| Cu2O(s) = | 1.282429 E-11 | 3.411946 E-10 | 0.0000 |
| CNO = | 5.158994 E-12 | 1.372568 E-10 | 0.0000 |
| CuO(s) = | 2.938461 E-12 | 7.817875 E-11 | 0.0000 |
| B2O3(l) = | 3.325219 E-13 | 8.846858 E-12 | 0.0000 |
| BHO2(s) = | 3.296009 E-14 | 8.769143 E-13 | 0.0000 |
| B2O3(s) = | 1.996961 E-14 | 5.312983 E-13 | 0.0000 |
| Cu(OH)2(s) = | 1.254179 E-14 | 3.336786 E-13 | 0.0000 |
| ICN = | 1.119006 E-14 | 2.977153 E-13 | 0.0000 |
| BH2 = | 5.893590 E-15 | 1.568010 E-13 | 0.0000 |
| CH3OH = | 4.314891 E-15 | 1.147991 E-13 | 0.0000 |
| CH4 = | 4.203188 E-15 | 1.118273 E-13 | 0.0000 |
| BN = | 1.076864 E-16 | 2.865035 E-15 | 0.0000 |
| BN(s) = | 1.018905 E-18 | 2.710832 E-17 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9574.74 kJ/kg
- Temperature at nozzle exit = 1321.7 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 41.490 mol/kg expl.
- Total mole number of products = 41.713 mol/kg expl.
- Volume of gaseous products (at SATP) = 1028.50 L/kg expl.
- Mass of gaseous products = 984.3 g/kg expl.
- Mass of condensed products = 15.8 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.723 g
- Mean molecular mass of all products = 23.974 g
- Specific gas constant = 344.948 J/kg K
- Specific heat capacity at p=const. (Cp) = 2001.66 J/kgK
- Specific heat capacity at V=const. (Cv) = 1656.71 J/molK
- Specific heat ratio (Cp/Cv) = 1.2082

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 237.40 s
- Exhaust (or nozzle exit) velocity = 2328.9 m/s
- Characteristic exhaust velocity (c*) = 1410.3 m/s
- Thrust coefficient (Cf) = 1.651
- Nozzle area expansion ratio (Ae/At) = 8.92
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 734.41 m/s
- Mach number at nozzle exit = 3.171

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.197809 E00 | 3.186812 E01 | 76.3987 |
| CO2 = | 2.695175 E-01 | 7.170603 E00 | 17.1904 |
| N2 = | 5.796793 E-02 | 1.542256 E00 | 3.6973 |
| B(OH)3 = | 1.864810 E-02 | 4.961390 E-01 | 1.1894 |
| B2O3(l) = | 8.244039 E-03 | 2.193355 E-01 | 0.5258 |
| BHO2 = | 6.161657 E-03 | 1.639330 E-01 | 0.3930 |
| OH = | 5.942915 E-03 | 1.581133 E-01 | 0.3791 |
| I = | 3.098106 E-03 | 8.242617 E-02 | 0.1976 |
| NO = | 2.408963 E-04 | 6.409129 E-03 | 0.0154 |
| Cu2O(s) = | 1.232905 E-04 | 3.280185 E-03 | 0.0079 |
| BO2 = | 3.269462 E-05 | 8.698514 E-04 | 0.0021 |
| O2 = | 1.732313 E-05 | 4.608877 E-04 | 0.0011 |
| I2 = | 1.403686 E-05 | 3.734554 E-04 | 0.0009 |
| CuO(s) = | 1.008645 E-05 | 2.683535 E-04 | 0.0006 |
| O = | 7.744752 E-06 | 2.060518 E-04 | 0.0005 |
| CuO = | 3.872348 E-06 | 1.030251 E-04 | 0.0002 |
| INO = | 7.744508 E-07 | 2.060453 E-05 | 0.0000 |
| B2O3 = | 5.497351 E-07 | 1.462589 E-05 | 0.0000 |
| Cu(OH)2(s) = | 3.871597 E-08 | 1.030051 E-06 | 0.0000 |
| IH = | 1.129704 E-09 | 3.005615 E-08 | 0.0000 |
| CO = | 8.070326 E-10 | 2.147138 E-08 | 0.0000 |
| H2 = | 7.074720 E-10 | 1.882253 E-08 | 0.0000 |
| Cu2O(l) = | 6.290186 E-11 | 1.673525 E-09 | 0.0000 |
| B2O3(s) = | 6.444836 E-12 | 1.714670 E-10 | 0.0000 |
| BHO2(s) = | 2.463928 E-13 | 6.555364 E-12 | 0.0000 |
| CH4 = | 1.124755 E-13 | 2.992448 E-12 | 0.0000 |
| H = | 2.837876 E-14 | 7.550264 E-13 | 0.0000 |
| HCN = | 3.108958 E-15 | 8.271489 E-14 | 0.0000 |
| BN(s) = | 2.799526 E-15 | 7.448233 E-14 | 0.0000 |
| NH3 = | 2.227518 E-15 | 5.926387 E-14 | 0.0000 |
| ICN = | 1.546785 E-15 | 4.115275 E-14 | 0.0000 |
| CH3OH = | 2.323362 E-16 | 6.181384 E-15 | 0.0000 |
| BH2 = | 1.936207 E-16 | 5.151345 E-15 | 0.0000 |
| BN = | 1.161848 E-16 | 3.091136 E-15 | 0.0000 |
| CHNO = | 1.161519 E-16 | 3.090260 E-15 | 0.0000 |
| CNO = | 7.744081 E-17 | 2.060339 E-15 | 0.0000 |
| NH2 = | 7.743021 E-17 | 2.060057 E-15 | 0.0000 |
| N = | 7.683223 E-17 | 2.044148 E-15 | 0.0000 |
| BO = | 3.870371 E-17 | 1.029725 E-15 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 35

**Combustion conditions (Number 35):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 13.43 %**
2. **AKC-266, 1.16 %**
3. **Hydrogen peroxide ($H_2O_2$), 81.14 %**
4. **Water ($H_2O$, liquid), 4.27 %**

C(0.231) H(2.398) N(0.100) O(1.847) B(0.035) Cu(0.000) I(0.003)

Molecular weight = 36.87
Oxygen balance = 5.707277 %
Enthalpy of formation = -6759.43 kJ/kg
Internal energy of formation = -6613.42 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3940.44 kJ/kg
- Total enthalpy of combustion prod. = -6759.36 kJ/kg
- Entropy of combustion products = 10.77 kJ/K kg
- Isobaric combustion temperature = 2331.6 K
- Mole number of gaseous products = 42.472 mol/kg expl.
- Total mole number of products = 42.474 mol/kg expl.
- Volume of gaseous products (at SATP) = 1052.83 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.538 g
- Mean molecular mass of all products = 23.544 g
- Specific gas constant = 353.111 J/kg K
- Specific heat capacity at p=const. (Cp) = 2269.84 J/kgK
- Specific heat capacity at V=const. (Cv) = 1916.73 J/molK
- Specific heat ratio (Cp/Cv) = 1.1842

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.171429 E00 | 3.176973 E01 | 74.7982 |
| CO2 = | 2.294330 E-01 | 6.222334 E00 | 14.6498 |
| O2 = | 6.416937 E-02 | 1.740305 E00 | 4.0973 |
| N2 = | 4.859794 E-02 | 1.318000 E00 | 3.1031 |
| BHO2 = | 3.068853 E-02 | 8.322879 E-01 | 1.9595 |
| OH = | 8.033199 E-03 | 2.178643 E-01 | 0.5129 |
| B(OH)3 = | 4.311488 E-03 | 1.169297 E-01 | 0.2753 |
| NO = | 2.515011 E-03 | 6.820832 E-02 | 0.1606 |
| I = | 2.470013 E-03 | 6.698795 E-02 | 0.1577 |
| CO = | 1.888120 E-03 | 5.120672 E-02 | 0.1206 |
| H2 = | 1.582268 E-03 | 4.291187 E-02 | 0.1010 |
| BO2 = | 2.456336 E-04 | 6.661703 E-03 | 0.0157 |
| O = | 2.259079 E-04 | 6.126733 E-03 | 0.0144 |
| IH = | 2.020061 E-04 | 5.478504 E-03 | 0.0129 |
| B2O3 = | 1.103133 E-04 | 2.991751 E-03 | 0.0070 |
| Cu2O(l) = | 7.806771 E-05 | 2.117234 E-03 | 0.0050 |

| | | | |
|---|---|---|---|
| H = | 7.069463 E-05 | 1.917273 E-03 | 0.0045 |
| CuO = | 6.681911 E-05 | 1.812167 E-03 | 0.0043 |
| I2 = | 1.697713 E-06 | 4.604282 E-05 | 0.0001 |
| BO = | 2.422204 E-07 | 6.569134 E-06 | 0.0000 |
| INO = | 4.065842 E-08 | 1.102676 E-06 | 0.0000 |
| NH3 = | 9.356937 E-09 | 2.537647 E-07 | 0.0000 |
| N = | 1.330465 E-09 | 3.608286 E-08 | 0.0000 |
| NH2 = | 1.150599 E-09 | 3.120481 E-08 | 0.0000 |
| CHNO = | 2.106170 E-10 | 5.712036 E-09 | 0.0000 |
| Cu2O(s) = | 1.003993 E-11 | 2.722878 E-10 | 0.0000 |
| CuO(s) = | 5.264442 E-12 | 1.427742 E-10 | 0.0000 |
| CNO = | 2.959754 E-12 | 8.026996 E-11 | 0.0000 |
| HCN = | 2.020261 E-12 | 5.479045 E-11 | 0.0000 |
| B2O3(l) = | 2.600375 E-13 | 7.052345 E-12 | 0.0000 |
| Cu(OH)2(s) = | 3.778434 E-14 | 1.024730 E-12 | 0.0000 |
| BHO2(s) = | 3.585451 E-14 | 9.723919 E-13 | 0.0000 |
| B2O3(s) = | 1.532604 E-14 | 4.156497 E-13 | 0.0000 |
| ICN = | 2.157697 E-15 | 5.851781 E-14 | 0.0000 |
| BH2 = | 6.286658 E-16 | 1.704972 E-14 | 0.0000 |
| CH3OH = | 2.416802 E-16 | 6.554484 E-15 | 0.0000 |
| CH4 = | 1.024258 E-16 | 2.777838 E-15 | 0.0000 |
| BN = | 2.692444 E-17 | 7.302038 E-16 | 0.0000 |
| BN(s) = | 2.074373 E-19 | 5.625802 E-18 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7208.32 kJ/kg
- Temperature at nozzle throat = 2149.1 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 42.393 mol/kg expl.
- Total mole number of products = 42.395 mol/kg expl.
- Volume of gaseous products (at SATP) = 1050.87 L/kg expl.
- Mass of gaseous products = 999.6 g/kg expl.
- Mass of condensed products = 0.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.580 g
- Mean molecular mass of all products = 23.588 g
- Specific gas constant = 352.452 J/kg K
- Specific heat capacity at p=const. (Cp) = 2230.47 J/kgK
- Specific heat capacity at V=const. (Cv) = 1878.02 J/molK
- Specific heat ratio (Cp/Cv) = 1.1877

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 947.6 m/s
- Sound velocity at throat) = 948.5 m/s
- Mach number at nozzle throat = 0.999
- Critical pressure ratio (pt/pc) = 0.566
- Pressure ratio (pc/pt) = 1.767

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.173068 E00 | 3.181417 E01 | 75.0418 |
| CO2 = | 2.305603 E-01 | 6.252909 E00 | 14.7491 |
| O2 = | 6.451062 E-02 | 1.749560 E00 | 4.1268 |
| N2 = | 4.900623 E-02 | 1.329073 E00 | 3.1350 |
| BHO2 = | 2.993300 E-02 | 8.117976 E-01 | 1.9148 |
| B(OH)3 = | 5.229603 E-03 | 1.418294 E-01 | 0.3345 |

| | | | |
|---|---|---|---|
| OH = | 4.603032 E-03 | 1.248365 E-01 | 0.2945 |
| I = | 2.520911 E-03 | 6.836833 E-02 | 0.1613 |
| NO = | 1.698441 E-03 | 4.606255 E-02 | 0.1087 |
| CO = | 7.607670 E-04 | 2.063237 E-02 | 0.0487 |
| H2 = | 7.084652 E-04 | 1.921392 E-02 | 0.0453 |
| IH = | 1.506060 E-04 | 4.084509 E-03 | 0.0096 |
| BO2 = | 1.371997 E-04 | 3.720923 E-03 | 0.0088 |
| O = | 9.972347 E-05 | 2.704549 E-03 | 0.0064 |
| Cu2O(l) = | 9.901819 E-05 | 2.685421 E-03 | 0.0063 |
| B2O3 = | 8.333160 E-05 | 2.259994 E-03 | 0.0053 |
| CuO = | 2.491814 E-05 | 6.757921 E-04 | 0.0016 |
| H = | 2.357484 E-05 | 6.393610 E-04 | 0.0015 |
| I2 = | 1.957134 E-06 | 5.307842 E-05 | 0.0001 |
| BO = | 5.502092 E-08 | 1.492194 E-06 | 0.0000 |
| INO = | 2.329298 E-08 | 6.317169 E-07 | 0.0000 |
| NH3 = | 2.011353 E-09 | 5.454888 E-08 | 0.0000 |
| N = | 2.225428 E-10 | 6.035469 E-09 | 0.0000 |
| NH2 = | 1.756627 E-10 | 4.764059 E-09 | 0.0000 |
| CHNO = | 3.043845 E-11 | 8.255055 E-10 | 0.0000 |
| Cu2O(s) = | 1.539337 E-11 | 4.174757 E-10 | 0.0000 |
| CuO(s) = | 7.272293 E-12 | 1.972281 E-10 | 0.0000 |
| B2O3(l) = | 5.362025 E-13 | 1.454207 E-11 | 0.0000 |
| CNO = | 2.682824 E-13 | 7.275951 E-12 | 0.0000 |
| HCN = | 1.378722 E-13 | 3.739162 E-12 | 0.0000 |
| BHO2(s) = | 4.722827 E-14 | 1.280854 E-12 | 0.0000 |
| B2O3(s) = | 3.351096 E-14 | 9.088337 E-13 | 0.0000 |
| Cu(OH)2(s) = | 3.132558 E-14 | 8.495649 E-13 | 0.0000 |
| ICN = | 1.804851 E-16 | 4.894845 E-15 | 0.0000 |
| BH2 = | 1.948876 E-17 | 5.285446 E-16 | 0.0000 |
| CH3OH = | 1.489075 E-17 | 4.038444 E-16 | 0.0000 |
| CH4 = | 3.084855 E-18 | 8.366278 E-17 | 0.0000 |
| BN = | 1.044113 E-18 | 2.831684 E-17 | 0.0000 |
| BN(s) = | 7.288318 E-20 | 1.976627 E-18 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9329.88 kJ/kg
- Temperature at nozzle exit = 1222.7 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 41.751 mol/kg expl.
- Total mole number of products = 41.947 mol/kg expl.
- Volume of gaseous products (at SATP) = 1034.97 L/kg expl.
- Mass of gaseous products = 986.3 g/kg expl.
- Mass of condensed products = 13.7 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.624 g
- Mean molecular mass of all products = 23.840 g
- Specific gas constant = 347.121 J/kg K
- Specific heat capacity at p=const. (Cp) = 1949.95 J/kgK
- Specific heat capacity at V=const. (Cv) = 1602.83 J/molK
- Specific heat ratio (Cp/Cv) = 1.2166

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 231.13 s
- Exhaust (or nozzle exit) velocity = 2267.4 m/s
- Characteristic exhaust velocity (c*) = 1380.4 m/s
- Thrust coefficient (Cf) = 1.643
- Nozzle area expansion ratio (Ae/At) = 8.77
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 709.99 m/s
- Mach number at nozzle exit = 3.194

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.168432 E00 | 3.168843 E01 | 75.5437 |
| CO2 = | 2.313211 E-01 | 6.273540 E00 | 14.9558 |
| O2 = | 6.575003 E-02 | 1.783173 E00 | 4.2510 |
| N2 = | 4.983791 E-02 | 1.351629 E00 | 3.2222 |
| B(OH)3 = | 1.979566 E-02 | 5.368679 E-01 | 1.2799 |
| B2O3(l) = | 6.997117 E-03 | 1.897652 E-01 | 0.4524 |
| I = | 2.542819 E-03 | 6.896248 E-02 | 0.1644 |
| BHO2 = | 1.676559 E-03 | 4.546911 E-02 | 0.1084 |
| CuO(s) = | 2.229627 E-04 | 6.046857 E-03 | 0.0144 |
| I2 = | 5.965914 E-05 | 1.617985 E-03 | 0.0039 |
| NO = | 3.510461 E-05 | 9.520543 E-04 | 0.0023 |
| IH = | 1.331802 E-05 | 3.611911 E-04 | 0.0009 |
| OH = | 1.153499 E-05 | 3.128345 E-04 | 0.0007 |
| H2 = | 9.659711 E-08 | 2.619761 E-06 | 0.0000 |
| CO = | 3.059794 E-08 | 8.298311 E-07 | 0.0000 |
| B2O3 = | 2.957153 E-08 | 8.019942 E-07 | 0.0000 |
| BO2 = | 1.443218 E-08 | 3.914077 E-07 | 0.0000 |
| O = | 9.423498 E-09 | 2.555699 E-07 | 0.0000 |
| Cu2O(l) = | 3.780358 E-10 | 1.025252 E-08 | 0.0000 |
| H = | 1.227975 E-10 | 3.330327 E-09 | 0.0000 |
| B2O3(s) = | 8.095160 E-11 | 2.195447 E-09 | 0.0000 |
| CuO = | 5.377152 E-11 | 1.458310 E-09 | 0.0000 |
| BN(s) = | 3.849108 E-11 | 1.043897 E-09 | 0.0000 |
| INO = | 3.311576 E-11 | 8.981155 E-10 | 0.0000 |
| Cu(OH)2(s) = | 2.683241 E-11 | 7.277079 E-10 | 0.0000 |
| Cu2O(s) = | 1.959743 E-11 | 5.314918 E-10 | 0.0000 |
| BN = | 5.186298 E-12 | 1.406549 E-10 | 0.0000 |
| BHO2(s) = | 4.870607 E-12 | 1.320932 E-10 | 0.0000 |
| BH2 = | 4.788484 E-12 | 1.298660 E-10 | 0.0000 |
| CH4 = | 4.592311 E-12 | 1.245457 E-10 | 0.0000 |
| CH3OH = | 4.082219 E-12 | 1.107118 E-10 | 0.0000 |
| ICN = | 3.095153 E-12 | 8.394206 E-11 | 0.0000 |
| HCN = | 2.779268 E-12 | 7.537511 E-11 | 0.0000 |
| CNO = | 2.388028 E-12 | 6.476448 E-11 | 0.0000 |
| CHNO = | 1.408729 E-12 | 3.820541 E-11 | 0.0000 |
| NH2 = | 1.226883 E-12 | 3.327366 E-11 | 0.0000 |
| N = | 1.203750 E-12 | 3.264628 E-11 | 0.0000 |
| BO = | 6.841160 E-13 | 1.855356 E-11 | 0.0000 |
| NH3 = | 5.892891 E-13 | 1.598181 E-11 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 36

**Combustion conditions (Number 36):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 11.5 %**
2. **AKC-266, 1.00 %**
3. **Hydrogen peroxide ($H_2O_2$), 83.13 %**
4. **Water ($H_2O$, liquid), 4.37 %**

C(0.194) H(2.334) N(0.084) O(1.857) B(0.030) Cu(0.000) I(0.002)

Molecular weight = 36.19
Oxygen balance = 11.30523 %
Enthalpy of formation = -6655.17 kJ/kg
Internal energy of formation = -6508.77 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3608.42 kJ/kg
- Total enthalpy of combustion prod. = -6655.12 kJ/kg
- Entropy of combustion products = 10.66 kJ/K kg
- Isobaric combustion temperature = 2194.3 K
- Mole number of gaseous products = 42.679 mol/kg expl.
- Total mole number of products = 42.682 mol/kg expl.
- Volume of gaseous products (at SATP) = 1057.98 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.423 g
- Mean molecular mass of all products = 23.430 g
- Specific gas constant = 354.835 J/kg K
- Specific heat capacity at p=const. (Cp) = 2225.91 J/kgK
- Specific heat capacity at V=const. (Cv) = 1871.08 J/molK
- Specific heat ratio (Cp/Cv) = 1.1896

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.143415 E00 | 3.159531 E01 | 74.0257 |
| CO2 = | 1.941100 E-01 | 5.363729 E00 | 12.5669 |
| O2 = | 1.255487 E-01 | 3.469214 E00 | 8.1281 |
| N2 = | 4.069268 E-02 | 1.124437 E00 | 2.6345 |
| BHO2 = | 2.365918 E-02 | 6.537602 E-01 | 1.5317 |
| B(OH)3 = | 5.887279 E-03 | 1.626797 E-01 | 0.3811 |
| OH = | 5.546367 E-03 | 1.532595 E-01 | 0.3591 |
| NO = | 2.422011 E-03 | 6.692602 E-02 | 0.1568 |
| I = | 2.096464 E-03 | 5.793037 E-02 | 0.1357 |
| CO = | 3.087788 E-04 | 8.532305 E-03 | 0.0200 |
| H2 = | 2.999844 E-04 | 8.289295 E-03 | 0.0194 |
| IH = | 1.639544 E-04 | 4.530456 E-03 | 0.0106 |
| BO2 = | 1.445399 E-04 | 3.993986 E-03 | 0.0094 |
| O = | 1.386444 E-04 | 3.831079 E-03 | 0.0090 |
| Cu2O(l) = | 8.404394 E-05 | 2.322337 E-03 | 0.0054 |
| B2O3 = | 6.560658 E-05 | 1.812868 E-03 | 0.0042 |

| | | | |
|---|---|---|---|
| CuO = | 2.056330 E-05 | 5.682136 E-04 | 0.0013 |
| H = | 1.399844 E-05 | 3.868107 E-04 | 0.0009 |
| I2 = | 1.610181 E-06 | 4.449319 E-05 | 0.0001 |
| INO = | 5.807830 E-08 | 1.604844 E-06 | 0.0000 |
| BO = | 3.896345 E-08 | 1.076654 E-06 | 0.0000 |
| NH3 = | 1.688890 E-09 | 4.666811 E-08 | 0.0000 |
| B2O3(l) = | 8.870852 E-10 | 2.451231 E-08 | 0.0000 |
| CuO(s) = | 3.767277 E-10 | 1.040990 E-08 | 0.0000 |
| Cu2O(s) = | 2.681306 E-10 | 7.409096 E-09 | 0.0000 |
| N = | 2.164013 E-10 | 5.979691 E-09 | 0.0000 |
| NH2 = | 1.674973 E-10 | 4.628355 E-09 | 0.0000 |
| B2O3(s) = | 1.256276 E-10 | 3.471395 E-09 | 0.0000 |
| Cu(OH)2(s) = | 6.434892 E-11 | 1.778116 E-09 | 0.0000 |
| CHNO = | 1.943705 E-11 | 5.370925 E-10 | 0.0000 |
| BN(s) = | 1.804572 E-11 | 4.986468 E-10 | 0.0000 |
| BN = | 1.523613 E-11 | 4.210111 E-10 | 0.0000 |
| CH4 = | 1.468579 E-11 | 4.058040 E-10 | 0.0000 |
| BH2 = | 1.262521 E-11 | 3.488652 E-10 | 0.0000 |
| CH3OH = | 1.261669 E-11 | 3.486296 E-10 | 0.0000 |
| ICN = | 9.914136 E-12 | 2.739515 E-10 | 0.0000 |
| BHO2(s) = | 4.092200 E-12 | 1.130774 E-10 | 0.0000 |
| HCN = | 3.822018 E-12 | 1.056116 E-10 | 0.0000 |
| CNO = | 2.594041 E-12 | 7.167961 E-11 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7080.19 kJ/kg
- Temperature at nozzle throat = 2013.5 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 42.606 mol/kg expl.
- Total mole number of products = 42.609 mol/kg expl.
- Volume of gaseous products (at SATP) = 1056.17 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.462 g
- Mean molecular mass of all products = 23.469 g
- Specific gas constant = 354.230 J/kg K
- Specific heat capacity at p=const. (Cp) = 2183.53 J/kgK
- Specific heat capacity at V=const. (Cv) = 1829.30 J/molK
- Specific heat ratio (Cp/Cv) = 1.1936

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 922.0 m/s
- Sound velocity at throat) = 922.7 m/s
- Mach number at nozzle throat = 0.999
- Critical pressure ratio (pt/pc) = 0.565
- Pressure ratio (pc/pt) = 1.770

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.143064 E00 | 3.158561 E01 | 74.1291 |
| CO2 = | 1.942619 E-01 | 5.367926 E00 | 12.5981 |
| O2 = | 1.265768 E-01 | 3.497623 E00 | 8.2087 |
| N2 = | 4.113948 E-02 | 1.136783 E00 | 2.6679 |
| BHO2 = | 2.202268 E-02 | 6.085398 E-01 | 1.4282 |
| B(OH)3 = | 7.659162 E-03 | 2.116411 E-01 | 0.4967 |

| | | | |
|---|---|---|---|
| OH = | 2.875643 E-03 | 7.946097 E-02 | 0.1865 |
| I = | 2.165501 E-03 | 5.983804 E-02 | 0.1404 |
| NO = | 1.528491 E-03 | 4.223590 E-02 | 0.0991 |
| H2 = | 1.867495 E-04 | 5.160341 E-03 | 0.0121 |
| CO = | 1.569029 E-04 | 4.335607 E-03 | 0.0102 |
| IH = | 9.286359 E-05 | 2.566045 E-03 | 0.0060 |
| Cu2O(l) = | 9.027478 E-05 | 2.494510 E-03 | 0.0059 |
| BO2 = | 6.481601 E-05 | 1.791023 E-03 | 0.0042 |
| O = | 5.215288 E-05 | 1.441110 E-03 | 0.0034 |
| B2O3 = | 3.780046 E-05 | 1.044518 E-03 | 0.0025 |
| CuO = | 8.091793 E-06 | 2.235958 E-04 | 0.0005 |
| H = | 5.041436 E-06 | 1.393071 E-04 | 0.0003 |
| I2 = | 2.653136 E-06 | 7.331256 E-05 | 0.0002 |
| INO = | 2.558822 E-08 | 7.070643 E-07 | 0.0000 |
| BO = | 6.466970 E-09 | 1.786980 E-07 | 0.0000 |
| BN = | 2.624808 E-09 | 7.252979 E-08 | 0.0000 |
| CH4 = | 9.889469 E-10 | 2.732699 E-08 | 0.0000 |
| BN(s) = | 6.827728 E-10 | 1.886666 E-08 | 0.0000 |
| NH3 = | 3.116568 E-10 | 8.611829 E-09 | 0.0000 |
| BH2 = | 6.354774 E-11 | 1.755977 E-09 | 0.0000 |
| N = | 3.226775 E-11 | 8.916359 E-10 | 0.0000 |
| CH3OH = | 3.109416 E-11 | 8.592067 E-10 | 0.0000 |
| NH2 = | 2.114270 E-11 | 5.842240 E-10 | 0.0000 |
| Cu2O(s) = | 1.999327 E-11 | 5.524624 E-10 | 0.0000 |
| CuO(s) = | 1.307000 E-11 | 3.611557 E-10 | 0.0000 |
| CHNO = | 2.855442 E-12 | 7.890275 E-11 | 0.0000 |
| B2O3(l) = | 1.018620 E-12 | 2.814692 E-11 | 0.0000 |
| BHO2(s) = | 7.708682 E-14 | 2.130095 E-12 | 0.0000 |
| B2O3(s) = | 6.801218 E-14 | 1.879341 E-12 | 0.0000 |
| Cu(OH)2(s) = | 5.720085 E-14 | 1.580598 E-12 | 0.0000 |
| CNO = | 1.755753 E-14 | 4.851569 E-13 | 0.0000 |
| ICN = | 1.239417 E-14 | 3.424808 E-13 | 0.0000 |
| HCN = | 3.699412 E-15 | 1.022237 E-13 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9059.16 kJ/kg
- Temperature at nozzle exit = 1110.7 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 42.092 mol/kg expl.
- Total mole number of products = 42.217 mol/kg expl.
- Volume of gaseous products (at SATP) = 1043.42 L/kg expl.
- Mass of gaseous products = 991.2 g/kg expl.
- Mass of condensed products = 8.8 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.549 g
- Mean molecular mass of all products = 23.688 g
- Specific gas constant = 349.953 J/kg K
- Specific heat capacity at p=const. (Cp) = 1889.91 J/kgK
- Specific heat capacity at V=const. (Cv) = 1539.96 J/molK
- Specific heat ratio (Cp/Cv) = 1.2272

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 223.52 s
- Exhaust (or nozzle exit) velocity = 2192.7 m/s
- Characteristic exhaust velocity (c*) = 1340.4 m/s
- Thrust coefficient (Cf) = 1.636
- Nozzle area expansion ratio (Ae/At) = 8.59
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 681.16 m/s
- Mach number at nozzle exit = 3.219

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.135844 E00 | 3.138612 E01 | 74.3450 |
| CO2 = | 1.944188 E-01 | 5.372262 E00 | 12.7254 |
| O2 = | 1.278653 E-01 | 3.533226 E00 | 8.3692 |
| N2 = | 4.189487 E-02 | 1.157657 E00 | 2.7422 |
| B(OH)3 = | 2.083196 E-02 | 5.756373 E-01 | 1.3635 |
| B2O3(l) = | 4.354981 E-03 | 1.203387 E-01 | 0.2850 |
| I = | 1.981807 E-03 | 5.476213 E-02 | 0.1297 |
| BHO2 = | 2.803271 E-04 | 7.746115 E-03 | 0.0183 |
| CuO(s) = | 1.402106 E-04 | 3.874358 E-03 | 0.0092 |
| I2 = | 1.373793 E-04 | 3.796121 E-03 | 0.0090 |
| Cu2O(s) = | 2.421541 E-05 | 6.691302 E-04 | 0.0016 |
| NO = | 1.769631 E-05 | 4.889919 E-04 | 0.0012 |
| IH = | 7.130395 E-06 | 1.970300 E-04 | 0.0005 |
| OH = | 2.701765 E-06 | 7.465628 E-05 | 0.0002 |
| H2 = | 5.698499 E-09 | 1.574633 E-07 | 0.0000 |
| CO = | 1.211794 E-09 | 3.348480 E-08 | 0.0000 |
| O = | 1.203351 E-09 | 3.325150 E-08 | 0.0000 |
| B2O3(s) = | 9.952092 E-10 | 2.750004 E-08 | 0.0000 |
| BO2 = | 8.527376 E-10 | 2.356320 E-08 | 0.0000 |
| INO = | 6.188703 E-10 | 1.710088 E-08 | 0.0000 |
| B2O3 = | 4.702809 E-10 | 1.299500 E-08 | 0.0000 |
| BN(s) = | 3.395396 E-11 | 9.382299 E-10 | 0.0000 |
| Cu2O(l) = | 7.978672 E-12 | 2.204700 E-10 | 0.0000 |
| BHO2(s) = | 6.793472 E-12 | 1.877200 E-10 | 0.0000 |
| BN = | 6.328019 E-12 | 1.748584 E-10 | 0.0000 |
| BH2 = | 5.929600 E-12 | 1.638492 E-10 | 0.0000 |
| CH4 = | 5.536410 E-12 | 1.529844 E-10 | 0.0000 |
| CH3OH = | 4.867814 E-12 | 1.345095 E-10 | 0.0000 |
| Cu(OH)2(s) = | 4.738690 E-12 | 1.309415 E-10 | 0.0000 |
| ICN = | 3.704118 E-12 | 1.023537 E-10 | 0.0000 |
| HCN = | 3.529399 E-12 | 9.752583 E-11 | 0.0000 |
| CNO = | 2.992414 E-12 | 8.268763 E-11 | 0.0000 |
| H = | 2.193679 E-12 | 6.061664 E-11 | 0.0000 |
| CHNO = | 1.890247 E-12 | 5.223209 E-11 | 0.0000 |
| CuO = | 1.713493 E-12 | 4.734794 E-11 | 0.0000 |
| NH2 = | 1.698016 E-12 | 4.692027 E-11 | 0.0000 |
| N = | 1.683561 E-12 | 4.652084 E-11 | 0.0000 |
| BO = | 1.312979 E-12 | 3.628078 E-11 | 0.0000 |
| NH3 = | 9.623822 E-13 | 2.659294 E-11 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 37

**Combustion conditions (Number 37):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 9.20 %**
2. **AKC-266, 0.80 %**
3. **Hydrogen peroxide ($H_2O_2$), 85.50 %**
4. **Water ($H_2O$, liquid), 4.50 %**

C(0.152) H(2.262) N(0.066) O(1.868) B(0.023) Cu(0.000) I(0.002)

Molecular weight = 35.4
Oxygen balance = 17.97923 %
Enthalpy of formation = -6531.30 kJ/kg
Internal energy of formation = -6384.42 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3197.15 kJ/kg
- Total enthalpy of combustion prod. = -6532.21 kJ/kg
- Entropy of combustion products = 10.50 kJ/K kg
- Isobaric combustion temperature = 2017.9 K
- Mole number of gaseous products = 42.948 mol/kg expl.
- Total mole number of products = 42.950 mol/kg expl.
- Volume of gaseous products (at SATP) = 1064.64 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.277 g
- Mean molecular mass of all products = 23.283 g
- Specific gas constant = 357.071 J/kg K
- Specific heat capacity at p=const. (Cp) = 2167.60 J/kgK
- Specific heat capacity at V=const. (Cv) = 1810.53 J/molK
- Specific heat ratio (Cp/Cv) = 1.1972

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.109101 E00 | 3.132989 E01 | 72.9448 |
| O2 = | 1.974594 E-01 | 5.577833 E00 | 12.9868 |
| CO2 = | 1.520937 E-01 | 4.296342 E00 | 10.0031 |
| N2 = | 3.194173 E-02 | 9.022902 E-01 | 2.1008 |
| BHO2 = | 1.464957 E-02 | 4.138211 E-01 | 0.9635 |
| B(OH)3 = | 8.599410 E-03 | 2.429162 E-01 | 0.5656 |
| OH = | 2.802516 E-03 | 7.916550 E-02 | 0.1843 |
| NO = | 1.701337 E-03 | 4.805938 E-02 | 0.1119 |
| I = | 1.670421 E-03 | 4.718606 E-02 | 0.1099 |
| H2 = | 9.919664 E-05 | 2.802107 E-03 | 0.0065 |
| IH = | 9.558615 E-05 | 2.700118 E-03 | 0.0063 |
| Cu2O(l) = | 7.155593 E-05 | 2.021312 E-03 | 0.0047 |
| CO = | 5.191566 E-05 | 1.466514 E-03 | 0.0034 |
| O = | 5.046762 E-05 | 1.425610 E-03 | 0.0033 |
| BO2 = | 4.752343 E-05 | 1.342442 E-03 | 0.0031 |
| B2O3 = | 2.069149 E-05 | 5.844933 E-04 | 0.0014 |

| | | | |
|---|---|---|---|
| CuO = | 4.553194 E-06 | 1.286186 E-04 | 0.0003 |
| H = | 2.869003 E-06 | 8.104362 E-05 | 0.0002 |
| I2 = | 2.716530 E-06 | 7.673656 E-05 | 0.0002 |
| INO = | 5.259270 E-08 | 1.485639 E-06 | 0.0000 |
| BO = | 2.547169 E-09 | 7.195244 E-08 | 0.0000 |
| Cu2O(s) = | 1.774356 E-09 | 5.012201 E-08 | 0.0000 |
| B2O3(l) = | 1.095329 E-09 | 3.094086 E-08 | 0.0000 |
| CuO(s) = | 3.870365 E-10 | 1.093301 E-08 | 0.0000 |
| NH3 = | 1.996197 E-10 | 5.638857 E-09 | 0.0000 |
| Cu(OH)2(s) = | 1.314853 E-10 | 3.714198 E-09 | 0.0000 |
| B2O3(s) = | 1.264624 E-10 | 3.572310 E-09 | 0.0000 |
| BHO2(s) = | 4.555553 E-11 | 1.286853 E-09 | 0.0000 |
| BN = | 2.052923 E-11 | 5.799097 E-10 | 0.0000 |
| BN(s) = | 1.990420 E-11 | 5.622540 E-10 | 0.0000 |
| CH4 = | 1.975454 E-11 | 5.580265 E-10 | 0.0000 |
| N = | 1.844636 E-11 | 5.210729 E-10 | 0.0000 |
| BH2 = | 1.795348 E-11 | 5.071499 E-10 | 0.0000 |
| CH3OH = | 1.686274 E-11 | 4.763386 E-10 | 0.0000 |
| NH2 = | 1.448838 E-11 | 4.092678 E-10 | 0.0000 |
| ICN = | 1.338529 E-11 | 3.781078 E-10 | 0.0000 |
| HCN = | 7.883421 E-12 | 2.226909 E-10 | 0.0000 |
| CNO = | 5.833404 E-12 | 1.647820 E-10 | 0.0000 |
| CHNO = | 7.439230 E-13 | 2.101434 E-11 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -6926.66 kJ/kg
- Temperature at nozzle throat = 1845.0 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 42.861 mol/kg expl.
- Total mole number of products = 42.863 mol/kg expl.
- Volume of gaseous products (at SATP) = 1062.49 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.325 g
- Mean molecular mass of all products = 23.330 g
- Specific gas constant = 356.348 J/kg K
- Specific heat capacity at p=const. (Cp) = 2122.91 J/kgK
- Specific heat capacity at V=const. (Cv) = 1766.56 J/molK
- Specific heat ratio (Cp/Cv) = 1.2017

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 888.2 m/s
- Sound velocity at throat ) = 888.9 m/s
- Mach number at nozzle throat = 0.999
- Critical pressure ratio (pt/pc) = 0.563
- Pressure ratio (pc/pt) = 1.775

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.107277 E00 | 3.127837 E01 | 72.9724 |
| O2 = | 1.981420 E-01 | 5.597117 E00 | 13.0581 |
| CO2 = | 1.521242 E-01 | 4.297206 E00 | 10.0254 |
| N2 = | 3.228114 E-02 | 9.118778 E-01 | 2.1274 |
| BHO2 = | 1.207089 E-02 | 3.409786 E-01 | 0.7955 |
| B(OH)3 = | 1.123277 E-02 | 3.173033 E-01 | 0.7403 |

| | | | |
|---|---|---|---|
| I = | 1.711557 E-03 | 4.834808 E-02 | 0.1128 |
| OH = | 1.299708 E-03 | 3.671416 E-02 | 0.0857 |
| NO = | 1.022578 E-03 | 2.888579 E-02 | 0.0674 |
| Cu2O(l) = | 7.310158 E-05 | 2.064974 E-03 | 0.0048 |
| IH = | 5.207611 E-05 | 1.471046 E-03 | 0.0034 |
| H2 = | 3.645422 E-05 | 1.029759 E-03 | 0.0024 |
| CO = | 2.135668 E-05 | 6.032836 E-04 | 0.0014 |
| BO2 = | 1.662291 E-05 | 4.695640 E-04 | 0.0011 |
| O = | 1.610430 E-05 | 4.549144 E-04 | 0.0011 |
| B2O3 = | 8.799282 E-06 | 2.485622 E-04 | 0.0006 |
| I2 = | 3.918600 E-06 | 1.106926 E-04 | 0.0003 |
| CuO = | 1.421130 E-06 | 4.014408 E-05 | 0.0001 |
| H = | 6.428457 E-07 | 1.815911 E-05 | 0.0000 |
| INO = | 2.218798 E-08 | 6.267662 E-07 | 0.0000 |
| BN = | 1.934472 E-09 | 5.464498 E-08 | 0.0000 |
| CH4 = | 6.336219 E-10 | 1.789856 E-08 | 0.0000 |
| BO = | 2.939098 E-10 | 8.302365 E-09 | 0.0000 |
| BH2 = | 1.510307 E-10 | 4.266317 E-09 | 0.0000 |
| NH3 = | 3.264064 E-11 | 9.220331 E-10 | 0.0000 |
| Cu2O(s) = | 3.040660 E-11 | 8.589259 E-10 | 0.0000 |
| CuO(s) = | 2.790705 E-11 | 7.883185 E-10 | 0.0000 |
| BN(s) = | 2.191214 E-11 | 6.189743 E-10 | 0.0000 |
| CH3OH = | 2.017671 E-11 | 5.699518 E-10 | 0.0000 |
| N = | 2.074994 E-12 | 5.861444 E-11 | 0.0000 |
| B2O3(l) = | 1.848820 E-12 | 5.222548 E-11 | 0.0000 |
| NH2 = | 1.350933 E-12 | 3.816118 E-11 | 0.0000 |
| CHNO = | 1.449579 E-13 | 4.094771 E-12 | 0.0000 |
| B2O3(s) = | 1.379569 E-13 | 3.897006 E-12 | 0.0000 |
| BHO2(s) = | 1.329671 E-13 | 3.756056 E-12 | 0.0000 |
| Cu(OH)2(s) = | 1.204527 E-13 | 3.402550 E-12 | 0.0000 |
| ICN = | 3.166863 E-14 | 8.945758 E-13 | 0.0000 |
| CNO = | 4.675967 E-16 | 1.320867 E-14 | 0.0000 |
| HCN = | 4.069751 E-17 | 1.149624 E-15 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8725.46 kJ/kg
- Temperature at nozzle exit = 974.8 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 42.500 mol/kg expl.
- Total mole number of products = 42.505 mol/kg expl.
- Volume of gaseous products (at SATP) = 1053.53 L/kg expl.
- Mass of gaseous products = 999.6 g/kg expl.
- Mass of condensed products = 0.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.520 g
- Mean molecular mass of all products = 23.527 g
- Specific gas constant = 353.346 J/kg K
- Specific heat capacity at p=const. (Cp) = 1813.67 J/kgK
- Specific heat capacity at V=const. (Cv) = 1460.33 J/molK
- Specific heat ratio (Cp/Cv) = 1.2420

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 213.50 s
- Exhaust (or nozzle exit) velocity = 2094.4 m/s
- Characteristic exhaust velocity (c*) = 1286.1 m/s
- Thrust coefficient (Cf) = 1.628
- Nozzle area expansion ratio (Ae/At) = 8.36
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 643.35 m/s
- Mach number at nozzle exit = 3.255

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.096010 E00 | 3.096009 E01 | 72.8380 |
| O2 = | 1.989103 E-01 | 5.618818 E00 | 13.2191 |
| CO2 = | 1.521456 E-01 | 4.297809 E00 | 10.1112 |
| N2 = | 3.279056 E-02 | 9.262680 E-01 | 2.1792 |
| B(OH)3 = | 2.323635 E-02 | 6.563806 E-01 | 1.5442 |
| I = | 1.062933 E-03 | 3.002572 E-02 | 0.0706 |
| I2 = | 3.535959 E-04 | 9.988379 E-03 | 0.0235 |
| CuO(s) = | 1.477426 E-04 | 4.173432 E-03 | 0.0098 |
| B2O3(l) = | 4.148169 E-05 | 1.171775 E-03 | 0.0028 |
| BHO2 = | 1.854446 E-05 | 5.238439 E-04 | 0.0012 |
| NO = | 3.723428 E-06 | 1.051794 E-04 | 0.0002 |
| IH = | 1.367973 E-06 | 3.864250 E-05 | 0.0001 |
| OH = | 2.276931 E-07 | 6.431876 E-06 | 0.0000 |
| Cu2O(s) = | 5.908529 E-09 | 1.669041 E-07 | 0.0000 |
| INO = | 3.279020 E-10 | 9.262576 E-09 | 0.0000 |
| H2 = | 1.106333 E-10 | 3.125170 E-09 | 0.0000 |
| CO = | 1.117659 E-11 | 3.157164 E-10 | 0.0000 |
| O = | 8.083084 E-12 | 2.283310 E-10 | 0.0000 |
| BO2 = | 4.291869 E-12 | 1.212367 E-10 | 0.0000 |
| B2O3(s) = | 2.677056 E-12 | 7.562150 E-11 | 0.0000 |
| BHO2(s) = | 1.336050 E-12 | 3.774076 E-11 | 0.0000 |
| B2O3 = | 9.754350 E-13 | 2.755409 E-11 | 0.0000 |
| BN = | 7.794098 E-13 | 2.201677 E-11 | 0.0000 |
| BH2 = | 7.373290 E-13 | 2.082807 E-11 | 0.0000 |
| CH4 = | 6.632877 E-13 | 1.873656 E-11 | 0.0000 |
| Cu2O(l) = | 6.059176 E-13 | 1.711596 E-11 | 0.0000 |
| CH3OH = | 5.749529 E-13 | 1.624127 E-11 | 0.0000 |
| ICN = | 4.387356 E-13 | 1.239341 E-11 | 0.0000 |
| HCN = | 4.363848 E-13 | 1.232700 E-11 | 0.0000 |
| CNO = | 3.644820 E-13 | 1.029589 E-11 | 0.0000 |
| BN(s) = | 3.567459 E-13 | 1.007736 E-11 | 0.0000 |
| CHNO = | 2.342539 E-13 | 6.617206 E-12 | 0.0000 |
| N = | 2.176012 E-13 | 6.146801 E-12 | 0.0000 |
| NH2 = | 2.151619 E-13 | 6.077896 E-12 | 0.0000 |
| BO = | 2.030733 E-13 | 5.736416 E-12 | 0.0000 |
| NH3 = | 1.253254 E-13 | 3.540192 E-12 | 0.0000 |
| CuO = | 3.752479 E-14 | 1.060001 E-12 | 0.0000 |
| Cu(OH)2(s) = | 3.203740 E-14 | 9.049927 E-13 | 0.0000 |
| H = | 8.686009 E-15 | 2.453624 E-13 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculations Number 38-48 Were Conducted for [EMIM][$BH_3CN$] and Hydrogen Peroxide (conc. 95%) Bipropellant System with Promoter 5 (8 wt.% in fuel)

(The enthalpy of formation value for [EMIM][$BH_3CN$] fuel was obtained from bomb calorimetry experiments)

# Calculation Number 38

**Combustion conditions (Number 38):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 36.80 %**
2. **Hydrogen peroxide ($H_2O_2$), 57.00 %**
3. **Water ($H_2O$, liquid), 3.00 %**
4. **AKC_298, 3.20 %**

C(0.838) H(3.430) N(0.352) O(1.685) B(0.125) Fe(0.001) I(0.008)

Molecular weight = 47.91
Oxygen balance = -63.30979 %
Enthalpy of formation = -8177.49 kJ/kg
Internal energy of formation = -8036.05 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -941.95 kJ/kg
- Total enthalpy of combustion prod. = -8176.49 kJ/kg
- Entropy of combustion products = 8.33 kJ/K kg
- Isobaric combustion temperature = 850.5 K
- Mole number of gaseous products = 37.338 mol/kg expl.
- Total mole number of products = 37.369 mol/kg expl.
- Volume of gaseous products (at SATP) = 925.58 L/kg expl.
- Mass of gaseous products = 997.8 g/kg expl.
- Mass of condensed products = 2.2 g/kg expl.
- Mean molecular mass of gaseous prod. = 26.724 g
- Mean molecular mass of all products = 26.761 g
- Specific gas constant = 310.431 J/kg K
- Specific heat capacity at p=const. (Cp) = 1938.12 J/kgK
- Specific heat capacity at V=const. (Cv) = 1627.69 J/molK
- Specific heat ratio (Cp/Cv) = 1.1907

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 5.395171 E-01 | 1.126214 E01 | 30.1378 |
| CH4 = | 4.403944 E-01 | 9.193004 E00 | 24.6007 |
| CO2 = | 3.715554 E-01 | 7.756025 E00 | 20.7553 |
| N2 = | 1.752278 E-01 | 3.657789 E00 | 9.7883 |
| B(OH)3 = | 1.250047 E-01 | 2.609408 E00 | 6.9828 |
| H2 = | 1.013563 E-01 | 2.115761 E00 | 5.6618 |
| CO = | 2.614354 E-02 | 5.457329 E-01 | 1.4604 |
| IH = | 8.330859 E-03 | 1.739024 E-01 | 0.4654 |
| FeO(s) = | 1.395571 E-03 | 2.913181 E-02 | 0.0780 |
| NH3 = | 1.151357 E-03 | 2.403397 E-02 | 0.0643 |
| B2O3(s) = | 3.221333 E-05 | 6.724366 E-04 | 0.0018 |
| BHO2(s) = | 2.793692 E-05 | 5.831687 E-04 | 0.0016 |
| I2 = | 1.720094 E-05 | 3.590607 E-04 | 0.0010 |
| I = | 8.105588 E-06 | 1.691999 E-04 | 0.0005 |
| B2O3(l) = | 6.673672 E-06 | 1.393094 E-04 | 0.0004 |
| CH3OH = | 1.814658 E-07 | 3.788004 E-06 | 0.0000 |

| | | | |
|---|---|---|---|
| BHO2 = | 1.160236 E-07 | 2.421933 E-06 | 0.0000 |
| HCN = | 6.788034 E-08 | 1.416967 E-06 | 0.0000 |
| CHNO = | 1.777458 E-08 | 3.710351 E-07 | 0.0000 |
| FeO(l) = | 8.176783 E-10 | 1.706861 E-08 | 0.0000 |
| Fe(s) = | 1.252477 E-10 | 2.614481 E-09 | 0.0000 |
| Fe(OH)2 = | 8.345313 E-11 | 1.742041 E-09 | 0.0000 |
| BN(s) = | 2.261217 E-11 | 4.720173 E-10 | 0.0000 |
| Fe(l) = | 1.528677 E-11 | 3.191033 E-10 | 0.0000 |
| BN = | 6.213112 E-12 | 1.296955 E-10 | 0.0000 |
| N = | 3.399656 E-12 | 7.096606 E-11 | 0.0000 |
| BH2 = | 3.089758 E-12 | 6.449710 E-11 | 0.0000 |
| FeO = | 2.881876 E-12 | 6.015766 E-11 | 0.0000 |
| BO = | 2.442575 E-12 | 5.098749 E-11 | 0.0000 |
| INO = | 2.121005 E-12 | 4.427488 E-11 | 0.0000 |
| BO2 = | 1.983296 E-12 | 4.140028 E-11 | 0.0000 |
| CNO = | 1.934981 E-12 | 4.039172 E-11 | 0.0000 |
| Fe = | 1.901657 E-12 | 3.969610 E-11 | 0.0000 |
| NO = | 1.226110 E-12 | 2.559440 E-11 | 0.0000 |
| H = | 1.118069 E-12 | 2.333911 E-11 | 0.0000 |
| B2O3 = | 9.238796 E-13 | 1.928551 E-11 | 0.0000 |
| NH2 = | 3.783782 E-13 | 7.898449 E-12 | 0.0000 |
| ICN = | 1.304750 E-13 | 2.723598 E-12 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -8322.59 kJ/kg
- Temperature at nozzle throat = 791.0 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 37.204 mol/kg expl.
- Total mole number of products = 37.382 mol/kg expl.
- Volume of gaseous products (at SATP) = 922.25 L/kg expl.
- Mass of gaseous products = 987.5 g/kg expl.
- Mass of condensed products = 12.5 g/kg expl.
- Mean molecular mass of gaseous prod. = 26.544 g
- Mean molecular mass of all products = 26.751 g
- Specific gas constant = 309.314 J/kg K
- Specific heat capacity at p=const. (Cp) = 1901.20 J/kgK
- Specific heat capacity at V=const. (Cv) = 1591.89 J/molK
- Specific heat ratio (Cp/Cv) = 1.1943

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 540.5 m/s
- Sound velocity at throat) = 540.6 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.563
- Pressure ratio (pc/pt) = 1.777

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 5.630292 E-01 | 1.175294 E01 | 31.4400 |
| CH4 = | 4.472995 E-01 | 9.337144 E00 | 24.9775 |
| CO2 = | 3.762230 E-01 | 7.853460 E00 | 21.0086 |
| N2 = | 1.753662 E-01 | 3.660679 E00 | 9.7926 |
| B(OH)3 = | 1.108308 E-01 | 2.313536 E00 | 6.1889 |
| H2 = | 8.571883 E-02 | 1.789336 E00 | 4.7866 |
| CO = | 1.457095 E-02 | 3.041611 E-01 | 0.8137 |

| | | | |
|---|---|---|---|
| IH = | 8.341559 E-03 | 1.741257 E-01 | 0.4658 |
| B2O3(l) = | 7.139882 E-03 | 1.490413 E-01 | 0.3987 |
| FeO(s) = | 1.395561 E-03 | 2.913162 E-02 | 0.0779 |
| NH3 = | 8.746893 E-04 | 1.825869 E-02 | 0.0488 |
| I2 = | 1.380702 E-05 | 2.882145 E-04 | 0.0008 |
| I = | 4.193618 E-06 | 8.753959 E-05 | 0.0002 |
| CH3OH = | 6.543004 E-08 | 1.365818 E-06 | 0.0000 |
| BHO2 = | 2.279790 E-08 | 4.758942 E-07 | 0.0000 |
| HCN = | 1.557305 E-08 | 3.250793 E-07 | 0.0000 |
| BN = | 5.904949 E-09 | 1.232628 E-07 | 0.0000 |
| CHNO = | 4.755742 E-09 | 9.927365 E-08 | 0.0000 |
| B2O3(s) = | 4.138364 E-10 | 8.638621 E-09 | 0.0000 |
| BHO2(s) = | 1.659035 E-10 | 3.463150 E-09 | 0.0000 |
| Fe(OH)2 = | 2.692276 E-11 | 5.619987 E-10 | 0.0000 |
| FeO(l) = | 2.023137 E-11 | 4.223194 E-10 | 0.0000 |
| Fe(s) = | 1.763380 E-12 | 3.680965 E-11 | 0.0000 |
| Fe(l) = | 6.686872 E-13 | 1.395850 E-11 | 0.0000 |
| H = | 1.291045 E-13 | 2.694988 E-12 | 0.0000 |
| BN(s) = | 1.411575 E-14 | 2.946590 E-13 | 0.0000 |
| ICN = | 1.054286 E-14 | 2.200767 E-13 | 0.0000 |
| NH2 = | 7.015876 E-16 | 1.464528 E-14 | 0.0000 |
| B2O3 = | 7.977656 E-19 | 1.665294 E-17 | 0.0000 |
| NO = | 7.827624 E-20 | 1.633976 E-18 | 0.0000 |
| Fe = | 6.151824 E-23 | 1.284161 E-21 | 0.0000 |
| CNO = | 3.310345 E-23 | 6.910174 E-22 | 0.0000 |
| BO2 = | 1.276342 E-23 | 2.664298 E-22 | 0.0000 |
| INO = | 6.623492 E-24 | 1.382619 E-22 | 0.0000 |
| BH2 = | 1.231844 E-25 | 2.571410 E-24 | 0.0000 |
| BO = | 7.085502 E-26 | 1.479062 E-24 | 0.0000 |
| FeO = | 1.494986 E-27 | 3.120707 E-26 | 0.0000 |
| N = | 0.000000 E00 | 0.000000 E00 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9046.10 kJ/kg
- Temperature at nozzle exit = 510.7 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 36.144 mol/kg expl.
- Total mole number of products = 38.724 mol/kg expl.
- Volume of gaseous products (at SATP) = 895.96 L/kg expl.
- Mass of gaseous products = 886.1 g/kg expl.
- Mass of condensed products = 113.8 g/kg expl.
- Mean molecular mass of gaseous prod. = 24.517 g
- Mean molecular mass of all products = 25.823 g
- Specific gas constant = 300.497 J/kg K
- Specific heat capacity at p=const. (Cp) = 1723.55 J/kgK
- Specific heat capacity at V=const. (Cv) = 1423.05 J/molK
- Specific heat ratio (Cp/Cv) = 1.2112

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 134.43 s
- Exhaust (or nozzle exit) velocity = 1318.8 m/s
- Characteristic exhaust velocity (c*) = 776.9 m/s
- Thrust coefficient (Cf) = 1.697
- Nozzle area expansion ratio (Ae/At) = 8.86
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 428.11 m/s
- Mach number at nozzle exit = 3.080

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 6.937554 E-01 | 1.448178 E01 | 37.3972 |
| CH4 = | 4.695093 E-01 | 9.800764 E00 | 25.3091 |
| CO2 = | 3.685238 E-01 | 7.692743 E00 | 19.8654 |
| N2 = | 1.757456 E-01 | 3.668597 E00 | 9.4736 |
| BHO2(s) = | 1.222365 E-01 | 2.551624 E00 | 6.5892 |
| H2 = | 1.260437 E-02 | 2.631097 E-01 | 0.6794 |
| IH = | 8.188875 E-03 | 1.709385 E-01 | 0.4414 |
| B(OH)3 = | 2.874001 E-03 | 5.999328 E-02 | 0.1549 |
| FeO(s) = | 1.395628 E-03 | 2.913301 E-02 | 0.0752 |
| NH3 = | 1.159460 E-04 | 2.420313 E-03 | 0.0063 |
| I2 = 9.219075 E-05 | | 1.924434 E-03 | 0.0050 |
| CO = | 6.038712 E-05 | 1.260550 E-03 | 0.0033 |
| I = 1.100594 E-07 | | 2.297434 E-06 | 0.0000 |
| FeO(l) = | 5.910749 E-09 | 1.233838 E-07 | 0.0000 |
| Fe(s) = | 6.563022 E-10 | 1.369997 E-08 | 0.0000 |
| B2O3(s) = | 3.707575 E-10 | 7.739371 E-09 | 0.0000 |
| Fe(l) = | 7.295841 E-11 | 1.522969 E-09 | 0.0000 |
| BN(s) = | 6.686884 E-11 | 1.395852 E-09 | 0.0000 |
| B2O3(l) = | 4.271666 E-11 | 8.916881 E-10 | 0.0000 |
| CH3OH = | 2.066294 E-11 | 4.313282 E-10 | 0.0000 |
| Fe(OH)2 = | 1.484265 E-11 | 3.098326 E-10 | 0.0000 |
| BN = | 1.352742 E-11 | 2.823778 E-10 | 0.0000 |
| BH2 = | 8.204967 E-12 | 1.712744 E-10 | 0.0000 |
| N = 7.661602 E-12 | | 1.599320 E-10 | 0.0000 |
| FeO = | 7.335569 E-12 | 1.531262 E-10 | 0.0000 |
| BO = | 7.135650 E-12 | 1.489530 E-10 | 0.0000 |
| BO2 = | 6.092556 E-12 | 1.271789 E-10 | 0.0000 |
| Fe = 5.842749 E-12 | | 1.219644 E-10 | 0.0000 |
| CNO = | 5.266425 E-12 | 1.099339 E-10 | 0.0000 |
| B2O3 = | 4.947593 E-12 | 1.032784 E-10 | 0.0000 |
| INO = | 4.868295 E-12 | 1.016231 E-10 | 0.0000 |
| NO = | 3.955861 E-12 | 8.257654 E-11 | 0.0000 |
| NH2 = | 2.552011 E-12 | 5.327191 E-11 | 0.0000 |
| H = 1.857824 E-12 | | 3.878111 E-11 | 0.0000 |
| ICN = | 1.840323 E-12 | 3.841579 E-11 | 0.0000 |
| BHO2 = | 5.110321 E-13 | 1.066753 E-11 | 0.0000 |
| HCN = | 1.082511 E-13 | 2.259686 E-12 | 0.0000 |
| CHNO = | 8.058522 E-14 | 1.682175 E-12 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 39

**Combustion conditions (Number 39):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 30.73 %**
2. **Hydrogen peroxide ($H_2O_2$), 63.27 %**
3. **Water ($H_2O$, liquid), 3.33 %**
4. **AKC_298, 2.67 %**

C(0.649) H(3.108) N(0.272) O(1.736) B(0.097) Fe(0.001) I(0.006)

Molecular weight = 44.45
Oxygen balance = -45.49397 %
Enthalpy of formation = -7823.62 kJ/kg
Internal energy of formation = -7680.97 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -1386.81 kJ/kg
- Total enthalpy of combustion prod. = -7823.17 kJ/kg
- Entropy of combustion products = 9.50 kJ/K kg
- Isobaric combustion temperature = 1060.6 K
- Mole number of gaseous products = 43.621 mol/kg expl.
- Total mole number of products = 43.645 mol/kg expl.
- Volume of gaseous products (at SATP) = 1081.32 L/kg expl.
- Mass of gaseous products = 998.3 g/kg expl.
- Mass of condensed products = 1.8 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.885 g
- Mean molecular mass of all products = 22.912 g
- Specific gas constant = 362.664 J/kg K
- Specific heat capacity at p=const. (Cp) = 2040.29 J/kgK
- Specific heat capacity at V=const. (Cv) = 1677.63 J/molK
- Specific heat ratio (Cp/Cv) = 1.2162

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 6.650776 E-01 | 1.496202 E01 | 34.2808 |
| H2 = | 3.842096 E-01 | 8.643433 E00 | 19.8037 |
| CO2 = | 3.065728 E-01 | 6.896864 E00 | 15.8020 |
| CH4 = | 1.770163 E-01 | 3.982276 E00 | 9.1242 |
| CO = | 1.657838 E-01 | 3.729582 E00 | 8.5452 |
| N2 = | 1.354981 E-01 | 3.048254 E00 | 6.9841 |
| B(OH)3 = | 9.689921 E-02 | 2.179909 E00 | 4.9946 |
| IH = | 6.442823 E-03 | 1.449420 E-01 | 0.3321 |
| NH3 = | 1.440385 E-03 | 3.240386 E-02 | 0.0742 |
| FeO(s) = | 1.080459 E-03 | 2.430671 E-02 | 0.0557 |
| I = | 3.106012 E-05 | 6.987489 E-04 | 0.0016 |
| BHO2 = | 1.582948 E-05 | 3.561103 E-04 | 0.0008 |
| B2O3(l) = | 1.019969 E-05 | 2.294590 E-04 | 0.0005 |
| I2 = | 4.431261 E-06 | 9.968859 E-05 | 0.0002 |
| HCN = | 1.810187 E-06 | 4.072315 E-05 | 0.0001 |
| CH3OH = | 7.234349 E-07 | 1.627487 E-05 | 0.0000 |

| | | | |
|---|---|---|---|
| CHNO = | 2.112547 E-07 | 4.752525 E-06 | 0.0000 |
| Fe(OH)2 = | 1.752858 E-08 | 3.943346 E-07 | 0.0000 |
| FeO(l) = | 1.781294 E-09 | 4.007318 E-08 | 0.0000 |
| H = | 1.126469 E-09 | 2.534180 E-08 | 0.0000 |
| Fe(s) = | 4.446096 E-11 | 1.000223 E-09 | 0.0000 |
| B2O3(s) = | 2.138068 E-11 | 4.809939 E-10 | 0.0000 |
| BN(s) = | 1.378779 E-11 | 3.101793 E-10 | 0.0000 |
| BHO2(s) = | 6.238505 E-12 | 1.403455 E-10 | 0.0000 |
| BN = | 4.049909 E-12 | 9.110943 E-11 | 0.0000 |
| Fe(l) = | 3.350869 E-12 | 7.538337 E-11 | 0.0000 |
| NH2 = | 2.638162 E-12 | 5.934983 E-11 | 0.0000 |
| N = | 2.073899 E-12 | 4.665580 E-11 | 0.0000 |
| B2O3 = | 1.737767 E-12 | 3.909395 E-11 | 0.0000 |
| BH2 = | 1.567201 E-12 | 3.525679 E-11 | 0.0000 |
| FeO = | 1.438093 E-12 | 3.235228 E-11 | 0.0000 |
| INO = | 1.394101 E-12 | 3.136261 E-11 | 0.0000 |
| BO = | 1.017145 E-12 | 2.288237 E-11 | 0.0000 |
| CNO = | 1.004903 E-12 | 2.260695 E-11 | 0.0000 |
| BO2 = | 7.592287 E-13 | 1.708011 E-11 | 0.0000 |
| ICN = | 6.285987 E-13 | 1.414137 E-11 | 0.0000 |
| Fe = | 5.738225 E-13 | 1.290909 E-11 | 0.0000 |
| NO = | 3.913627 E-13 | 8.804353 E-12 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -8040.53 kJ/kg
- Temperature at nozzle throat = 996.7 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 43.004 mol/kg expl.
- Total mole number of products = 43.077 mol/kg expl.
- Volume of gaseous products (at SATP) = 1066.04 L/kg expl.
- Mass of gaseous products = 994.9 g/kg expl.
- Mass of condensed products = 5.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.135 g
- Mean molecular mass of all products = 23.215 g
- Specific gas constant = 357.539 J/kg K
- Specific heat capacity at p=const. (Cp) = 2010.28 J/kgK
- Specific heat capacity at V=const. (Cv) = 1652.74 J/molK
- Specific heat ratio (Cp/Cv) = 1.2163

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 659.3 m/s
- Sound velocity at throat) = 658.4 m/s
- Mach number at nozzle throat = 1.001
- Critical pressure ratio (pt/pc) = 0.556
- Pressure ratio (pc/pt) = 1.799

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 6.675742 E-01 | 1.501819 E01 | 34.8636 |
| H2 = | 3.587345 E-01 | 8.070327 E00 | 18.7347 |
| CO2 = | 3.253876 E-01 | 7.320135 E00 | 16.9932 |
| CH4 = | 1.919385 E-01 | 4.317974 E00 | 10.0239 |
| N2 = | 1.356587 E-01 | 3.051867 E00 | 7.0847 |
| CO = | 1.320484 E-01 | 2.970647 E00 | 6.8961 |
| B(OH)3 = | 9.264205 E-02 | 2.084137 E00 | 4.8382 |

| | | | |
|---|---|---|---|
| IH = | 6.454572 E-03 | 1.452063 E-01 | 0.3371 |
| B2O3(l) = | 2.143467 E-03 | 4.822085 E-02 | 0.1119 |
| NH3 = | 1.120383 E-03 | 2.520488 E-02 | 0.0585 |
| FeO(s) = | 1.080448 E-03 | 2.430647 E-02 | 0.0564 |
| I = | 2.241605 E-05 | 5.042862 E-04 | 0.0012 |
| BHO2 = | 6.484674 E-06 | 1.458835 E-04 | 0.0003 |
| I2 = | 2.878914 E-06 | 6.476594 E-05 | 0.0002 |
| HCN = | 7.704090 E-07 | 1.733163 E-05 | 0.0000 |
| CH3OH = | 3.436255 E-07 | 7.730426 E-06 | 0.0000 |
| CHNO = | 8.957229 E-08 | 2.015077 E-06 | 0.0000 |
| Fe(OH)2 = | 9.542462 E-09 | 2.146735 E-07 | 0.0000 |
| BN = | 3.213825 E-09 | 7.230033 E-08 | 0.0000 |
| H = | 2.840894 E-10 | 6.391063 E-09 | 0.0000 |
| B2O3(s) = | 5.199156 E-11 | 1.169636 E-09 | 0.0000 |
| FeO(l) = | 5.087041 E-11 | 1.144414 E-09 | 0.0000 |
| Fe(s) = | 1.377420 E-11 | 3.098734 E-10 | 0.0000 |
| BHO2(s) = | 1.343275 E-11 | 3.021919 E-10 | 0.0000 |
| Fe(l) = | 6.796073 E-12 | 1.528889 E-10 | 0.0000 |
| ICN = | 8.475289 E-13 | 1.906657 E-11 | 0.0000 |
| NH2 = | 8.434784 E-13 | 1.897545 E-11 | 0.0000 |
| B2O3 = | 2.296504 E-13 | 5.166367 E-12 | 0.0000 |
| BN(s) = | 7.517269 E-14 | 1.691134 E-12 | 0.0000 |
| NO = | 8.198762 E-16 | 1.844448 E-14 | 0.0000 |
| Fe = | 1.599311 E-16 | 3.597916 E-15 | 0.0000 |
| BO2 = | 1.200666 E-17 | 2.701098 E-16 | 0.0000 |
| CNO = | 1.184249 E-18 | 2.664166 E-17 | 0.0000 |
| BO = | 6.790460 E-19 | 1.527627 E-17 | 0.0000 |
| INO = | 2.390264 E-20 | 5.377296 E-19 | 0.0000 |
| FeO = | 1.638661 E-20 | 3.686441 E-19 | 0.0000 |
| BH2 = | 1.962146 E-21 | 4.414173 E-20 | 0.0000 |
| N = | 9.098295 E-24 | 2.046812 E-22 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9087.81 kJ/kg
- Temperature at nozzle exit = 675.8 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 40.305 mol/kg expl.
- Total mole number of products = 41.179 mol/kg expl.
- Volume of gaseous products (at SATP) = 999.11 L/kg expl.
- Mass of gaseous products = 939.1 g/kg expl.
- Mass of condensed products = 60.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.300 g
- Mean molecular mass of all products = 24.285 g
- Specific gas constant = 335.093 J/kg K
- Specific heat capacity at p=const. (Cp) = 1819.45 J/kgK
- Specific heat capacity at V=const. (Cv) = 1484.36 J/molK
- Specific heat ratio (Cp/Cv) = 1.2257

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 162.12 s
- Exhaust (or nozzle exit) velocity = 1590.4 m/s
- Characteristic exhaust velocity (c*) = 912.2 m/s
- Thrust coefficient (Cf) = 1.743
- Nozzle area expansion ratio (Ae/At) = 8.62
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 524.81 m/s

- Mach number at nozzle exit = 3.030

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 8.066755 E-01 | 1.814750 E01 | 44.0700 |
| CO2 = | 3.714521 E-01 | 8.356431 E00 | 20.2930 |
| CH4 = | 2.702094 E-01 | 6.078809 E00 | 14.7620 |
| H2 = | 1.713495 E-01 | 3.854792 E00 | 9.3611 |
| N2 = | 1.361168 E-01 | 3.062173 E00 | 7.4363 |
| B2O3(s) = | 3.777739 E-02 | 8.498650 E-01 | 2.0638 |
| B(OH)3 = | 2.138060 E-02 | 4.809920 E-01 | 1.1681 |
| CO = | 7.714198 E-03 | 1.735437 E-01 | 0.4214 |
| IH = | 6.477604 E-03 | 1.457244 E-01 | 0.3539 |
| FeO(s) = | 1.080483 E-03 | 2.430725 E-02 | 0.0590 |
| NH3 = | 2.049441 E-04 | 4.610557 E-03 | 0.0112 |
| I = 2.992115 E-06 | | 6.731260 E-05 | 0.0002 |
| I2 = 1.075025 E-06 | | 2.418447 E-05 | 0.0001 |
| B2O3(l) = | 3.385351 E-08 | 7.615910 E-07 | 0.0000 |
| FeO(l) = | 2.239106 E-09 | 5.037241 E-08 | 0.0000 |
| CH3OH = | 1.298673 E-09 | 2.921580 E-08 | 0.0000 |
| BHO2 = | 1.030846 E-09 | 2.319058 E-08 | 0.0000 |
| HCN = | 2.603697 E-10 | 5.857449 E-09 | 0.0000 |
| Fe(s) = | 2.421019 E-10 | 5.446485 E-09 | 0.0000 |
| CHNO = | 6.582344 E-11 | 1.480808 E-09 | 0.0000 |
| BHO2(s) = | 4.488130 E-11 | 1.009679 E-09 | 0.0000 |
| BN(s) = | 2.948066 E-11 | 6.632165 E-10 | 0.0000 |
| Fe(l) = | 2.642780 E-11 | 5.945371 E-10 | 0.0000 |
| BN = | 8.709700 E-12 | 1.959392 E-10 | 0.0000 |
| N = 4.937009 E-12 | | 1.110662 E-10 | 0.0000 |
| BH2 = | 4.720611 E-12 | 1.061980 E-10 | 0.0000 |
| FeO = | 4.350021 E-12 | 9.786095 E-11 | 0.0000 |
| BO = | 3.880695 E-12 | 8.730268 E-11 | 0.0000 |
| INO = | 3.376536 E-12 | 7.596079 E-11 | 0.0000 |
| BO2 = | 3.299922 E-12 | 7.423722 E-11 | 0.0000 |
| Fe(OH)2 = | 3.290197 E-12 | 7.401844 E-11 | 0.0000 |
| CNO = | 3.269223 E-12 | 7.354661 E-11 | 0.0000 |
| Fe = 3.069498 E-12 | | 6.905346 E-11 | 0.0000 |
| NO = | 2.270061 E-12 | 5.106878 E-11 | 0.0000 |
| B2O3 = | 2.084397 E-12 | 4.689196 E-11 | 0.0000 |
| NH2 = | 1.232390 E-12 | 2.772467 E-11 | 0.0000 |
| ICN = | 9.363646 E-13 | 2.106508 E-11 | 0.0000 |
| H = 4.595273 E-13 | | 1.033783 E-11 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 40

**Combustion conditions (Number 40):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 26.86 %**
2. **Hydrogen peroxide ($H_2O_2$), 67.26 %**
3. **Water ($H_2O$, liquid), 3.54 %**
4. **AKC_298, 2.34 %**

C(0.543) H(2.926) N(0.228) O(1.764) B(0.081) Fe(0.001) I(0.005)

Molecular weight = 42.5
Oxygen balance = -34.14476 %
Enthalpy of formation = -7598.98 kJ/kg
Internal energy of formation = -7455.56 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -1672.11 kJ/kg
- Total enthalpy of combustion prod. = -7600.57 kJ/kg
- Entropy of combustion products = 10.13 kJ/K kg
- Isobaric combustion temperature = 1193.9 K
- Mole number of gaseous products = 47.466 mol/kg expl.
- Total mole number of products = 47.488 mol/kg expl.
- Volume of gaseous products (at SATP) = 1176.63 L/kg expl.
- Mass of gaseous products = 998.4 g/kg expl.
- Mass of condensed products = 1.6 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.035 g
- Mean molecular mass of all products = 21.058 g
- Specific gas constant = 394.629 J/kg K
- Specific heat capacity at p=const. (Cp) = 2071.12 J/kgK
- Specific heat capacity at V=const. (Cv) = 1676.49 J/molK
- Specific heat ratio (Cp/Cv) = 1.2354

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 7.537500 E-01 | 1.773461 E01 | 37.3457 |
| H2 = | 5.201451 E-01 | 1.223824 E01 | 25.7714 |
| CO2 = | 2.559921 E-01 | 6.023113 E00 | 12.6835 |
| CO = | 2.549024 E-01 | 5.997474 E00 | 12.6295 |
| N2 = | 1.133416 E-01 | 2.666759 E00 | 5.6157 |
| B(OH)3 = | 8.082791 E-02 | 1.901760 E00 | 4.0047 |
| CH4 = | 3.184193 E-02 | 7.491931 E-01 | 1.5777 |
| IH = | 5.363395 E-03 | 1.261927 E-01 | 0.2657 |
| NH3 = | 1.001439 E-03 | 2.356237 E-02 | 0.0496 |
| FeO(s) = | 9.051952 E-04 | 2.129789 E-02 | 0.0448 |
| BHO2 = | 1.292030 E-04 | 3.039954 E-03 | 0.0064 |
| I = | 6.446877 E-05 | 1.516854 E-03 | 0.0032 |
| B2O3(l) = | 3.472669 E-05 | 8.170673 E-04 | 0.0017 |
| HCN = | 3.090942 E-06 | 7.272526 E-05 | 0.0002 |
| I2 = | 2.240229 E-06 | 5.270925 E-05 | 0.0001 |
| CH3OH = | 4.963099 E-07 | 1.167743 E-05 | 0.0000 |

| | | | |
|---|---|---|---|
| CHNO = | 3.712117 E-07 | 8.734059 E-06 | 0.0000 |
| Fe(OH)2 = | 2.243537 E-07 | 5.278708 E-06 | 0.0000 |
| H = | 2.146033 E-08 | 5.049296 E-07 | 0.0000 |
| FeO(l) = | 2.583015 E-09 | 6.077450 E-08 | 0.0000 |
| B2O3(s) = | 4.552768 E-10 | 1.071199 E-08 | 0.0000 |
| Fe(s) = | 2.644487 E-10 | 6.222083 E-09 | 0.0000 |
| B2O3 = | 2.030030 E-10 | 4.776358 E-09 | 0.0000 |
| BN(s) = | 1.624407 E-10 | 3.821988 E-09 | 0.0000 |
| NH2 = | 5.495657 E-11 | 1.293046 E-09 | 0.0000 |
| Fe(l) = | 3.693146 E-11 | 8.689423 E-10 | 0.0000 |
| BHO2(s) = | 3.641738 E-11 | 8.568467 E-10 | 0.0000 |
| BN = | 3.364114 E-11 | 7.915259 E-10 | 0.0000 |
| N = | 1.707584 E-11 | 4.017691 E-10 | 0.0000 |
| INO = | 1.264467 E-11 | 2.975102 E-10 | 0.0000 |
| BH2 = | 1.195948 E-11 | 2.813888 E-10 | 0.0000 |
| ICN = | 1.022676 E-11 | 2.406203 E-10 | 0.0000 |
| FeO = | 1.001734 E-11 | 2.356931 E-10 | 0.0000 |
| CNO = | 8.579635 E-12 | 2.018660 E-10 | 0.0000 |
| BO = | 6.306920 E-12 | 1.483924 E-10 | 0.0000 |
| BO2 = | 4.318094 E-12 | 1.015983 E-10 | 0.0000 |
| Fe = | 2.195725 E-12 | 5.166213 E-11 | 0.0000 |
| NO = | 2.170623 E-12 | 5.107152 E-11 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7867.11 kJ/kg
- Temperature at nozzle throat = 1108.9 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 46.825 mol/kg expl.
- Total mole number of products = 46.847 mol/kg expl.
- Volume of gaseous products (at SATP) = 1160.75 L/kg expl.
- Mass of gaseous products = 998.5 g/kg expl.
- Mass of condensed products = 1.5 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.324 g
- Mean molecular mass of all products = 21.347 g
- Specific gas constant = 389.306 J/kg K
- Specific heat capacity at p=const. (Cp) = 2039.74 J/kgK
- Specific heat capacity at V=const. (Cv) = 1650.43 J/molK
- Specific heat ratio (Cp/Cv) = 1.2359

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 730.1 m/s
- Sound velocity at throat) = 730.4 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.553
- Pressure ratio (pc/pt) = 1.807

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 7.423581 E-01 | 1.746658 E01 | 37.2846 |
| H2 = | 5.043352 E-01 | 1.186626 E01 | 25.3300 |
| CO2 = | 2.808330 E-01 | 6.607583 E00 | 14.1047 |
| CO = | 2.164324 E-01 | 5.092332 E00 | 10.8702 |
| N2 = | 1.134257 E-01 | 2.668738 E00 | 5.6968 |
| B(OH)3 = | 8.097364 E-02 | 1.905189 E00 | 4.0669 |
| CH4 = | 4.547288 E-02 | 1.069909 E00 | 2.2839 |

| | | | |
|---|---|---|---|
| IH = | 5.384323 E-03 | 1.266851 E-01 | 0.2704 |
| FeO(s) = | 9.052928 E-04 | 2.130019 E-02 | 0.0455 |
| NH3 = | 8.349437 E-04 | 1.964498 E-02 | 0.0419 |
| BHO2 = | 5.296116 E-05 | 1.246097 E-03 | 0.0027 |
| I = | 4.469814 E-05 | 1.051681 E-03 | 0.0022 |
| I2 = | 1.661466 E-06 | 3.909182 E-05 | 0.0001 |
| HCN = | 1.603322 E-06 | 3.772377 E-05 | 0.0001 |
| CH3OH = | 2.839806 E-07 | 6.681641 E-06 | 0.0000 |
| CHNO = | 1.667206 E-07 | 3.922687 E-06 | 0.0000 |
| Fe(OH)2 = | 9.765296 E-08 | 2.297628 E-06 | 0.0000 |
| H = | 5.170867 E-09 | 1.216628 E-07 | 0.0000 |
| BN = | 4.529043 E-09 | 1.065616 E-07 | 0.0000 |
| B2O3(l) = | 1.553247 E-09 | 3.654558 E-08 | 0.0000 |
| FeO(l) = | 8.196569 E-11 | 1.928530 E-09 | 0.0000 |
| B2O3 = | 2.564945 E-11 | 6.034934 E-10 | 0.0000 |
| B2O3(s) = | 2.537736 E-11 | 5.970915 E-10 | 0.0000 |
| Fe(s) = | 2.527248 E-11 | 5.946237 E-10 | 0.0000 |
| Fe(l) = | 1.362869 E-11 | 3.206628 E-10 | 0.0000 |
| NH2 = | 1.017769 E-11 | 2.394658 E-10 | 0.0000 |
| BHO2(s) = | 6.079046 E-12 | 1.430309 E-10 | 0.0000 |
| ICN = | 2.462675 E-12 | 5.794308 E-11 | 0.0000 |
| BN(s) = | 8.162222 E-14 | 1.920449 E-12 | 0.0000 |
| Fe = | 3.940563 E-14 | 9.271558 E-13 | 0.0000 |
| NO = | 3.810385 E-14 | 8.965267 E-13 | 0.0000 |
| BO2 = | 2.697949 E-15 | 6.347871 E-14 | 0.0000 |
| BO = | 2.777622 E-16 | 6.535330 E-15 | 0.0000 |
| CNO = | 5.035311 E-17 | 1.184734 E-15 | 0.0000 |
| FeO = | 8.202965 E-18 | 1.930035 E-16 | 0.0000 |
| BH2 = | 8.990451 E-19 | 2.115319 E-17 | 0.0000 |
| INO = | 7.226357 E-19 | 1.700254 E-17 | 0.0000 |
| N = | 4.097434 E-21 | 9.640650 E-20 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9118.82 kJ/kg
- Temperature at nozzle exit = 751.0 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 43.265 mol/kg expl.
- Total mole number of products = 43.941 mol/kg expl.
- Volume of gaseous products (at SATP) = 1072.50 L/kg expl.
- Mass of gaseous products = 952.9 g/kg expl.
- Mass of condensed products = 47.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.025 g
- Mean molecular mass of all products = 22.758 g
- Specific gas constant = 359.705 J/kg K
- Specific heat capacity at p=const. (Cp) = 1873.65 J/kgK
- Specific heat capacity at V=const. (Cv) = 1513.95 J/molK
- Specific heat ratio (Cp/Cv) = 1.2376

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 177.63 s
- Exhaust (or nozzle exit) velocity = 1742.6 m/s
- Characteristic exhaust velocity (c*) = 999.4 m/s
- Thrust coefficient (Cf) = 1.744
- Nozzle area expansion ratio (Ae/At) = 8.42
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 577.81 m/s
- Mach number at nozzle exit = 3.016

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 8.183565 E-01 | 1.925471 E01 | 43.8194 |
| CO2 = | 3.781167 E-01 | 8.896523 E00 | 20.2465 |
| H2 = | 3.329875 E-01 | 7.834698 E00 | 17.8300 |
| CH4 = | 1.353255 E-01 | 3.184006 E00 | 7.2461 |
| N2 = | 1.137404 E-01 | 2.676142 E00 | 6.0903 |
| CO = | 2.929822 E-02 | 6.893433 E-01 | 1.5688 |
| B(OH)3 = | 2.537070 E-02 | 5.969347 E-01 | 1.3585 |
| B2O3(s) = | 2.310090 E-02 | 5.435297 E-01 | 1.2370 |
| IH = | 5.420715 E-03 | 1.275413 E-01 | 0.2903 |
| B2O3(l) = | 4.727020 E-03 | 1.112197 E-01 | 0.2531 |
| FeO(s) = | 9.054070 E-04 | 2.130288 E-02 | 0.0485 |
| NH3 = | 2.072870 E-04 | 4.877153 E-03 | 0.0111 |
| I = 5.563863 E-06 | 1.309094 E-04 | 0.0003 | |
| I2 = 3.032298 E-06 | 7.134546 E-05 | 0.0002 | |
| BHO2 = | 2.777507 E-08 | 6.535060 E-07 | 0.0000 |
| HCN = | 3.034775 E-09 | 7.140373 E-08 | 0.0000 |
| CH3OH = | 2.488416 E-09 | 5.854873 E-08 | 0.0000 |
| FeO(l) = | 1.295595 E-09 | 3.048343 E-08 | 0.0000 |
| CHNO = | 2.930361 E-10 | 6.894702 E-09 | 0.0000 |
| Fe(s) = | 1.729112 E-10 | 4.068344 E-09 | 0.0000 |
| Fe(l) = | 1.653829 E-10 | 3.891214 E-09 | 0.0000 |
| BN(s) = | 3.151909 E-11 | 7.415972 E-10 | 0.0000 |
| BHO2(s) = | 1.062485 E-11 | 2.499868 E-10 | 0.0000 |
| BN = | 7.297515 E-12 | 1.716997 E-10 | 0.0000 |
| N = 4.097798 E-12 | 9.641508 E-11 | 0.0000 | |
| BH2 = | 3.729808 E-12 | 8.775682 E-11 | 0.0000 |
| FeO = | 3.420558 E-12 | 8.048062 E-11 | 0.0000 |
| BO = | 2.936284 E-12 | 6.908640 E-11 | 0.0000 |
| INO = | 2.922174 E-12 | 6.875438 E-11 | 0.0000 |
| CNO = | 2.665212 E-12 | 6.270846 E-11 | 0.0000 |
| BO2 = | 2.486745 E-12 | 5.850941 E-11 | 0.0000 |
| Fe(OH)2 = | 2.449905 E-12 | 5.764262 E-11 | 0.0000 |
| Fe = 2.215386 E-12 | 5.212474 E-11 | 0.0000 | |
| NO = | 1.742766 E-12 | 4.100469 E-11 | 0.0000 |
| B2O3 = | 1.313966 E-12 | 3.091565 E-11 | 0.0000 |
| NH2 = | 8.447990 E-13 | 1.987686 E-11 | 0.0000 |
| ICN = | 6.946709 E-13 | 1.634457 E-11 | 0.0000 |
| H = 3.138563 E-14 | 7.384571 E-13 | 0.0000 | |

Notes:

- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 41

**Combustion conditions (Number 41):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 23.00 %**
2. **Hydrogen peroxide ($H_2O_2$), 71.25 %**
3. **Water ($H_2O$, liquid), 3.75 %**
4. **AKC_298, 2.00 %**

C(0.445) H(2.760) N(0.187) O(1.790) B(0.066) Fe(0.001) I(0.004)

Molecular weight = 40.72
Oxygen balance = -22.81186 %
Enthalpy of formation = -7373.58 kJ/kg
Internal energy of formation = -7229.39 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -2436.13 kJ/kg
- Total enthalpy of combustion prod. = -7373.67 kJ/kg
- Entropy of combustion products = 10.60 kJ/K kg
- Isobaric combustion temperature = 1581.0 K
- Mole number of gaseous products = 46.531 mol/kg expl.
- Total mole number of products = 46.548 mol/kg expl.
- Volume of gaseous products (at SATP) = 1153.45 L/kg expl.
- Mass of gaseous products = 998.7 g/kg expl.
- Mass of condensed products = 1.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.464 g
- Mean molecular mass of all products = 21.483 g
- Specific gas constant = 386.855 J/kg K
- Specific heat capacity at p=const. (Cp) = 2157.03 J/kgK
- Specific heat capacity at V=const. (Cv) = 1770.18 J/molK
- Specific heat ratio (Cp/Cv) = 1.2185

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 9.433417 E-01 | 2.316939 E01 | 49.7751 |
| H2 = | 3.415821 E-01 | 8.389589 E00 | 18.0235 |
| CO = | 2.362665 E-01 | 5.802935 E00 | 12.4665 |
| CO2 = | 2.088915 E-01 | 5.130578 E00 | 11.0221 |
| N2 = | 9.331874 E-02 | 2.291999 E00 | 4.9239 |
| B(OH)3 = | 5.941507 E-02 | 1.459292 E00 | 3.1350 |
| BHO2 = | 7.038380 E-03 | 1.728695 E-01 | 0.3714 |
| IH = | 3.989387 E-03 | 9.798323 E-02 | 0.2105 |
| FeO(s) = | 6.919555 E-04 | 1.699510 E-02 | 0.0365 |
| I = | 4.531702 E-04 | 1.113030 E-02 | 0.0239 |
| NH3 = | 1.312318 E-04 | 3.223180 E-03 | 0.0069 |
| CH4 = | 2.762761 E-05 | 6.785610 E-04 | 0.0015 |
| Fe(OH)2 = | 2.623065 E-05 | 6.442504 E-04 | 0.0014 |
| FeO(l) = | 2.311584 E-05 | 5.677476 E-04 | 0.0012 |
| H = | 4.430548 E-06 | 1.088186 E-04 | 0.0002 |
| I2 = | 2.646757 E-06 | 6.500693 E-05 | 0.0001 |

| | | | |
|---|---|---|---|
| B2O3 = | 2.018835 E-06 | 4.958455 E-05 | 0.0001 |
| HCN = | 1.205524 E-06 | 2.960884 E-05 | 0.0001 |
| OH = | 4.086882 E-07 | 1.003778 E-05 | 0.0000 |
| CHNO = | 3.267376 E-07 | 8.024993 E-06 | 0.0000 |
| CH3OH = | 1.699919 E-08 | 4.175166 E-07 | 0.0000 |
| Fe = 6.409235 E-09 | 1.574171 E-07 | 0.0000 | |
| BO2 = | 3.361954 E-09 | 8.257286 E-08 | 0.0000 |
| NH2 = | 2.887445 E-09 | 7.091847 E-08 | 0.0000 |
| NO = | 2.694993 E-09 | 6.619165 E-08 | 0.0000 |
| BO = | 5.124465 E-10 | 1.258619 E-08 | 0.0000 |
| B2O3(l) = | 6.326970 E-11 | 1.553966 E-09 | 0.0000 |
| FeO = | 2.261800 E-11 | 5.555201 E-10 | 0.0000 |
| ICN = | 1.844567 E-11 | 4.530436 E-10 | 0.0000 |
| Fe(s) = | 1.445184 E-11 | 3.549513 E-10 | 0.0000 |
| Fe(l) = | 1.065061 E-11 | 2.615894 E-10 | 0.0000 |
| B2O3(s) = | 3.198869 E-12 | 7.856733 E-11 | 0.0000 |
| O2 = | 2.862986 E-12 | 7.031773 E-11 | 0.0000 |
| O = 1.310072 E-12 | 3.217665 E-11 | 0.0000 | |
| BHO2(s) = | 1.104901 E-12 | 2.713744 E-11 | 0.0000 |
| CNO = | 3.487917 E-13 | 8.566663 E-12 | 0.0000 |
| BH2 = | 1.773540 E-13 | 4.355987 E-12 | 0.0000 |
| INO = | 7.393170 E-14 | 1.815835 E-12 | 0.0000 |
| BN(s) = | 1.798816 E-14 | 4.418067 E-13 | 0.0000 |
| N = 1.485457 E-14 | 3.648427 E-13 | 0.0000 | |
| BN = | 1.051836 E-19 | 2.583411 E-18 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7712.92 kJ/kg
- Temperature at nozzle throat = 1436.4 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 46.435 mol/kg expl.
- Total mole number of products = 46.453 mol/kg expl.
- Volume of gaseous products (at SATP) = 1151.09 L/kg expl.
- Mass of gaseous products = 998.7 g/kg expl.
- Mass of condensed products = 1.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.508 g
- Mean molecular mass of all products = 21.527 g
- Specific gas constant = 386.064 J/kg K
- Specific heat capacity at p=const. (Cp) = 2113.79 J/kgK
- Specific heat capacity at V=const. (Cv) = 1727.73 J/molK
- Specific heat ratio (Cp/Cv) = 1.2235

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 823.7 m/s
- Sound velocity at throat ) = 823.7 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.559
- Pressure ratio (pc/pt) = 1.790

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 9.222375 E-01 | 2.265105 E01 | 48.7608 |
| H2 = | 3.588338 E-01 | 8.813308 E00 | 18.9724 |
| CO2 = | 2.262772 E-01 | 5.557588 E00 | 11.9638 |
| CO = | 2.188542 E-01 | 5.375272 E00 | 11.5713 |

| | | | | |
|---|---|---|---|---|
| N2 = | 9.332382 E-02 | | 2.292124 E00 | 4.9342 |
| B(OH)3 = | 6.317449 E-02 | | 1.551627 E00 | 3.3402 |
| IH = | 4.127188 E-03 | | 1.013678 E-01 | 0.2182 |
| BHO2 = | 3.282415 E-03 | | 8.061931 E-02 | 0.1735 |
| FeO(s) = | 7.306742 E-04 | | 1.794607 E-02 | 0.0386 |
| I = | 3.168510 E-04 | | 7.782170 E-03 | 0.0168 |
| NH3 = | 1.217463 E-04 | | 2.990208 E-03 | 0.0064 |
| CH4 = | 5.485647 E-05 | | 1.347328 E-03 | 0.0029 |
| Fe(OH)2 = | 1.062239 E-05 | | 2.608963 E-04 | 0.0006 |
| I2 = | 1.905710 E-06 | | 4.680609 E-05 | 0.0001 |
| H = | 1.095416 E-06 | | 2.690449 E-05 | 0.0001 |
| HCN = | 6.984172 E-07 | | 1.715381 E-05 | 0.0000 |
| B2O3 = | 2.984418 E-07 | | 7.330020 E-06 | 0.0000 |
| CHNO = | 1.670142 E-07 | | 4.102031 E-06 | 0.0000 |
| OH = | 5.875525 E-08 | | 1.443086 E-06 | 0.0000 |
| CH3OH = | 1.230291 E-08 | | 3.021716 E-07 | 0.0000 |
| FeO(l) = | 1.094284 E-08 | | 2.687667 E-07 | 0.0000 |
| Fe = | 8.190109 E-10 | | 2.011570 E-08 | 0.0000 |
| NH2 = | 6.654761 E-10 | | 1.634474 E-08 | 0.0000 |
| NO = | 2.852827 E-10 | | 7.006822 E-09 | 0.0000 |
| BO2 = | 2.493566 E-10 | | 6.124440 E-09 | 0.0000 |
| B2O3(l) = | 1.436702 E-10 | | 3.528681 E-09 | 0.0000 |
| BO = | 3.205096 E-11 | | 7.872029 E-10 | 0.0000 |
| Fe(s) = | 2.358120 E-11 | | 5.791772 E-10 | 0.0000 |
| Fe(l) = | 1.756328 E-11 | | 4.313713 E-10 | 0.0000 |
| B2O3(s) = | 7.580731 E-12 | | 1.861901 E-10 | 0.0000 |
| ICN = | 6.699522 E-12 | | 1.645468 E-10 | 0.0000 |
| FeO = | 2.252968 E-12 | | 5.533508 E-11 | 0.0000 |
| BHO2(s) = | 1.551667 E-12 | | 3.811045 E-11 | 0.0000 |
| O2 = | 1.641447 E-13 | | 4.031553 E-12 | 0.0000 |
| O = | 1.462504 E-13 | | 3.592053 E-12 | 0.0000 |
| CNO = | 4.347997 E-14 | | 1.067911 E-12 | 0.0000 |
| BN(s) = | 2.279233 E-14 | | 5.598018 E-13 | 0.0000 |
| BH2 = | 1.155171 E-14 | | 2.837212 E-13 | 0.0000 |
| INO = | 4.649303 E-15 | | 1.141914 E-13 | 0.0000 |
| N = | 5.523651 E-16 | | 1.356663 E-14 | 0.0000 |
| BN = | 8.440433 E-22 | | 2.073053 E-20 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9230.32 kJ/kg
- Temperature at nozzle exit = 814.0 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 45.537 mol/kg expl.
- Total mole number of products = 46.080 mol/kg expl.
- Volume of gaseous products (at SATP) = 1128.81 L/kg expl.
- Mass of gaseous products = 962.2 g/kg expl.
- Mass of condensed products = 37.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.129 g
- Mean molecular mass of all products = 21.702 g
- Specific gas constant = 378.593 J/kg K
- Specific heat capacity at p=const. (Cp) = 1902.89 J/kgK
- Specific heat capacity at V=const. (Cv) = 1524.29 J/molK
- Specific heat ratio (Cp/Cv) = 1.2484

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 196.43 s
- Exhaust (or nozzle exit) velocity = 1927.0 m/s

- Characteristic exhaust velocity (c*) = 1176.2 m/s
- Thrust coefficient (Cf) = 1.638
- Nozzle area expansion ratio (Ae/At) = 8.26
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 614.02 m/s
- Mach number at nozzle exit = 3.138

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 8.706105 E-01 | 2.138304 E01 | 46.4041 |
| H2 = | 4.166376 E-01 | 1.023303 E01 | 22.2070 |
| CO2 = | 3.660329 E-01 | 8.990125 E00 | 19.5098 |
| N2 = | 9.331790 E-02 | 2.291978 E00 | 4.9739 |
| CO = | 5.183774 E-02 | 1.273185 E00 | 2.7630 |
| CH4 = | 2.731648 E-02 | 6.709195 E-01 | 1.4560 |
| B(OH)3 = | 2.369712 E-02 | 5.820245 E-01 | 1.2631 |
| B2O3(l) = | 2.137975 E-02 | 5.251074 E-01 | 1.1396 |
| IH = | 4.426388 E-03 | 1.087164 E-01 | 0.2359 |
| FeO(s) = | 7.413912 E-04 | 1.820929 E-02 | 0.0395 |
| NH3 = | 1.344472 E-04 | 3.302153 E-03 | 0.0072 |
| I = | 1.598902 E-05 | 3.927058 E-04 | 0.0009 |
| I2 = | 2.736592 E-06 | 6.721337 E-05 | 0.0001 |
| B2O3(s) = | 3.020643 E-07 | 7.418992 E-06 | 0.0000 |
| BHO2 = | 2.717893 E-07 | 6.675411 E-06 | 0.0000 |
| FeO(l) = | 7.988723 E-09 | 1.962108 E-07 | 0.0000 |
| HCN = | 7.079388 E-09 | 1.738767 E-07 | 0.0000 |
| CH3OH = | 1.917010 E-09 | 4.708364 E-08 | 0.0000 |
| CHNO = | 7.060523 E-10 | 1.734133 E-08 | 0.0000 |
| Fe(l) = | 1.456385 E-10 | 3.577022 E-09 | 0.0000 |
| Fe(s) = | 1.423253 E-10 | 3.495647 E-09 | 0.0000 |
| Fe(OH)2 = | 2.629066 E-11 | 6.457243 E-10 | 0.0000 |
| BN(s) = | 2.451699 E-11 | 6.021611 E-10 | 0.0000 |
| BN = | 6.380222 E-12 | 1.567045 E-10 | 0.0000 |
| N = | 3.515911 E-12 | 8.635419 E-11 | 0.0000 |
| BH2 = | 3.127352 E-12 | 7.681080 E-11 | 0.0000 |
| O = | 2.957516 E-12 | 7.263946 E-11 | 0.0000 |
| O2 = | 2.936450 E-12 | 7.212207 E-11 | 0.0000 |
| FeO = | 2.785156 E-12 | 6.840616 E-11 | 0.0000 |
| INO = | 2.546658 E-12 | 6.254840 E-11 | 0.0000 |
| H = | 2.400172 E-12 | 5.895057 E-11 | 0.0000 |
| BO = | 2.313520 E-12 | 5.682229 E-11 | 0.0000 |
| CNO = | 2.280447 E-12 | 5.601000 E-11 | 0.0000 |
| BO2 = | 1.924204 E-12 | 4.726033 E-11 | 0.0000 |
| Fe = | 1.662284 E-12 | 4.082732 E-11 | 0.0000 |
| NO = | 1.347348 E-12 | 3.309219 E-11 | 0.0000 |
| BHO2(s) = | 9.259731 E-13 | 2.274280 E-11 | 0.0000 |
| B2O3 = | 8.129672 E-13 | 1.996727 E-11 | 0.0000 |
| NH2 = | 5.995154 E-13 | 1.472468 E-11 | 0.0000 |
| ICN = | 5.611649 E-13 | 1.378276 E-11 | 0.0000 |
| OH = | 4.661246 E-13 | 1.144847 E-11 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 42

**Combustion conditions (Number 42):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 20.70 %**
2. **Hydrogen peroxide ($H_2O_2$), 73.62 %**
3. **Water ($H_2O$, liqid), 3.88 %**
4. **AKC_298, 1.80 %**

C(0.391) H(2.667) N(0.164) O(1.805) B(0.058) Fe(0.001) I(0.004)

Molecular weight = 39.72
Oxygen balance = -16.06457 %
Enthalpy of formation = -7240.12 kJ/kg
Internal energy of formation = -7095.47 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -2945.23 kJ/kg
- Total enthalpy of combustion prod. = -7240.48 kJ/kg
- Entropy of combustion products = 10.76 kJ/K kg
- Isobaric combustion temperature = 1834.1 K
- Mole number of gaseous products = 45.413 mol/kg expl.
- Total mole number of products = 45.425 mol/kg expl.
- Volume of gaseous products (at SATP) = 1125.75 L/kg expl.
- Mass of gaseous products = 999.1 g/kg expl.
- Mass of condensed products = 0.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.001 g
- Mean molecular mass of all products = 22.014 g
- Specific gas constant = 377.565 J/kg K
- Specific heat capacity at p=const. (Cp) = 2206.99 J/kgK
- Specific heat capacity at V=const. (Cv) = 1829.42 J/molK
- Specific heat ratio (Cp/Cv) = 1.2064

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.052710 E00 | 2.650376 E01 | 58.3456 |
| H2 = | 2.157627 E-01 | 5.432194 E00 | 11.9585 |
| CO2 = | 2.096601 E-01 | 5.278550 E00 | 11.6202 |
| CO = | 1.812084 E-01 | 4.562229 E00 | 10.0433 |
| N2 = | 8.197275 E-02 | 2.063803 E00 | 4.5433 |
| B(OH)3 = | 3.419177 E-02 | 8.608360 E-01 | 1.8951 |
| BHO2 = | 2.408610 E-02 | 6.064084 E-01 | 1.3350 |
| IH = | 2.907709 E-03 | 7.320652 E-02 | 0.1612 |
| I = | 9.922165 E-04 | 2.498074 E-02 | 0.0550 |
| FeO(l) = | 4.775234 E-04 | 1.202246 E-02 | 0.0265 |
| Fe(OH)2 = | 1.602508 E-04 | 4.034585 E-03 | 0.0089 |
| H = | 3.709415 E-05 | 9.339082 E-04 | 0.0021 |
| NH3 = | 3.601632 E-05 | 9.067720 E-04 | 0.0020 |
| B2O3 = | 3.538988 E-05 | 8.910003 E-04 | 0.0020 |
| FeO(s) = | 1.286904 E-05 | 3.239999 E-04 | 0.0007 |
| OH = | 1.174161 E-05 | 2.956149 E-04 | 0.0007 |

| | | | |
|---|---|---|---|
| I2 = | 2.620152 E-06 | 6.596677 E-05 | 0.0001 |
| CH4 = | 4.828657 E-07 | 1.215697 E-05 | 0.0000 |
| HCN = | 3.865142 E-07 | 9.731153 E-06 | 0.0000 |
| BO2 = | 3.012313 E-07 | 7.584009 E-06 | 0.0000 |
| CHNO = | 2.199096 E-07 | 5.536598 E-06 | 0.0000 |
| Fe = | 2.129251 E-07 | 5.360752 E-06 | 0.0000 |
| NO = | 1.852076 E-07 | 4.662916 E-06 | 0.0000 |
| BO = | 3.269726 E-08 | 8.232090 E-07 | 0.0000 |
| NH2 = | 1.447312 E-08 | 3.643854 E-07 | 0.0000 |
| FeO = | 4.825092 E-09 | 1.214799 E-07 | 0.0000 |
| O2 = | 2.450157 E-09 | 6.168688 E-08 | 0.0000 |
| CH3OH = | 1.892277 E-09 | 4.764130 E-08 | 0.0000 |
| O = | 1.396742 E-09 | 3.516536 E-08 | 0.0000 |
| ICN = | 1.631928 E-11 | 4.108655 E-10 | 0.0000 |
| B2O3(l) = | 1.310718 E-11 | 3.299954 E-10 | 0.0000 |
| CNO = | 6.437164 E-12 | 1.620665 E-10 | 0.0000 |
| Fe(s) = | 4.922473 E-12 | 1.239316 E-10 | 0.0000 |
| Fe(l) = | 4.712381 E-12 | 1.186422 E-10 | 0.0000 |
| BH2 = | 2.142812 E-12 | 5.394893 E-11 | 0.0000 |
| N = | 1.817014 E-12 | 4.574642 E-11 | 0.0000 |
| INO = | 1.220374 E-12 | 3.072498 E-11 | 0.0000 |
| B2O3(s) = | 6.414162 E-13 | 1.614874 E-11 | 0.0000 |
| BHO2(s) = | 1.531268 E-13 | 3.855226 E-12 | 0.0000 |
| BN(s) = | 1.860400 E-15 | 4.683873 E-14 | 0.0000 |
| BN = | 9.014461 E-18 | 2.269544 E-16 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7622.19 kJ/kg
- Temperature at nozzle throat = 1678.5 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 45.232 mol/kg expl.
- Total mole number of products = 45.246 mol/kg expl.
- Volume of gaseous products (at SATP) = 1121.27 L/kg expl.
- Mass of gaseous products = 999.0 g/kg expl.
- Mass of condensed products = 1.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.086 g
- Mean molecular mass of all products = 22.101 g
- Specific gas constant = 376.062 J/kg K
- Specific heat capacity at p=const. (Cp) = 2165.08 J/kgK
- Specific heat capacity at V=const. (Cv) = 1789.01 J/molK
- Specific heat ratio (Cp/Cv) = 1.2102

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 873.7 m/s
- Sound velocity at throat ) = 874.0 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.561
- Pressure ratio (pc/pt) = 1.782

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.035264 E00 | 2.606453 E01 | 57.6060 |
| H2 = | 2.261014 E-01 | 5.692486 E00 | 12.5811 |
| CO2 = | 2.200753 E-01 | 5.540770 E00 | 12.2458 |

| | | | |
|---|---|---|---|
| CO = | 1.707933 E-01 | 4.300011 E00 | 9.5036 |
| N2 = | 8.197563 E-02 | 2.063876 E00 | 4.5614 |
| B(OH)3 = | 4.126688 E-02 | 1.038964 E00 | 2.2962 |
| BHO2 = | 1.705524 E-02 | 4.293947 E-01 | 0.9490 |
| IH = | 3.091136 E-03 | 7.782461 E-02 | 0.1720 |
| I = | 8.099934 E-04 | 2.039296 E-02 | 0.0451 |
| FeO(s) = | 4.601713 E-04 | 1.158559 E-02 | 0.0256 |
| Fe(OH)2 = | 1.026089 E-04 | 2.583354 E-03 | 0.0057 |
| FeO(l) = | 8.801481 E-05 | 2.215923 E-03 | 0.0049 |
| NH3 = | 3.067607 E-05 | 7.723223 E-04 | 0.0017 |
| B2O3 = | 1.340019 E-05 | 3.373725 E-04 | 0.0007 |
| H = | 1.279829 E-05 | 3.222188 E-04 | 0.0007 |
| OH = | 2.608328 E-06 | 6.566908 E-05 | 0.0001 |
| I2 = | 2.018003 E-06 | 5.080665 E-05 | 0.0001 |
| CH4 = | 6.816576 E-07 | 1.716189 E-05 | 0.0000 |
| HCN = | 2.319194 E-07 | 5.838964 E-06 | 0.0000 |
| CHNO = | 1.145604 E-07 | 2.884253 E-06 | 0.0000 |
| Fe = | 6.509433 E-08 | 1.638860 E-06 | 0.0000 |
| BO2 = | 5.063903 E-08 | 1.274924 E-06 | 0.0000 |
| NO = | 2.902900 E-08 | 7.308545 E-07 | 0.0000 |
| BO = | 5.054155 E-09 | 1.272469 E-07 | 0.0000 |
| NH2 = | 3.730229 E-09 | 9.391486 E-08 | 0.0000 |
| CH3OH = | 1.224680 E-09 | 3.083339 E-08 | 0.0000 |
| FeO = | 8.414285 E-10 | 2.118439 E-08 | 0.0000 |
| O2 = | 2.079845 E-10 | 5.236364 E-09 | 0.0000 |
| O = | 1.092965 E-10 | 2.751726 E-09 | 0.0000 |
| B2O3(l) = | 3.614478 E-11 | 9.100062 E-10 | 0.0000 |
| Fe(s) = | 1.550546 E-11 | 3.903764 E-10 | 0.0000 |
| Fe(l) = | 1.384537 E-11 | 3.485806 E-10 | 0.0000 |
| ICN = | 6.275386 E-12 | 1.579935 E-10 | 0.0000 |
| B2O3(s) = | 2.430586 E-12 | 6.119413 E-11 | 0.0000 |
| CNO = | 9.113270 E-13 | 2.294421 E-11 | 0.0000 |
| BHO2(s) = | 6.232147 E-13 | 1.569049 E-11 | 0.0000 |
| INO = | 4.432760 E-13 | 1.116023 E-11 | 0.0000 |
| BH2 = | 3.803064 E-13 | 9.574860 E-12 | 0.0000 |
| N = | 1.624571 E-13 | 4.090132 E-12 | 0.0000 |
| BN(s) = | 5.452322 E-15 | 1.372715 E-13 | 0.0000 |
| BN = | 1.146159 E-18 | 2.885650 E-17 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9360.85 kJ/kg
- Temperature at nozzle exit = 907.4 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 45.203 mol/kg expl.
- Total mole number of products = 45.657 mol/kg expl.
- Volume of gaseous products (at SATP) = 1120.54 L/kg expl.
- Mass of gaseous products = 968.4 g/kg expl.
- Mass of condensed products = 31.7 g/kg expl.
- Mean molecular mass of gaseous prod. = 21.423 g
- Mean molecular mass of all products = 21.903 g
- Specific gas constant = 375.819 J/kg K
- Specific heat capacity at p=const. (Cp) = 1915.79 J/kgK
- Specific heat capacity at V=const. (Cv) = 1539.97 J/molK
- Specific heat ratio (Cp/Cv) = 1.2440

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 209.92 s

- Exhaust (or nozzle exit) velocity = 2059.3 m/s
- Characteristic exhaust velocity (c*) = 1263.8 m/s
- Thrust coefficient (Cf) = 1.629
- Nozzle area expansion ratio (Ae/At) = 8.32
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 642.42 m/s
- Mach number at nozzle exit = 3.206

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 9.591436 E-01 | 2.414807 E01 | 52.8899 |
| H2 = | 3.359318 E-01 | 8.457655 E00 | 18.5242 |
| CO2 = | 3.319002 E-01 | 8.356151 E00 | 18.3019 |
| N2 = | 8.197077 E-02 | 2.063753 E00 | 4.5201 |
| CO = | 5.843686 E-02 | 1.471247 E00 | 3.2224 |
| B(OH)3 = | 2.357223 E-02 | 5.934709 E-01 | 1.2998 |
| B2O3(l) = | 1.738628 E-02 | 4.377292 E-01 | 0.9587 |
| IH = | 3.869416 E-03 | 9.741911 E-02 | 0.2134 |
| FeO(s) = | 6.509139 E-04 | 1.638786 E-02 | 0.0359 |
| CH4 = | 5.325616 E-04 | 1.340814 E-02 | 0.0294 |
| NH3 = | 4.077753 E-05 | 1.026644 E-03 | 0.0022 |
| I = 3.294549 E-05 | | 8.294588 E-04 | 0.0018 |
| BHO2 = | 4.187501 E-06 | 1.054274 E-04 | 0.0002 |
| I2 = 1.402418 E-06 | | 3.530826 E-05 | 0.0001 |
| FeO(l) = | 5.125022 E-09 | 1.290311 E-07 | 0.0000 |
| HCN = | 4.571516 E-09 | 1.150957 E-07 | 0.0000 |
| CHNO = | 7.877787 E-10 | 1.983367 E-08 | 0.0000 |
| Fe(OH)2 = | 6.906966 E-10 | 1.738946 E-08 | 0.0000 |
| CH3OH = | 2.272326 E-10 | 5.720967 E-09 | 0.0000 |
| Fe(l) = | 1.196644 E-10 | 3.012754 E-09 | 0.0000 |
| H = 1.187282 E-10 | | 2.989184 E-09 | 0.0000 |
| Fe(s) = | 1.168209 E-10 | 2.941166 E-09 | 0.0000 |
| BN(s) = | 2.482539 E-11 | 6.250214 E-10 | 0.0000 |
| B2O3(s) = | 1.216814 E-11 | 3.063537 E-10 | 0.0000 |
| BN = | 5.331031 E-12 | 1.342178 E-10 | 0.0000 |
| N = 2.799846 E-12 | | 7.049087 E-11 | 0.0000 |
| BHO2(s) = | 2.523252 E-12 | 6.352717 E-11 | 0.0000 |
| BH2 = | 2.514635 E-12 | 6.331022 E-11 | 0.0000 |
| O = 2.170322 E-12 | | 5.464154 E-11 | 0.0000 |
| O2 = | 2.126215 E-12 | 5.353108 E-11 | 0.0000 |
| INO = | 2.042066 E-12 | 5.141248 E-11 | 0.0000 |
| FeO = | 2.004330 E-12 | 5.046242 E-11 | 0.0000 |
| CNO = | 1.859804 E-12 | 4.682372 E-11 | 0.0000 |
| BO = | 1.579962 E-12 | 3.977822 E-11 | 0.0000 |
| BO2 = | 1.212232 E-12 | 3.052001 E-11 | 0.0000 |
| Fe = 1.033673 E-12 | | 2.602448 E-11 | 0.0000 |
| NO = | 8.089973 E-13 | 2.036788 E-11 | 0.0000 |
| ICN = | 5.101547 E-13 | 1.284401 E-11 | 0.0000 |
| NH2 = | 3.423007 E-13 | 8.618002 E-12 | 0.0000 |
| B2O3 = | 2.033827 E-13 | 5.120504 E-12 | 0.0000 |
| OH = | 1.325484 E-14 | 3.337131 E-13 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 43

**Combustion conditions (Number 43):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 18.40 %**
2. **Hydrogen peroxide ($H_2O_2$), 76.00 %**
3. **Water ($H_2O$, liquid), 4.00 %**
4. **AKC_298, 1.60 %**

C(0.339) H(2.579) N(0.142) O(1.819) B(0.051) Fe(0.001) I(0.003)

Molecular weight = 38.78
Oxygen balance = -9.312554 %
Enthalpy of formation = -7105.62 kJ/kg
Internal energy of formation = -6960.51 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3483.91 kJ/kg
- Total enthalpy of combustion prod. = -7106.40 kJ/kg
- Entropy of combustion products = 10.85 kJ/K kg
- Isobaric combustion temperature = 2095.0 K
- Mole number of gaseous products = 44.213 mol/kg expl.
- Total mole number of products = 44.214 mol/kg expl.
- Volume of gaseous products (at SATP) = 1095.99 L/kg expl.
- Mass of gaseous products = 999.9 g/kg expl.
- Mass of condensed products = 0.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.616 g
- Mean molecular mass of all products = 22.617 g
- Specific gas constant = 367.586 J/kg K
- Specific heat capacity at p=const. (Cp) = 2253.75 J/kgK
- Specific heat capacity at V=const. (Cv) = 1886.17 J/molK
- Specific heat ratio (Cp/Cv) = 1.1949

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.139063 E00 | 2.937621 E01 | 66.4413 |
| CO2 = | 2.248196 E-01 | 5.798055 E00 | 13.1137 |
| CO = | 1.143600 E-01 | 2.949323 E00 | 6.6706 |
| H2 = | 1.101857 E-01 | 2.841668 E00 | 6.4271 |
| N2 = | 7.114113 E-02 | 1.834716 E00 | 4.1496 |
| BHO2 = | 3.702196 E-02 | 9.547893 E-01 | 2.1595 |
| B(OH)3 = | 1.337202 E-02 | 3.448619 E-01 | 0.7800 |
| IH = | 1.739275 E-03 | 4.485558 E-02 | 0.1015 |
| I = | 1.645227 E-03 | 4.243009 E-02 | 0.0960 |
| Fe(OH)2 = | 5.263096 E-04 | 1.357342 E-02 | 0.0307 |
| OH = | 1.719144 E-04 | 4.433639 E-03 | 0.0100 |
| H = | 1.646761 E-04 | 4.246965 E-03 | 0.0096 |
| B2O3 = | 1.156278 E-04 | 2.982019 E-03 | 0.0067 |
| FeO(s) = | 2.582016 E-05 | 6.658970 E-04 | 0.0015 |
| FeO(l) = | 1.053458 E-05 | 2.716848 E-04 | 0.0006 |
| NH3 = | 8.348815 E-06 | 2.153143 E-04 | 0.0005 |

| | | | |
|---|---|---|---|
| BO2 = | 7.069174 E-06 | 1.823127 E-04 | 0.0004 |
| NO = | 5.960931 E-06 | 1.537313 E-04 | 0.0003 |
| I2 = | 2.116537 E-06 | 5.458510 E-05 | 0.0001 |
| Fe = | 1.949090 E-06 | 5.026666 E-05 | 0.0001 |
| O2 = | 7.191811 E-07 | 1.854754 E-05 | 0.0000 |
| BO = | 4.314245 E-07 | 1.112636 E-05 | 0.0000 |
| FeO = | 1.757694 E-07 | 4.533060 E-06 | 0.0000 |
| O = | 1.753982 E-07 | 4.523486 E-06 | 0.0000 |
| CHNO = | 1.107535 E-07 | 2.856312 E-06 | 0.0000 |
| HCN = | 8.244833 E-08 | 2.126327 E-06 | 0.0000 |
| NH2 = | 2.899101 E-08 | 7.476727 E-07 | 0.0000 |
| CH4 = | 6.659628 E-09 | 1.717505 E-07 | 0.0000 |
| CH3OH = | 1.572641 E-10 | 4.055812 E-09 | 0.0000 |
| INO = | 1.120848 E-10 | 2.890645 E-09 | 0.0000 |
| N = | 1.032974 E-10 | 2.664019 E-09 | 0.0000 |
| CNO = | 2.797184 E-11 | 7.213885 E-10 | 0.0000 |
| ICN = | 8.167142 E-12 | 2.106291 E-10 | 0.0000 |
| BH2 = | 6.433567 E-12 | 1.659205 E-10 | 0.0000 |
| Fe(l) = | 2.631485 E-12 | 6.786550 E-11 | 0.0000 |
| Fe(s) = | 2.433555 E-12 | 6.276091 E-11 | 0.0000 |
| B2O3(l) = | 2.306461 E-12 | 5.948320 E-11 | 0.0000 |
| B2O3(s) = | 1.438022 E-13 | 3.708630 E-12 | 0.0000 |
| BHO2(s) = | 1.250028 E-13 | 3.223797 E-12 | 0.0000 |
| BN = | 1.413562 E-15 | 3.645550 E-14 | 0.0000 |
| BN(s) = | 3.721515 E-16 | 9.597717 E-15 | 0.0000 |
| B(OH)3(s) = | 1.404558 E-17 | 3.622329 E-16 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7527.77 kJ/kg
- Temperature at nozzle throat = 1918.1 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 44.099 mol/kg expl.
- Total mole number of products = 44.103 mol/kg expl.
- Volume of gaseous products (at SATP) = 1093.18 L/kg expl.
- Mass of gaseous products = 999.7 g/kg expl.
- Mass of condensed products = 0.3 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.670 g
- Mean molecular mass of all products = 22.674 g
- Specific gas constant = 366.643 J/kg K
- Specific heat capacity at p=const. (Cp) = 2211.03 J/kgK
- Specific heat capacity at V=const. (Cv) = 1844.39 J/molK
- Specific heat ratio (Cp/Cv) = 1.1988

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 918.0 m/s
- Sound velocity at throat) = 918.2 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.564
- Pressure ratio (pc/pt) = 1.773

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.129047 E00 | 2.911792 E01 | 66.0222 |
| CO2 = | 2.308350 E-01 | 5.953190 E00 | 13.4983 |
| H2 = | 1.160943 E-01 | 2.994050 E00 | 6.7887 |

| | | | |
|---|---|---|---|
| CO = | 1.083447 E-01 | 2.794190 E00 | 6.3356 |
| N2 = | 7.114436 E-02 | 1.834800 E00 | 4.1602 |
| BHO2 = | 3.292075 E-02 | 8.490198 E-01 | 1.9251 |
| B(OH)3 = | 1.756389 E-02 | 4.529694 E-01 | 1.0271 |
| IH = | 1.918787 E-03 | 4.948515 E-02 | 0.1122 |
| I = | 1.466474 E-03 | 3.782008 E-02 | 0.0858 |
| Fe(OH)2 = | 4.176180 E-04 | 1.077029 E-02 | 0.0244 |
| FeO(l) = | 1.462541 E-04 | 3.771866 E-03 | 0.0086 |
| B2O3 = | 7.312871 E-05 | 1.885975 E-03 | 0.0043 |
| H = | 6.755078 E-05 | 1.742122 E-03 | 0.0040 |
| OH = | 5.097846 E-05 | 1.314725 E-03 | 0.0030 |
| NH3 = | 6.738462 E-06 | 1.737837 E-04 | 0.0004 |
| BO2 = | 1.741397 E-06 | 4.491030 E-05 | 0.0001 |
| I2 = | 1.737415 E-06 | 4.480761 E-05 | 0.0001 |
| NO = | 1.211129 E-06 | 3.123479 E-05 | 0.0001 |
| Fe = | 8.679858 E-07 | 2.238519 E-05 | 0.0001 |
| BO = | 1.020734 E-07 | 2.632453 E-06 | 0.0000 |
| O2 = | 7.964865 E-08 | 2.054124 E-06 | 0.0000 |
| CHNO = | 5.624142 E-08 | 1.450456 E-06 | 0.0000 |
| FeO = | 4.883794 E-08 | 1.259521 E-06 | 0.0000 |
| HCN = | 4.773141 E-08 | 1.230984 E-06 | 0.0000 |
| O = | 2.041689 E-08 | 5.265477 E-07 | 0.0000 |
| NH2 = | 9.501588 E-09 | 2.450442 E-07 | 0.0000 |
| CH4 = | 7.820695 E-09 | 2.016942 E-07 | 0.0000 |
| FeO(s) = | 2.888461 E-10 | 7.449286 E-09 | 0.0000 |
| CH3OH = | 9.246751 E-11 | 2.384720 E-09 | 0.0000 |
| INO = | 1.606635 E-11 | 4.143482 E-10 | 0.0000 |
| N = | 1.075248 E-11 | 2.773043 E-10 | 0.0000 |
| CNO = | 6.617033 E-12 | 1.706520 E-10 | 0.0000 |
| Fe(l) = | 6.115155 E-12 | 1.577087 E-10 | 0.0000 |
| Fe(s) = | 5.940377 E-12 | 1.532012 E-10 | 0.0000 |
| B2O3(l) = | 5.586183 E-12 | 1.440666 E-10 | 0.0000 |
| ICN = | 2.970833 E-12 | 7.661723 E-11 | 0.0000 |
| BH2 = | 1.278429 E-12 | 3.297044 E-11 | 0.0000 |
| B2O3(s) = | 3.813237 E-13 | 9.834267 E-12 | 0.0000 |
| BHO2(s) = | 1.919460 E-13 | 4.950250 E-12 | 0.0000 |
| BN(s) = | 6.578751 E-16 | 1.696647 E-14 | 0.0000 |
| BN = | 8.096486 E-17 | 2.088068 E-15 | 0.0000 |
| B(OH)3(s) = | 1.234904 E-17 | 3.184793 E-16 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9486.90 kJ/kg
- Temperature at nozzle exit = 1074.5 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 43.606 mol/kg expl.
- Total mole number of products = 43.994 mol/kg expl.
- Volume of gaseous products (at SATP) = 1080.95 L/kg expl.
- Mass of gaseous products = 973.0 g/kg expl.
- Mass of condensed products = 27.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.314 g
- Mean molecular mass of all products = 22.731 g
- Specific gas constant = 362.541 J/kg K
- Specific heat capacity at p=const. (Cp) = 1948.75 J/kgK
- Specific heat capacity at V=const. (Cv) = 1586.20 J/molK
- Specific heat ratio (Cp/Cv) = 1.2286

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 222.42 s
- Exhaust (or nozzle exit) velocity = 2182.0 m/s
- Characteristic exhaust velocity (c*) = 1332.5 m/s
- Thrust coefficient (Cf) = 1.637
- Nozzle area expansion ratio (Ae/At) = 8.57
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 683.37 m/s
- Mach number at nozzle exit = 3.193

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.079460 E00 | 2.783906 E01 | 63.2798 |
| CO2 = | 2.913013 E-01 | 7.512606 E00 | 17.0766 |
| H2 = | 1.759394 E-01 | 4.537444 E00 | 10.3139 |
| N2 = | 7.114597 E-02 | 1.834841 E00 | 4.1707 |
| CO = | 4.787788 E-02 | 1.234761 E00 | 2.8067 |
| B(OH)3 = | 2.154260 E-02 | 5.555795 E-01 | 1.2629 |
| B2O3(l) = | 1.446105 E-02 | 3.729477 E-01 | 0.8477 |
| IH = | 3.177346 E-03 | 8.194315 E-02 | 0.1863 |
| FeO(s) = | 5.647803 E-04 | 1.456558 E-02 | 0.0331 |
| I = | 2.056697 E-04 | 5.304183 E-03 | 0.0121 |
| BHO2 = | 1.680452 E-04 | 4.333855 E-03 | 0.0099 |
| NH3 = | 4.852808 E-06 | 1.251530 E-04 | 0.0003 |
| I2 = | 2.859934 E-06 | 7.375716 E-05 | 0.0002 |
| CH4 = | 6.203457 E-07 | 1.599860 E-05 | 0.0000 |
| Fe(OH)2 = | 3.326259 E-08 | 8.578360 E-07 | 0.0000 |
| H = | 8.270400 E-09 | 2.132921 E-07 | 0.0000 |
| FeO(l) = | 2.248293 E-09 | 5.798304 E-08 | 0.0000 |
| HCN = | 1.326759 E-09 | 3.421687 E-08 | 0.0000 |
| CHNO = | 4.823259 E-10 | 1.243909 E-08 | 0.0000 |
| OH = | 1.562060 E-10 | 4.028522 E-09 | 0.0000 |
| B2O3 = | 1.464884 E-10 | 3.777908 E-09 | 0.0000 |
| Fe(s) = | 9.435150 E-11 | 2.433307 E-09 | 0.0000 |
| Fe(l) = | 9.432598 E-11 | 2.432649 E-09 | 0.0000 |
| B2O3(s) = | 4.356975 E-11 | 1.123656 E-09 | 0.0000 |
| BN(s) = | 2.350172 E-11 | 6.061049 E-10 | 0.0000 |
| CH3OH = | 1.092484 E-11 | 2.817494 E-10 | 0.0000 |
| BN = | 3.966886 E-12 | 1.023052 E-10 | 0.0000 |
| BHO2(s) = | 3.664348 E-12 | 9.450285 E-11 | 0.0000 |
| N = | 1.828086 E-12 | 4.714600 E-11 | 0.0000 |
| BH2 = | 1.777278 E-12 | 4.583566 E-11 | 0.0000 |
| CNO = | 1.321465 E-12 | 3.408033 E-11 | 0.0000 |
| INO = | 1.271271 E-12 | 3.278583 E-11 | 0.0000 |
| B(OH)3(s) = | 1.107570 E-12 | 2.856401 E-11 | 0.0000 |
| O = | 1.069617 E-12 | 2.758522 E-11 | 0.0000 |
| O2 = | 9.603011 E-13 | 2.476598 E-11 | 0.0000 |
| FeO = | 9.504500 E-13 | 2.451193 E-11 | 0.0000 |
| BO = | 6.115264 E-13 | 1.577115 E-11 | 0.0000 |
| ICN = | 4.564606 E-13 | 1.177203 E-11 | 0.0000 |
| BO2 = | 2.363969 E-13 | 6.096630 E-12 | 0.0000 |
| Fe = | 2.198940 E-13 | 5.671024 E-12 | 0.0000 |
| NO = | 4.372644 E-14 | 1.127697 E-12 | 0.0000 |
| NH2 = | 2.715608 E-14 | 7.003502 E-13 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 44

**Combustion conditions (Number 44):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 16.83 %**
2. **Hydrogen peroxide ($H_2O_2$), 77.62 %**
3. **Water ($H_2O$, liquid), 4.08 %**
4. **AKC_298, 1.47 %**

C(0.305) H(2.521) N(0.128) O(1.828) B(0.046) Fe(0.001) I(0.003)

Molecular weight = 38.16
Oxygen balance = -4.710632 %
Enthalpy of formation = -7014.44 kJ/kg
Internal energy of formation = -6869.03 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3885.98 kJ/kg
- Total enthalpy of combustion prod. = -7014.76 kJ/kg
- Entropy of combustion products = 10.87 kJ/K kg
- Isobaric combustion temperature = 2284.6 K
- Mole number of gaseous products = 43.233 mol/kg expl.
- Total mole number of products = 43.233 mol/kg expl.
- Volume of gaseous products (at SATP) = 1071.70 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.131 g
- Mean molecular mass of all products = 23.131 g
- Specific gas constant = 359.437 J/kg K
- Specific heat capacity at p=const. (Cp) = 2285.81 J/kgK
- Specific heat capacity at V=const. (Cv) = 1926.38 J/molK
- Specific heat ratio (Cp/Cv) = 1.1866

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.179479 E00 | 3.090936 E01 | 71.4952 |
| CO2 = | 2.436062 E-01 | 6.383930 E00 | 14.7664 |
| N2 = | 6.401203 E-02 | 1.677495 E00 | 3.8801 |
| CO = | 6.174036 E-02 | 1.617964 E00 | 3.7424 |
| H2 = | 5.038750 E-02 | 1.320452 E00 | 3.0543 |
| BHO2 = | 3.888462 E-02 | 1.019008 E00 | 2.3570 |
| B(OH)3 = | 6.330637 E-03 | 1.659003 E-01 | 0.3837 |
| I = | 2.051680 E-03 | 5.376620 E-02 | 0.1244 |
| OH = | 1.080143 E-03 | 2.830616 E-02 | 0.0655 |
| IH = | 1.009739 E-03 | 2.646116 E-02 | 0.0612 |
| Fe(OH)2 = | 5.077303 E-04 | 1.330555 E-02 | 0.0308 |
| H = | 3.225739 E-04 | 8.453352 E-03 | 0.0196 |
| B2O3 = | 1.661897 E-04 | 4.355158 E-03 | 0.0101 |
| NO = | 6.460831 E-05 | 1.693122 E-03 | 0.0039 |
| BO2 = | 4.172855 E-05 | 1.093536 E-03 | 0.0025 |
| O2 = | 3.588393 E-05 | 9.403720 E-04 | 0.0022 |

| | | | |
|---|---|---|---|
| O = | 4.371420 E-06 | 1.145572 E-04 | 0.0003 |
| Fe = | 2.249483 E-06 | 5.894981 E-05 | 0.0001 |
| NH3 = | 1.932830 E-06 | 5.065162 E-05 | 0.0001 |
| I2 = | 1.271269 E-06 | 3.331481 E-05 | 0.0001 |
| BO = | 1.270481 E-06 | 3.329415 E-05 | 0.0001 |
| FeO = | 6.805701 E-07 | 1.783498 E-05 | 0.0000 |
| CHNO = | 4.164959 E-08 | 1.091467 E-06 | 0.0000 |
| NH2 = | 3.362825 E-08 | 8.812600 E-07 | 0.0000 |
| HCN = | 1.276253 E-08 | 3.344541 E-07 | 0.0000 |
| N = | 9.412081 E-10 | 2.466524 E-08 | 0.0000 |
| INO = | 9.048159 E-10 | 2.371155 E-08 | 0.0000 |
| CH4 = | 1.216471 E-10 | 3.187876 E-09 | 0.0000 |
| CNO = | 8.033329 E-11 | 2.105209 E-09 | 0.0000 |
| FeO(l) = | 3.665228 E-11 | 9.605075 E-10 | 0.0000 |
| FeO(s) = | 1.300565 E-11 | 3.408251 E-10 | 0.0000 |
| CH3OH = | 1.263365 E-11 | 3.310767 E-10 | 0.0000 |
| BH2 = | 3.129465 E-12 | 8.201057 E-11 | 0.0000 |
| ICN = | 1.991634 E-12 | 5.219263 E-11 | 0.0000 |
| Fe(l) = | 6.118120 E-13 | 1.603311 E-11 | 0.0000 |
| B2O3(l) = | 5.121982 E-13 | 1.342264 E-11 | 0.0000 |
| Fe(s) = | 3.671094 E-13 | 9.620445 E-12 | 0.0000 |
| BHO2(s) = | 5.039258 E-14 | 1.320585 E-12 | 0.0000 |
| B2O3(s) = | 3.035987 E-14 | 7.956088 E-13 | 0.0000 |
| BN = | 5.308906 E-15 | 1.391249 E-13 | 0.0000 |
| BN(s) = | 6.061374 E-17 | 1.588440 E-15 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7462.42 kJ/kg
- Temperature at nozzle throat = 2095.2 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 43.170 mol/kg expl.
- Total mole number of products = 43.170 mol/kg expl.
- Volume of gaseous products (at SATP) = 1070.15 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.164 g
- Mean molecular mass of all products = 23.164 g
- Specific gas constant = 358.918 J/kg K
- Specific heat capacity at p=const. (Cp) = 2243.95 J/kgK
- Specific heat capacity at V=const. (Cv) = 1885.03 J/molK
- Specific heat ratio (Cp/Cv) = 1.1904

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 946.2 m/s
- Sound velocity at throat) = 946.1 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.566
- Pressure ratio (pc/pt) = 1.768

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.175303 E00 | 3.079991 E01 | 71.3452 |
| CO2 = | 2.467617 E-01 | 6.466621 E00 | 14.9793 |
| N2 = | 6.403662 E-02 | 1.678140 E00 | 3.8873 |
| CO = | 5.858495 E-02 | 1.535274 E00 | 3.5563 |

| | | | |
|---|---|---|---|
| H2 = | 5.308893 E-02 | 1.391245 E00 | 3.2227 |
| BHO2 = | 3.719983 E-02 | 9.748564 E-01 | 2.2582 |
| B(OH)3 = | 8.140058 E-03 | 2.133179 E-01 | 0.4941 |
| I = | 1.945947 E-03 | 5.099538 E-02 | 0.1181 |
| IH = | 1.115217 E-03 | 2.922531 E-02 | 0.0677 |
| Fe(OH)2 = | 5.089353 E-04 | 1.333713 E-02 | 0.0309 |
| OH = | 3.544921 E-04 | 9.289798 E-03 | 0.0215 |
| H = | 1.489898 E-04 | 3.904416 E-03 | 0.0090 |
| B2O3 = | 1.186271 E-04 | 3.108734 E-03 | 0.0072 |
| NO = | 1.587847 E-05 | 4.161102 E-04 | 0.0010 |
| BO2 = | 1.311443 E-05 | 3.436758 E-04 | 0.0008 |
| O2 = | 5.702189 E-06 | 1.494312 E-04 | 0.0003 |
| NH3 = | 1.536812 E-06 | 4.027361 E-05 | 0.0001 |
| Fe = | 1.442827 E-06 | 3.781063 E-05 | 0.0001 |
| I2 = | 1.398838 E-06 | 3.665787 E-05 | 0.0001 |
| O = | 6.554727 E-07 | 1.717728 E-05 | 0.0000 |
| BO = | 3.813398 E-07 | 9.993369 E-06 | 0.0000 |
| FeO = | 2.821149 E-07 | 7.393085 E-06 | 0.0000 |
| CHNO = | 2.162033 E-08 | 5.665811 E-07 | 0.0000 |
| NH2 = | 1.113682 E-08 | 2.918509 E-07 | 0.0000 |
| HCN = | 7.505641 E-09 | 1.966924 E-07 | 0.0000 |
| INO = | 1.822222 E-10 | 4.775304 E-09 | 0.0000 |
| N = | 1.271579 E-10 | 3.332293 E-09 | 0.0000 |
| CH4 = | 1.270861 E-10 | 3.330409 E-09 | 0.0000 |
| FeO(l) = | 1.112940 E-10 | 2.916563 E-09 | 0.0000 |
| FeO(s) = | 5.445604 E-11 | 1.427072 E-09 | 0.0000 |
| CNO = | 1.516261 E-11 | 3.973505 E-10 | 0.0000 |
| CH3OH = | 6.737446 E-12 | 1.765611 E-10 | 0.0000 |
| Fe(l) = | 1.397352 E-12 | 3.661892 E-11 | 0.0000 |
| B2O3(l) = | 1.271158 E-12 | 3.331189 E-11 | 0.0000 |
| Fe(s) = | 1.240343 E-12 | 3.250436 E-11 | 0.0000 |
| ICN = | 8.693224 E-13 | 2.278141 E-11 | 0.0000 |
| BH2 = | 7.788117 E-13 | 2.040949 E-11 | 0.0000 |
| B2O3(s) = | 8.100845 E-14 | 2.122902 E-12 | 0.0000 |
| BHO2(s) = | 7.573784 E-14 | 1.984781 E-12 | 0.0000 |
| BN = | 4.323707 E-16 | 1.133068 E-14 | 0.0000 |
| BN(s) = | 8.258137 E-17 | 2.164122 E-15 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9564.82 kJ/kg
- Temperature at nozzle exit = 1196.1 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 42.505 mol/kg expl.
- Total mole number of products = 42.827 mol/kg expl.
- Volume of gaseous products (at SATP) = 1053.66 L/kg expl.
- Mass of gaseous products = 977.6 g/kg expl.
- Mass of condensed products = 22.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 22.999 g
- Mean molecular mass of all products = 23.350 g
- Specific gas constant = 353.389 J/kg K
- Specific heat capacity at p=const. (Cp) = 1975.59 J/kgK
- Specific heat capacity at V=const. (Cv) = 1622.20 J/molK
- Specific heat ratio (Cp/Cv) = 1.2178

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 230.21 s
- Exhaust (or nozzle exit) velocity = 2258.3 m/s

- Characteristic exhaust velocity (c*) = 1378.2 m/s
- Thrust coefficient (Cf) = 1.639
- Nozzle area expansion ratio (Ae/At) = 8.75
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 709.35 m/s
- Mach number at nozzle exit = 3.184

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.145568 E00 | 3.002069 E01 | 70.0973 |
| CO2 = | 2.763868 E-01 | 7.242975 E00 | 16.9121 |
| H2 = | 8.190736 E-02 | 2.146459 E00 | 5.0119 |
| N2 = | 6.404491 E-02 | 1.678357 E00 | 3.9189 |
| CO = | 2.895984 E-02 | 7.589197 E-01 | 1.7721 |
| B(OH)3 = | 2.079402 E-02 | 5.449269 E-01 | 1.2724 |
| B2O3(l) = | 1.177435 E-02 | 3.085580 E-01 | 0.7205 |
| IH = | 2.459388 E-03 | 6.445058 E-02 | 0.1505 |
| BHO2 = | 1.247882 E-03 | 3.270191 E-02 | 0.0764 |
| I = 5.972846 E-04 | | 1.565241 E-02 | 0.0365 |
| FeO(s) = | 5.103627 E-04 | 1.337453 E-02 | 0.0312 |
| I2 = 3.644894 E-06 | | 9.551788 E-05 | 0.0002 |
| NH3 = | 8.748606 E-07 | 2.292654 E-05 | 0.0001 |
| Fe(OH)2 = | 3.527094 E-07 | 9.243080 E-06 | 0.0000 |
| H = 7.041304 E-08 | | 1.845240 E-06 | 0.0000 |
| B2O3 = | 1.483602 E-08 | 3.887919 E-07 | 0.0000 |
| OH = | 6.847620 E-09 | 1.794483 E-07 | 0.0000 |
| FeO(l) = | 5.322167 E-09 | 1.394724 E-07 | 0.0000 |
| CH4 = | 2.128316 E-09 | 5.577452 E-08 | 0.0000 |
| CHNO = | 2.099028 E-10 | 5.500701 E-09 | 0.0000 |
| HCN = | 2.048397 E-10 | 5.368016 E-09 | 0.0000 |
| Fe(s) = | 9.251994 E-11 | 2.424572 E-09 | 0.0000 |
| Fe(l) = | 9.048939 E-11 | 2.371359 E-09 | 0.0000 |
| B2O3(s) = | 4.844205 E-11 | 1.269469 E-09 | 0.0000 |
| BN(s) = | 2.371505 E-11 | 6.214751 E-10 | 0.0000 |
| NO = | 1.856192 E-11 | 4.864327 E-10 | 0.0000 |
| BO2 = | 9.234398 E-12 | 2.419961 E-10 | 0.0000 |
| BN = | 3.277205 E-12 | 8.588222 E-11 | 0.0000 |
| BHO2(s) = | 3.217822 E-12 | 8.432603 E-11 | 0.0000 |
| Fe = 1.920876 E-12 | | 5.033837 E-11 | 0.0000 |
| BH2 = | 1.470193 E-12 | 3.852779 E-11 | 0.0000 |
| N = 1.294199 E-12 | | 3.391571 E-11 | 0.0000 |
| CNO = | 1.064680 E-12 | 2.790094 E-11 | 0.0000 |
| NH2 = | 1.036958 E-12 | 2.717445 E-11 | 0.0000 |
| INO = | 8.107309 E-13 | 2.124597 E-11 | 0.0000 |
| ICN = | 5.095681 E-13 | 1.335371 E-11 | 0.0000 |
| O = 4.217378 E-13 | | 1.105203 E-11 | 0.0000 |
| FeO = | 3.664554 E-13 | 9.603307 E-12 | 0.0000 |
| CH3OH = | 2.934398 E-13 | 7.689864 E-12 | 0.0000 |
| O2 = | 2.368610 E-13 | 6.207164 E-12 | 0.0000 |
| BO = | 9.781919 E-14 | 2.563444 E-12 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 45

**Combustion conditions (Number 45):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 15.32 %**
2. **Hydrogen peroxide ($H_2O_2$), 79.16 %**
3. **Water ($H_2O$, liquid), 4.14 %**
4. **AKC_298, 1.38 %**

C(0.274) H(2.468) N(0.115) O(1.837) B(0.041) Fe(0.000) I(0.003)

Molecular weight = 37.61
Oxygen balance = -0.319364 %
Enthalpy of formation = -6929.48 kJ/kg
Internal energy of formation = -6783.83 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -4177.23 kJ/kg
- Total enthalpy of combustion prod. = -6929.48 kJ/kg
- Entropy of combustion products = 10.85 kJ/K kg
- Isobaric combustion temperature = 2422.1 K
- Mole number of gaseous products = 42.391 mol/kg expl.
- Total mole number of products = 42.391 mol/kg expl.
- Volume of gaseous products (at SATP) = 1050.82 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.590 g
- Mean molecular mass of all products = 23.590 g
- Specific gas constant = 352.436 J/kg K
- Specific heat capacity at p=const. (Cp) = 2304.50 J/kgK
- Specific heat capacity at V=const. (Cv) = 1952.06 J/molK
- Specific heat ratio (Cp/Cv) = 1.1805

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.197045 E00 | 3.183134 E01 | 75.0904 |
| CO2 = | 2.614006 E-01 | 6.951060 E00 | 16.3976 |
| N2 = | 5.698851 E-02 | 1.515416 E00 | 3.5749 |
| BHO2 = | 3.676843 E-02 | 9.777314 E-01 | 2.3065 |
| CO = | 1.273406 E-02 | 3.386190 E-01 | 0.7988 |
| H2 = | 9.135348 E-03 | 2.429235 E-01 | 0.5731 |
| OH = | 6.012653 E-03 | 1.598860 E-01 | 0.3772 |
| O2 = | 5.383778 E-03 | 1.431633 E-01 | 0.3377 |
| B(OH)3 = | 3.655669 E-03 | 9.721009 E-02 | 0.2293 |
| I = | 2.431589 E-03 | 6.465984 E-02 | 0.1525 |
| NO = | 9.444088 E-04 | 2.511334 E-02 | 0.0592 |
| Fe(OH)2 = | 4.702624 E-04 | 1.250503 E-02 | 0.0295 |
| IH = | 4.006566 E-04 | 1.065410 E-02 | 0.0251 |
| H = | 2.671797 E-04 | 7.104736 E-03 | 0.0168 |
| BO2 = | 2.155116 E-04 | 5.730798 E-03 | 0.0135 |
| B2O3 = | 1.717561 E-04 | 4.567268 E-03 | 0.0108 |

| | | | |
|---|---|---|---|
| O = | 1.082848 E-04 | 2.879466 E-03 | 0.0068 |
| FeO = | 1.485241 E-06 | 3.949492 E-05 | 0.0001 |
| BO = | 1.248188 E-06 | 3.319131 E-05 | 0.0001 |
| I2 = | 1.198975 E-06 | 3.188266 E-05 | 0.0001 |
| Fe = | 6.950706 E-07 | 1.848304 E-05 | 0.0000 |
| NH3 = | 1.244303 E-07 | 3.308799 E-06 | 0.0000 |
| INO = | 1.245697 E-08 | 3.312507 E-07 | 0.0000 |
| NH2 = | 1.016390 E-08 | 2.702743 E-07 | 0.0000 |
| CHNO = | 3.721609 E-09 | 9.896354 E-08 | 0.0000 |
| N = | 3.675989 E-09 | 9.775042 E-08 | 0.0000 |
| HCN = | 1.964643 E-10 | 5.224301 E-09 | 0.0000 |
| CNO = | 3.619430 E-11 | 9.624642 E-10 | 0.0000 |
| FeO(l) = | 1.784902 E-11 | 4.746339 E-10 | 0.0000 |
| FeO(s) = | 9.385819 E-12 | 2.495839 E-10 | 0.0000 |
| B2O3(l) = | 1.981841 E-13 | 5.270031 E-12 | 0.0000 |
| BH2 = | 9.491006 E-14 | 2.523810 E-12 | 0.0000 |
| ICN = | 8.292964 E-14 | 2.205232 E-12 | 0.0000 |
| CH4 = | 7.668728 E-14 | 2.039237 E-12 | 0.0000 |
| Fe(l) = | 7.012693 E-14 | 1.864787 E-12 | 0.0000 |
| CH3OH = | 6.931010 E-14 | 1.843066 E-12 | 0.0000 |
| Fe(s) = | 5.229429 E-14 | 1.390589 E-12 | 0.0000 |
| BHO2(s) = | 2.886910 E-14 | 7.676754 E-13 | 0.0000 |
| B2O3(s) = | 1.146358 E-14 | 3.048350 E-13 | 0.0000 |
| BN = | 1.795677 E-15 | 4.774992 E-14 | 0.0000 |
| BN(s) = | 2.507750 E-18 | 6.668509 E-17 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7397.08 kJ/kg
- Temperature at nozzle throat = 2247.9 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 42.259 mol/kg expl.
- Total mole number of products = 42.259 mol/kg expl.
- Volume of gaseous products (at SATP) = 1047.57 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.663 g
- Mean molecular mass of all products = 23.663 g
- Specific gas constant = 351.344 J/kg K
- Specific heat capacity at p=const. (Cp) = 2269.27 J/kgK
- Specific heat capacity at V=const. (Cv) = 1917.93 J/molK
- Specific heat ratio (Cp/Cv) = 1.1832

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 967.1 m/s
- Sound velocity at throat ) = 966.7 m/s
- Mach number at nozzle throat = 1.000
- Critical pressure ratio (pt/pc) = 0.566
- Pressure ratio (pc/pt) = 1.767

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.200684 E00 | 3.192811 E01 | 75.5529 |
| CO2 = | 2.658511 E-01 | 7.069407 E00 | 16.7287 |
| N2 = | 5.722308 E-02 | 1.521653 E00 | 3.6008 |
| BHO2 = | 3.644993 E-02 | 9.692618 E-01 | 2.2936 |

| | | | |
|---|---|---|---|
| CO = | 8.283536 E-03 | 2.202725 E-01 | 0.5212 |
| H2 = | 6.442775 E-03 | 1.713237 E-01 | 0.4054 |
| B(OH)3 = | 4.148446 E-03 | 1.103138 E-01 | 0.2610 |
| OH = | 3.143148 E-03 | 8.358133 E-02 | 0.1978 |
| O2 = | 2.778422 E-03 | 7.388268 E-02 | 0.1748 |
| I = | 2.472723 E-03 | 6.575365 E-02 | 0.1556 |
| NO = | 4.753776 E-04 | 1.264105 E-02 | 0.0299 |
| Fe(OH)2 = | 4.712672 E-04 | 1.253175 E-02 | 0.0297 |
| IH = | 3.593711 E-04 | 9.556252 E-03 | 0.0226 |
| B2O3 = | 1.370875 E-04 | 3.645377 E-03 | 0.0086 |
| H = | 1.237314 E-04 | 3.290217 E-03 | 0.0078 |
| BO2 = | 1.114070 E-04 | 2.962491 E-03 | 0.0070 |
| O = | 3.850837 E-05 | 1.023999 E-03 | 0.0024 |
| I2 = | 1.278707 E-06 | 3.400286 E-05 | 0.0001 |
| FeO = | 8.131816 E-07 | 2.162380 E-05 | 0.0001 |
| BO = | 4.186567 E-07 | 1.113275 E-05 | 0.0000 |
| Fe = | 3.623477 E-07 | 9.635403 E-06 | 0.0000 |
| NH3 = | 5.148625 E-08 | 1.369102 E-06 | 0.0000 |
| INO = | 5.088148 E-09 | 1.353020 E-07 | 0.0000 |
| NH2 = | 2.663011 E-09 | 7.081373 E-08 | 0.0000 |
| CHNO = | 1.097153 E-09 | 2.917504 E-08 | 0.0000 |
| N = | 7.680114 E-10 | 2.042265 E-08 | 0.0000 |
| HCN = | 4.287609 E-11 | 1.140144 E-09 | 0.0000 |
| FeO(l) = | 3.713175 E-11 | 9.873926 E-10 | 0.0000 |
| FeO(s) = | 1.966389 E-11 | 5.228943 E-10 | 0.0000 |
| CNO = | 6.139732 E-12 | 1.632653 E-10 | 0.0000 |
| B2O3(l) = | 3.620275 E-13 | 9.626889 E-12 | 0.0000 |
| Fe(l) = | 8.494506 E-14 | 2.258825 E-12 | 0.0000 |
| Fe(s) = | 6.972727 E-14 | 1.854160 E-12 | 0.0000 |
| BHO2(s) = | 3.494116 E-14 | 9.291413 E-13 | 0.0000 |
| B2O3(s) = | 2.184595 E-14 | 5.809188 E-13 | 0.0000 |
| ICN = | 1.745572 E-14 | 4.641754 E-13 | 0.0000 |
| CH4 = | 1.406460 E-14 | 3.740001 E-13 | 0.0000 |
| BH2 = | 1.066533 E-14 | 2.836080 E-13 | 0.0000 |
| CH3OH = | 1.038447 E-14 | 2.761396 E-13 | 0.0000 |
| BN = | 1.323490 E-16 | 3.519370 E-15 | 0.0000 |
| BN(s) = | 1.625040 E-18 | 4.321240 E-17 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9628.45 kJ/kg
- Temperature at nozzle exit = 1310.7 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 41.511 mol/kg expl.
- Total mole number of products = 41.740 mol/kg expl.
- Volume of gaseous products (at SATP) = 1029.02 L/kg expl.
- Mass of gaseous products = 984.1 g/kg expl.
- Mass of condensed products = 15.9 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.706 g
- Mean molecular mass of all products = 23.958 g
- Specific gas constant = 345.125 J/kg K
- Specific heat capacity at p=const. (Cp) = 1999.87 J/kgK
- Specific heat capacity at V=const. (Cv) = 1654.74 J/molK
- Specific heat ratio (Cp/Cv) = 1.2086

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 236.83 s
- Exhaust (or nozzle exit) velocity = 2323.3 m/s

- Characteristic exhaust velocity (c*) = 1406.2 m/s
- Thrust coefficient (Cf) = 1.652
- Nozzle area expansion ratio (Ae/At) = 8.91
- Pressure ratio (pc/pe) = 70.000
- Sound velocity at nozzle exit = 731.59 m/s
- Mach number at nozzle exit = 3.176

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.198194 E00 | 3.186188 E01 | 76.3347 |
| CO2 = | 2.709336 E-01 | 7.204558 E00 | 17.2607 |
| N2 = | 5.746079 E-02 | 1.527974 E00 | 3.6607 |
| B(OH)3 = | 1.922176 E-02 | 5.111373 E-01 | 1.2246 |
| B2O3(l) = | 8.120493 E-03 | 2.159369 E-01 | 0.5173 |
| BHO2 = | 5.520829 E-03 | 1.468077 E-01 | 0.3517 |
| H2 = | 3.708149 E-03 | 9.860561 E-02 | 0.2362 |
| CO = | 3.201035 E-03 | 8.512065 E-02 | 0.2039 |
| I = | 2.090414 E-03 | 5.558746 E-02 | 0.1332 |
| IH = | 7.228998 E-04 | 1.922306 E-02 | 0.0461 |
| FeO(s) = | 2.992816 E-04 | 7.958378 E-03 | 0.0191 |
| FeO(l) = | 1.707131 E-04 | 4.539534 E-03 | 0.0109 |
| I2 = | 1.067109 E-05 | 2.837613 E-04 | 0.0007 |
| Fe(OH)2 = | 2.535988 E-06 | 6.743597 E-05 | 0.0002 |
| B2O3 = | 3.989594 E-07 | 1.060897 E-05 | 0.0000 |
| OH = | 2.630318 E-07 | 6.994437 E-06 | 0.0000 |
| H = | 1.527514 E-07 | 4.061904 E-06 | 0.0000 |
| NH3 = | 1.544387 E-08 | 4.106772 E-07 | 0.0000 |
| Fe(s) = | 8.677360 E-09 | 2.307449 E-07 | 0.0000 |
| NO = | 3.493586 E-09 | 9.290003 E-08 | 0.0000 |
| BO2 = | 1.540744 E-09 | 4.097086 E-08 | 0.0000 |
| O2 = | 2.425447 E-10 | 6.449651 E-09 | 0.0000 |
| CH4 = | 1.417444 E-10 | 3.769210 E-09 | 0.0000 |
| Fe(l) = | 1.258875 E-10 | 3.347549 E-09 | 0.0000 |
| B2O3(s) = | 4.852812 E-11 | 1.290440 E-09 | 0.0000 |
| BN(s) = | 3.085463 E-11 | 8.204740 E-10 | 0.0000 |
| Fe = | 1.185065 E-11 | 3.151276 E-10 | 0.0000 |
| CHNO = | 9.260642 E-12 | 2.462553 E-10 | 0.0000 |
| BN = | 3.018836 E-12 | 8.027567 E-11 | 0.0000 |
| BHO2(s) = | 2.763590 E-12 | 7.348827 E-11 | 0.0000 |
| O = | 2.717624 E-12 | 7.226596 E-11 | 0.0000 |
| BO = | 2.035227 E-12 | 5.411995 E-11 | 0.0000 |
| BH2 = | 1.685133 E-12 | 4.481037 E-11 | 0.0000 |
| HCN = | 1.544864 E-12 | 4.108041 E-11 | 0.0000 |
| CNO = | 1.043043 E-12 | 2.773617 E-11 | 0.0000 |
| FeO = | 1.017556 E-12 | 2.705843 E-11 | 0.0000 |
| N = | 8.821762 E-13 | 2.345848 E-11 | 0.0000 |
| ICN = | 8.521849 E-13 | 2.266096 E-11 | 0.0000 |
| CH3OH = | 7.434221 E-13 | 1.976878 E-11 | 0.0000 |
| NH2 = | 2.572881 E-13 | 6.841702 E-12 | 0.0000 |
| INO = | 2.223242 E-13 | 5.911956 E-12 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 46

**Combustion conditions (Number 46):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 13.42 %**
2. **Hydrogen peroxide ($H_2O_2$), 81.14 %**
3. **Water ($H_2O$, liquid), 4.27 %**
4. **AKC_298, 1.17 %**

C(0.235) H(2.401) N(0.099) O(1.847) B(0.035) Fe(0.000) I(0.002)

Molecular weight = 36.87
Oxygen balance = 5.298504 %
Enthalpy of formation = -6815.83 kJ/kg
Internal energy of formation = -6669.73 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3936.55 kJ/kg
- Total enthalpy of combustion prod. = -6816.65 kJ/kg
- Entropy of combustion products = 10.77 kJ/K kg
- Isobaric combustion temperature = 2327.1 K
- Mole number of gaseous products = 42.468 mol/kg expl.
- Total mole number of products = 42.468 mol/kg expl.
- Volume of gaseous products (at SATP) = 1052.73 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.547 g
- Mean molecular mass of all products = 23.547 g
- Specific gas constant = 353.076 J/kg K
- Specific heat capacity at p=const. (Cp) = 2272.06 J/kgK
- Specific heat capacity at V=const. (Cv) = 1918.98 J/molK
- Specific heat ratio (Cp/Cv) = 1.1840

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.173048 E00 | 3.181199 E01 | 74.9088 |
| CO2 = | 2.333326 E-01 | 6.327771 E00 | 14.9002 |
| O2 = | 5.968703 E-02 | 1.618659 E00 | 3.8115 |
| N2 = | 4.815266 E-02 | 1.305857 E00 | 3.0749 |
| BHO2 = | 3.033125 E-02 | 8.225563 E-01 | 1.9369 |
| OH = | 7.768395 E-03 | 2.106719 E-01 | 0.4961 |
| B(OH)3 = | 4.344851 E-03 | 1.178284 E-01 | 0.2775 |
| NO = | 2.392376 E-03 | 6.487910 E-02 | 0.1528 |
| I = | 2.173430 E-03 | 5.894147 E-02 | 0.1388 |
| CO = | 1.937027 E-03 | 5.253043 E-02 | 0.1237 |
| H2 = | 1.602240 E-03 | 4.345131 E-02 | 0.1023 |
| Fe(OH)2 = | 3.920862 E-04 | 1.063303 E-02 | 0.0250 |
| BO2 = | 2.344507 E-04 | 6.358092 E-03 | 0.0150 |
| O = | 2.124111 E-04 | 5.760397 E-03 | 0.0136 |
| IH = | 1.804139 E-04 | 4.892664 E-03 | 0.0115 |
| B2O3 = | 1.070443 E-04 | 2.902946 E-03 | 0.0068 |

| | | | |
|---|---|---|---|
| H = | 6.954960 E-05 | 1.886123 E-03 | 0.0044 |
| I2 = | 1.335023 E-06 | 3.620461 E-05 | 0.0001 |
| FeO = | 6.718316 E-07 | 1.821947 E-05 | 0.0000 |
| BO = | 2.333198 E-07 | 6.327422 E-06 | 0.0000 |
| INO = | 3.433334 E-08 | 9.310893 E-07 | 0.0000 |
| NH3 = | 9.542447 E-09 | 2.587826 E-07 | 0.0000 |
| N = | 1.262683 E-09 | 3.424283 E-08 | 0.0000 |
| NH2 = | 1.138876 E-09 | 3.088529 E-08 | 0.0000 |
| CHNO = | 2.161556 E-10 | 5.861946 E-09 | 0.0000 |
| FeO(l) = | 2.089947 E-11 | 5.667747 E-10 | 0.0000 |
| FeO(s) = | 1.147950 E-11 | 3.113138 E-10 | 0.0000 |
| CNO = | 2.939806 E-12 | 7.972489 E-11 | 0.0000 |
| HCN = | 2.099577 E-12 | 5.693864 E-11 | 0.0000 |
| Fe3O4(s) = | 4.152524 E-13 | 1.126127 E-11 | 0.0000 |
| B2O3(l) = | 2.615708 E-13 | 7.093565 E-12 | 0.0000 |
| B2O3(s) = | 1.543381 E-14 | 4.185512 E-13 | 0.0000 |
| ICN = | 1.963753 E-15 | 5.325522 E-14 | 0.0000 |
| BHO2(s) = | 1.676851 E-15 | 4.547470 E-14 | 0.0000 |
| BH2 = | 6.229569 E-16 | 1.689403 E-14 | 0.0000 |
| CH3OH = | 3.584482 E-16 | 9.720792 E-15 | 0.0000 |
| CH4 = | 1.114217 E-16 | 3.021655 E-15 | 0.0000 |
| BN = | 3.495189 E-17 | 9.478640 E-16 | 0.0000 |
| BN(s) = | 2.110050 E-19 | 5.722266 E-18 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7264.65 kJ/kg
- Temperature at nozzle throat = 2145.0 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 42.389 mol/kg expl.
- Total mole number of products = 42.389 mol/kg expl.
- Volume of gaseous products (at SATP) = 1050.79 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.591 g
- Mean molecular mass of all products = 23.591 g
- Specific gas constant = 352.424 J/kg K
- Specific heat capacity at p=const. (Cp) = 2232.55 J/kgK
- Specific heat capacity at V=const. (Cv) = 1880.13 J/molK
- Specific heat ratio (Cp/Cv) = 1.1874

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 946.6 m/s
- Sound velocity at throat) = 947.4 m/s
- Mach number at nozzle throat = 0.999
- Critical pressure ratio (pt/pc) = 0.566
- Pressure ratio (pc/pt) = 1.767

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.174634 E00 | 3.185501 E01 | 75.1489 |
| CO2 = | 2.344908 E-01 | 6.359179 E00 | 15.0019 |
| O2 = | 5.994795 E-02 | 1.625734 E00 | 3.8353 |
| N2 = | 4.854222 E-02 | 1.316422 E00 | 3.1056 |
| BHO2 = | 2.955807 E-02 | 8.015883 E-01 | 1.8910 |
| B(OH)3 = | 5.274770 E-03 | 1.430470 E-01 | 0.3375 |

| | | | |
|---|---|---|---|
| OH = | 4.443451 E-03 | 1.205024 E-01 | 0.2843 |
| I = | 2.218914 E-03 | 6.017496 E-02 | 0.1420 |
| NO = | 1.613265 E-03 | 4.375028 E-02 | 0.1032 |
| CO = | 7.788471 E-04 | 2.112163 E-02 | 0.0498 |
| H2 = | 7.160853 E-04 | 1.941959 E-02 | 0.0458 |
| Fe(OH)2 = | 3.924413 E-04 | 1.064266 E-02 | 0.0251 |
| IH = | 1.345302 E-04 | 3.648338 E-03 | 0.0086 |
| BO2 = | 1.306135 E-04 | 3.542122 E-03 | 0.0084 |
| O = | 9.350299 E-05 | 2.535717 E-03 | 0.0060 |
| B2O3 = | 8.068459 E-05 | 2.188093 E-03 | 0.0052 |
| H = | 2.312361 E-05 | 6.270916 E-04 | 0.0015 |
| I2 = | 1.542161 E-06 | 4.182201 E-05 | 0.0001 |
| FeO = | 3.166492 E-07 | 8.587243 E-06 | 0.0000 |
| BO = | 5.274674 E-08 | 1.430444 E-06 | 0.0000 |
| INO = | 1.966435 E-08 | 5.332794 E-07 | 0.0000 |
| NH3 = | 2.046500 E-09 | 5.549924 E-08 | 0.0000 |
| N = | 2.102530 E-10 | 5.701872 E-09 | 0.0000 |
| NH2 = | 1.732396 E-10 | 4.698102 E-09 | 0.0000 |
| FeO(l) = | 4.930532 E-11 | 1.337116 E-09 | 0.0000 |
| CHNO = | 3.114125 E-11 | 8.445228 E-10 | 0.0000 |
| FeO(s) = | 2.714508 E-11 | 7.361500 E-10 | 0.0000 |
| Fe3O4(s) = | 1.100309 E-11 | 2.983940 E-10 | 0.0000 |
| B2O3(l) = | 5.402705 E-13 | 1.465165 E-11 | 0.0000 |
| CNO = | 2.652198 E-13 | 7.192522 E-12 | 0.0000 |
| HCN = | 1.425903 E-13 | 3.866919 E-12 | 0.0000 |
| BHO2(s) = | 4.767715 E-14 | 1.292961 E-12 | 0.0000 |
| B2O3(s) = | 3.382489 E-14 | 9.173004 E-13 | 0.0000 |
| ICN = | 1.636871 E-16 | 4.439046 E-15 | 0.0000 |
| BH2 = | 1.915815 E-17 | 5.195517 E-16 | 0.0000 |
| CH3OH = | 1.574034 E-17 | 4.268637 E-16 | 0.0000 |
| CH4 = | 3.337727 E-18 | 9.051616 E-17 | 0.0000 |
| BN = | 9.809387 E-19 | 2.660217 E-17 | 0.0000 |
| BN(s) = | 7.398988 E-20 | 2.006539 E-18 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9382.94 kJ/kg
- Temperature at nozzle exit = 1220.8 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 41.753 mol/kg expl.
- Total mole number of products = 41.941 mol/kg expl.
- Volume of gaseous products (at SATP) = 1035.02 L/kg expl.
- Mass of gaseous products = 986.4 g/kg expl.
- Mass of condensed products = 13.7 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.623 g
- Mean molecular mass of all products = 23.843 g
- Specific gas constant = 347.138 J/kg K
- Specific heat capacity at p=const. (Cp) = 1951.70 J/kgK
- Specific heat capacity at V=const. (Cv) = 1604.56 J/molK
- Specific heat ratio (Cp/Cv) = 1.2163

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 230.94 s
- Exhaust (or nozzle exit) velocity = 2265.5 m/s
- Characteristic exhaust velocity (c*) = 1379.2 m/s
- Thrust coefficient (Cf) = 1.643
- Nozzle area expansion ratio (Ae/At) = 8.77
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 709.39 m/s
- Mach number at nozzle exit = 3.194

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.170078 E00 | 3.173145 E01 | 75.6566 |
| CO2 = | 2.352696 E-01 | 6.380301 E00 | 15.2124 |
| O2 = | 6.107547 E-02 | 1.656312 E00 | 3.9491 |
| N2 = | 4.933165 E-02 | 1.337830 E00 | 3.1898 |
| B(OH)3 = | 1.988508 E-02 | 5.392655 E-01 | 1.2858 |
| B2O3(l) = | 6.802541 E-03 | 1.844788 E-01 | 0.4398 |
| I = 2.251402 E-03 | 6.105599 E-02 | 0.1456 | |
| BHO2 = | 1.634646 E-03 | 4.433012 E-02 | 0.1057 |
| Fe3O4(s) = | 1.309199 E-04 | 3.550431 E-03 | 0.0085 |
| I2 = 4.671262 E-05 | 1.266804 E-03 | 0.0030 | |
| NO = | 3.442823 E-05 | 9.336628 E-04 | 0.0022 |
| IH = | 1.172096 E-05 | 3.178619 E-04 | 0.0008 |
| OH = | 1.120668 E-05 | 3.039151 E-04 | 0.0007 |
| H2 = | 9.213471 E-08 | 2.498610 E-06 | 0.0000 |
| CO = | 3.152861 E-08 | 8.550276 E-07 | 0.0000 |
| B2O3 = | 2.797523 E-08 | 7.586630 E-07 | 0.0000 |
| BO2 = | 1.505579 E-08 | 4.082996 E-07 | 0.0000 |
| O = 1.210568 E-08 | 3.282952 E-07 | 0.0000 | |
| Fe(OH)2 = | 9.419765 E-09 | 2.554555 E-07 | 0.0000 |
| FeO(s) = | 1.008462 E-09 | 2.734857 E-08 | 0.0000 |
| INO = | 3.974176 E-10 | 1.077761 E-08 | 0.0000 |
| H = 1.187219 E-10 | 3.219631 E-09 | 0.0000 | |
| FeO(l) = | 1.107574 E-10 | 3.003640 E-09 | 0.0000 |
| B2O3(s) = | 8.147834 E-11 | 2.209619 E-09 | 0.0000 |
| BN(s) = | 4.361280 E-11 | 1.182740 E-09 | 0.0000 |
| BN = | 5.198758 E-12 | 1.409856 E-10 | 0.0000 |
| BH2 = | 4.796630 E-12 | 1.300803 E-10 | 0.0000 |
| BHO2(s) = | 4.774109 E-12 | 1.294695 E-10 | 0.0000 |
| CH4 = | 4.589957 E-12 | 1.244755 E-10 | 0.0000 |
| CH3OH = | 4.081051 E-12 | 1.106744 E-10 | 0.0000 |
| ICN = | 3.111243 E-12 | 8.437413 E-11 | 0.0000 |
| HCN = | 2.780194 E-12 | 7.539636 E-11 | 0.0000 |
| CNO = | 2.392283 E-12 | 6.487655 E-11 | 0.0000 |
| CHNO = | 1.409147 E-12 | 3.821480 E-11 | 0.0000 |
| NH2 = | 1.230741 E-12 | 3.337659 E-11 | 0.0000 |
| N = 1.211641 E-12 | 3.285862 E-11 | 0.0000 | |
| BO = | 6.919038 E-13 | 1.876381 E-11 | 0.0000 |
| FeO = | 6.747603 E-13 | 1.829889 E-11 | 0.0000 |
| NH3 = | 5.896946 E-13 | 1.599199 E-11 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 47

**Combustion conditions (Number 47):**

---

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

---

1. **[EMIM][$BH_3CN$], 11.50 %**
2. **Hydrogen peroxide ($H_2O_2$), 83.13 %**
3. **Water ($H_2O$, liquid), 4.37 %**
4. **AKC_298, 1.00 %**

C(0.198) H(2.338) N(0.083) O(1.857) B(0.030) Fe(0.000) I(0.002)

Molecular weight = 36.19
Oxygen balance = 10.93876 %
Enthalpy of formation = -6703.14 kJ/kg
Internal energy of formation = -6556.66 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3607.00 kJ/kg
- Total enthalpy of combustion prod. = -6703.42 kJ/kg
- Entropy of combustion products = 10.66 kJ/K kg
- Isobaric combustion temperature = 2191.5 K
- Mole number of gaseous products = 42.679 mol/kg expl.
- Total mole number of products = 42.679 mol/kg expl.
- Volume of gaseous products (at SATP) = 1057.97 L/kg expl.
- Mass of gaseous products = 1000.0 g/kg expl.
- Mass of condensed products = 0.0 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.431 g
- Mean molecular mass of all products = 23.431 g
- Specific gas constant = 354.832 J/kg K
- Specific heat capacity at p=const. (Cp) = 2228.10 J/kgK
- Specific heat capacity at V=const. (Cv) = 1873.27 J/molK
- Specific heat ratio (Cp/Cv) = 1.1894

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.144852 E00 | 3.163426 E01 | 74.1216 |
| CO2 = | 1.975423 E-01 | 5.458440 E00 | 12.7896 |
| O2 = | 1.215148 E-01 | 3.357667 E00 | 7.8673 |
| N2 = | 4.032339 E-02 | 1.114206 E00 | 2.6107 |
| BHO2 = | 2.337214 E-02 | 6.458133 E-01 | 1.5132 |
| B(OH)3 = | 5.896728 E-03 | 1.629369 E-01 | 0.3818 |
| OH = | 5.439544 E-03 | 1.503041 E-01 | 0.3522 |
| NO = | 2.360194 E-03 | 6.521629 E-02 | 0.1528 |
| I = | 1.827464 E-03 | 5.049602 E-02 | 0.1183 |
| Fe(OH)2 = | 3.293987 E-04 | 9.101864 E-03 | 0.0213 |
| CO = | 3.139742 E-04 | 8.675657 E-03 | 0.0203 |
| H2 = | 3.015380 E-04 | 8.332023 E-03 | 0.0195 |
| IH = | 1.474397 E-04 | 4.074016 E-03 | 0.0095 |
| BO2 = | 1.397811 E-04 | 3.862397 E-03 | 0.0090 |
| O = | 1.198123 E-04 | 3.310624 E-03 | 0.0078 |
| B2O3 = | 6.363879 E-05 | 1.758451 E-03 | 0.0041 |

| | | | |
|---|---|---|---|
| H = | 1.380713 E-05 | 3.815152 E-04 | 0.0009 |
| I2 = | 9.105769 E-07 | 2.516083 E-05 | 0.0001 |
| FeO = | 2.164915 E-07 | 5.982039 E-06 | 0.0000 |
| INO = | 5.114984 E-08 | 1.413360 E-06 | 0.0000 |
| BO = | 3.743778 E-08 | 1.034472 E-06 | 0.0000 |
| Fe3O4(s) = | 4.203022 E-09 | 1.161369 E-07 | 0.0000 |
| FeO(l) = | 2.649722 E-09 | 7.321646 E-08 | 0.0000 |
| NH3 = | 1.686786 E-09 | 4.660886 E-08 | 0.0000 |
| N = | 2.109291 E-10 | 5.828340 E-09 | 0.0000 |
| NH2 = | 1.652254 E-10 | 4.565467 E-09 | 0.0000 |
| B2O3(l) = | 8.146605 E-11 | 2.251050 E-09 | 0.0000 |
| CHNO = | 1.951718 E-11 | 5.392939 E-10 | 0.0000 |
| B2O3(s) = | 9.823902 E-12 | 2.714516 E-10 | 0.0000 |
| FeO(s) = | 2.487596 E-12 | 6.873663 E-11 | 0.0000 |
| BN(s) = | 1.583475 E-12 | 4.375418 E-11 | 0.0000 |
| BN = | 1.299191 E-12 | 3.589893 E-11 | 0.0000 |
| CH4 = | 1.235597 E-12 | 3.414170 E-11 | 0.0000 |
| BH2 = | 1.035734 E-12 | 2.861915 E-11 | 0.0000 |
| CH3OH = | 1.029440 E-12 | 2.844522 E-11 | 0.0000 |
| ICN = | 7.714023 E-13 | 2.131520 E-11 | 0.0000 |
| BHO2(s) = | 1.871680 E-13 | 5.171779 E-12 | 0.0000 |
| HCN = | 1.512035 E-13 | 4.178017 E-12 | 0.0000 |
| CNO = | 3.020738 E-14 | 8.346829 E-13 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -7127.70 kJ/kg
- Temperature at nozzle throat = 2011.2 K
- Pressure at nozzle throat = 4.0 MPa
- Mole number of gaseous products = 42.607 mol/kg expl.
- Total mole number of products = 42.607 mol/kg expl.
- Volume of gaseous products (at SATP) = 1056.18 L/kg expl.
- Mass of gaseous products = 999.9 g/kg expl.
- Mass of condensed products = 0.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.467 g
- Mean molecular mass of all products = 23.470 g
- Specific gas constant = 354.232 J/kg K
- Specific heat capacity at p=const. (Cp) = 2185.71 J/kgK
- Specific heat capacity at V=const. (Cv) = 1831.48 J/molK
- Specific heat ratio (Cp/Cv) = 1.1934

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 921.2 m/s
- Sound velocity at throat) = 922.1 m/s
- Mach number at nozzle throat = 0.999
- Critical pressure ratio (pt/pc) = 0.565
- Pressure ratio (pc/pt) = 1.770

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.144544 E00 | 3.162575 E01 | 74.2262 |
| CO2 = | 1.976970 E-01 | 5.462715 E00 | 12.8211 |
| O2 = | 1.224952 E-01 | 3.384756 E00 | 7.9441 |
| N2 = | 4.075989 E-02 | 1.126267 E00 | 2.6434 |
| BHO2 = | 2.173466 E-02 | 6.005667 E-01 | 1.4095 |
| B(OH)3 = | 7.665354 E-03 | 2.118072 E-01 | 0.4971 |

| | | | |
|---|---|---|---|
| OH = | 2.822392 E-03 | 7.798763 E-02 | 0.1830 |
| I = | 1.891069 E-03 | 5.225354 E-02 | 0.1226 |
| NO = | 1.487251 E-03 | 4.109536 E-02 | 0.0965 |
| Fe(OH)2 = | 2.639497 E-04 | 7.293393 E-03 | 0.0171 |
| H2 = | 1.868301 E-04 | 5.162442 E-03 | 0.0121 |
| CO = | 1.592511 E-04 | 4.400388 E-03 | 0.0103 |
| IH = | 8.159467 E-05 | 2.254604 E-03 | 0.0053 |
| BO2 = | 6.270469 E-05 | 1.732640 E-03 | 0.0041 |
| O = | 5.041423 E-05 | 1.393033 E-03 | 0.0033 |
| B2O3 = | 3.663832 E-05 | 1.012381 E-03 | 0.0024 |
| Fe3O4(s) = | 2.181517 E-05 | 6.027913 E-04 | 0.0014 |
| H = | 4.964716 E-06 | 1.371838 E-04 | 0.0003 |
| I2 = | 2.045172 E-06 | 5.651169 E-05 | 0.0001 |
| FeO = | 6.727916 E-08 | 1.859041 E-06 | 0.0000 |
| INO = | 2.187738 E-08 | 6.045103 E-07 | 0.0000 |
| BO = | 6.241589 E-09 | 1.724660 E-07 | 0.0000 |
| BN = | 2.811529 E-09 | 7.768747 E-08 | 0.0000 |
| CH4 = | 9.533313 E-10 | 2.634221 E-08 | 0.0000 |
| BN(s) = | 6.880638 E-10 | 1.901241 E-08 | 0.0000 |
| NH3 = | 3.116357 E-10 | 8.611040 E-09 | 0.0000 |
| FeO(l) = | 6.797132 E-11 | 1.878167 E-09 | 0.0000 |
| BH2 = | 6.711879 E-11 | 1.854610 E-09 | 0.0000 |
| FeO(s) = | 4.037114 E-11 | 1.115525 E-09 | 0.0000 |
| N = | 3.108269 E-11 | 8.588691 E-10 | 0.0000 |
| CH3OH = | 2.999962 E-11 | 8.289421 E-10 | 0.0000 |
| NH2 = | 2.079389 E-11 | 5.745717 E-10 | 0.0000 |
| CHNO = | 2.883579 E-12 | 7.967834 E-11 | 0.0000 |
| B2O3(l) = | 1.012700 E-12 | 2.798268 E-11 | 0.0000 |
| BHO2(s) = | 7.716786 E-14 | 2.132283 E-12 | 0.0000 |
| B2O3(s) = | 6.771323 E-14 | 1.871035 E-12 | 0.0000 |
| ICN = | 1.926530 E-14 | 5.323341 E-13 | 0.0000 |
| CNO = | 1.740653 E-14 | 4.809730 E-13 | 0.0000 |
| HCN = | 3.736614 E-15 | 1.032492 E-13 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -9105.47 kJ/kg
- Temperature at nozzle exit = 1109.9 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 42.088 mol/kg expl.
- Total mole number of products = 42.197 mol/kg expl.
- Volume of gaseous products (at SATP) = 1043.32 L/kg expl.
- Mass of gaseous products = 991.9 g/kg expl.
- Mass of condensed products = 8.1 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.567 g
- Mean molecular mass of all products = 23.699 g
- Specific gas constant = 349.918 J/kg K
- Specific heat capacity at p=const. (Cp) = 1891.57 J/kgK
- Specific heat capacity at V=const. (Cv) = 1541.65 J/molK
- Specific heat ratio (Cp/Cv) = 1.2270

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 223.43 s
- Exhaust (or nozzle exit) velocity = 2191.8 m/s
- Characteristic exhaust velocity (c*) = 1339.6 m/s
- Thrust coefficient (Cf) = 1.636
- Nozzle area expansion ratio (Ae/At) = 8.60
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 680.80 m/s
- Mach number at nozzle exit = 3.219

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.136352 E00 | 3.139940 E01 | 74.4108 |
| CO2 = | 1.978563 E-01 | 5.467115 E00 | 12.9561 |
| O2 = | 1.237387 E-01 | 3.419118 E00 | 8.1027 |
| N2 = | 4.149456 E-02 | 1.146567 E00 | 2.7172 |
| B(OH)3 = | 2.154522 E-02 | 5.953323 E-01 | 1.4108 |
| B2O3(l) = | 3.855842 E-03 | 1.065437 E-01 | 0.2525 |
| I = 1.779985 E-03 | | 4.918410 E-02 | 0.1166 |
| BHO2 = | 2.790897 E-04 | 7.711738 E-03 | 0.0183 |
| Fe3O4(s) = | 1.098327 E-04 | 3.034870 E-03 | 0.0072 |
| I2 = 9.501675 E-05 | | 2.625479 E-03 | 0.0062 |
| NO = | 1.791698 E-05 | 4.950776 E-04 | 0.0012 |
| IH = | 6.756877 E-06 | 1.867043 E-04 | 0.0004 |
| OH = | 2.608126 E-06 | 7.206709 E-05 | 0.0002 |
| H2 = | 5.475930 E-09 | 1.513095 E-07 | 0.0000 |
| FeO(s) = | 1.866139 E-09 | 5.156468 E-08 | 0.0000 |
| FeO(l) = | 1.710520 E-09 | 4.726466 E-08 | 0.0000 |
| B2O3(s) = | 1.278732 E-09 | 3.533361 E-08 | 0.0000 |
| CO = | 1.221410 E-09 | 3.374969 E-08 | 0.0000 |
| O = 1.056203 E-09 | | 2.918475 E-08 | 0.0000 |
| INO = | 7.259683 E-10 | 2.005978 E-08 | 0.0000 |
| BO2 = | 5.481208 E-10 | 1.514554 E-08 | 0.0000 |
| B2O3 = | 4.567232 E-10 | 1.262006 E-08 | 0.0000 |
| Fe(OH)2 = | 4.348800 E-10 | 1.201650 E-08 | 0.0000 |
| BN(s) = | 3.924352 E-10 | 1.084367 E-08 | 0.0000 |
| BHO2(s) = | 1.021008 E-10 | 2.821224 E-09 | 0.0000 |
| BN = | 6.565570 E-11 | 1.814182 E-09 | 0.0000 |
| BH2 = | 6.165020 E-11 | 1.703503 E-09 | 0.0000 |
| CH4 = | 5.765955 E-11 | 1.593234 E-09 | 0.0000 |
| CH3OH = | 5.097764 E-11 | 1.408601 E-09 | 0.0000 |
| ICN = | 3.941272 E-11 | 1.089043 E-09 | 0.0000 |
| HCN = | 3.760294 E-11 | 1.039035 E-09 | 0.0000 |
| CNO = | 3.224667 E-11 | 8.910321 E-10 | 0.0000 |
| CHNO = | 2.120628 E-11 | 5.859666 E-10 | 0.0000 |
| NH2 = | 1.930846 E-11 | 5.335265 E-10 | 0.0000 |
| N = 1.918155 E-11 | | 5.300198 E-10 | 0.0000 |
| BO = | 1.547546 E-11 | 4.276142 E-10 | 0.0000 |
| FeO = | 1.509874 E-11 | 4.172045 E-10 | 0.0000 |
| NH3 = | 1.193546 E-11 | 3.297977 E-10 | 0.0000 |
| H = 1.297172 E-13 | | 3.584314 E-12 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default)

# Calculation Number 48

**Combustion conditions (Number 48):**

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Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
**Expansion conditions: Equilibrium expansion**

**Reactant information:**

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1. **[EMIM][$BH_3CN$], 9.20 %**
2. **Hydrogen peroxide ($H_2O_2$), 85.50 %**
3. **Water ($H_2O$, liquid), 4.5 %**
4. **AKC_298, 0.80 %**

C(0.155) H(2.264) N(0.065) O(1.868) B(0.023) Fe(0.000) I(0.002)

Molecular weight = 35.4
Oxygen balance = 17.68607 %
Enthalpy of formation = -6569.68 kJ/kg
Internal energy of formation = -6422.73 kJ/kg

Parameters in combustion chamber:

---

- Heat of isobaric combustion = -3196.35 kJ/kg
- Total enthalpy of combustion prod. = -6569.87 kJ/kg
- Entropy of combustion products = 10.50 kJ/K kg
- Isobaric combustion temperature = 2016.4 K
- Mole number of gaseous products = 42.949 mol/kg expl.
- Total mole number of products = 42.950 mol/kg expl.
- Volume of gaseous products (at SATP) = 1064.66 L/kg expl.
- Mass of gaseous products = 999.8 g/kg expl.
- Mass of condensed products = 0.2 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.279 g
- Mean molecular mass of all products = 23.283 g
- Specific gas constant = 357.076 J/kg K
- Specific heat capacity at p=const. (Cp) = 2169.43 J/kgK
- Specific heat capacity at V=const. (Cv) = 1812.35 J/molK
- Specific heat ratio (Cp/Cv) = 1.1970

Composition of combustion products in chamber:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.110372 E00 | 3.136521 E01 | 73.0276 |
| O2 = | 1.942368 E-01 | 5.486699 E00 | 12.7747 |
| CO2 = | 1.547826 E-01 | 4.372217 E00 | 10.1798 |
| N2 = | 3.164201 E-02 | 8.938068 E-01 | 2.0811 |
| BHO2 = | 1.445976 E-02 | 4.084516 E-01 | 0.9510 |
| B(OH)3 = | 8.567491 E-03 | 2.420100 E-01 | 0.5635 |
| OH = | 2.771591 E-03 | 7.829046 E-02 | 0.1823 |
| NO = | 1.674087 E-03 | 4.728872 E-02 | 0.1101 |
| I = | 1.457722 E-03 | 4.117695 E-02 | 0.0959 |
| Fe(OH)2 = | 1.526674 E-04 | 4.312469 E-03 | 0.0100 |
| IH = | 8.576209 E-05 | 2.422563 E-03 | 0.0056 |
| H2 = | 7.171097 E-05 | 2.025654 E-03 | 0.0047 |
| CO = | 5.220349 E-05 | 1.474617 E-03 | 0.0034 |
| O = | 4.950931 E-05 | 1.398513 E-03 | 0.0033 |
| BO2 = | 4.636006 E-05 | 1.309555 E-03 | 0.0030 |
| Fe3O4(s) = | 3.504506 E-05 | 9.899344 E-04 | 0.0023 |

| | | | |
|---|---|---|---|
| B2O3 = | 2.006933 E-05 | 5.669080 E-04 | 0.0013 |
| H = | 2.838299 E-06 | 8.017478 E-05 | 0.0002 |
| I2 = | 1.710078 E-06 | 4.830539 E-05 | 0.0001 |
| INO = | 4.596966 E-08 | 1.298527 E-06 | 0.0000 |
| FeO = | 2.367020 E-08 | 6.686233 E-07 | 0.0000 |
| BO = | 2.491089 E-09 | 7.036698 E-08 | 0.0000 |
| B2O3(l) = | 1.098796 E-09 | 3.103820 E-08 | 0.0000 |
| NH3 = | 1.988851 E-10 | 5.618003 E-09 | 0.0000 |
| B2O3(s) = | 1.263528 E-10 | 3.569149 E-09 | 0.0000 |
| FeO(s) = | 8.455662 E-11 | 2.388511 E-09 | 0.0000 |
| FeO(l) = | 4.907436 E-11 | 1.386227 E-09 | 0.0000 |
| BHO2(s) = | 4.513016 E-11 | 1.274813 E-09 | 0.0000 |
| BN = | 2.057689 E-11 | 5.812452 E-10 | 0.0000 |
| BN(s) = | 1.991824 E-11 | 5.626400 E-10 | 0.0000 |
| CH4 = | 1.973943 E-11 | 5.575889 E-10 | 0.0000 |
| N = | 1.818175 E-11 | 5.135887 E-10 | 0.0000 |
| BH2 = | 1.798620 E-11 | 5.080648 E-10 | 0.0000 |
| CH3OH = | 1.685012 E-11 | 4.759733 E-10 | 0.0000 |
| NH2 = | 1.433699 E-11 | 4.049837 E-10 | 0.0000 |
| ICN = | 1.348786 E-11 | 3.809980 E-10 | 0.0000 |
| HCN = | 7.879814 E-12 | 2.225848 E-10 | 0.0000 |
| CNO = | 5.838152 E-12 | 1.649130 E-10 | 0.0000 |
| CHNO = | 7.375988 E-13 | 2.083530 E-11 | 0.0000 |

Parameters at the nozzle throat:

---

- Total enthalpy of combustion prod. = -6963.97 kJ/kg
- Temperature at nozzle throat = 1843.9 K
- Pressure at nozzle throat = 3.9 MPa
- Mole number of gaseous products = 42.863 mol/kg expl.
- Total mole number of products = 42.865 mol/kg expl.
- Volume of gaseous products (at SATP) = 1062.53 L/kg expl.
- Mass of gaseous products = 999.6 g/kg expl.
- Mass of condensed products = 0.4 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.320 g
- Mean molecular mass of all products = 23.330 g
- Specific gas constant = 356.361 J/kg K
- Specific heat capacity at p=const. (Cp) = 2124.77 J/kgK
- Specific heat capacity at V=const. (Cv) = 1768.41 J/molK
- Specific heat ratio (Cp/Cv) = 1.2015

Characteristic parameters at the nozzle throat:

.....

- Flow velocity at nozzle throat = 887.8 m/s
- Sound velocity at throat) = 888.6 m/s
- Mach number at nozzle throat = 0.999
- Critical pressure ratio (pt/pc) = 0.563
- Pressure ratio (pc/pt) = 1.775

Composition of combustion products at nozzle throat:

---

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.108639 E00 | 3.131626 E01 | 73.0583 |
| O2 = | 1.949062 E-01 | 5.505609 E00 | 12.8441 |
| CO2 = | 1.548131 E-01 | 4.373079 E00 | 10.2020 |
| N2 = | 3.197619 E-02 | 9.032466 E-01 | 2.1072 |
| BHO2 = | 1.190712 E-02 | 3.363461 E-01 | 0.7847 |
| B(OH)3 = | 1.117334 E-02 | 3.156185 E-01 | 0.7363 |

| | | | |
|---|---|---|---|
| I = | 1.495273 E-03 | 4.223770 E-02 | 0.0985 |
| OH = | 1.287018 E-03 | 3.635502 E-02 | 0.0848 |
| NO = | 1.005770 E-03 | 2.841047 E-02 | 0.0663 |
| Fe3O4(s) = | 6.856720 E-05 | 1.936850 E-03 | 0.0045 |
| Fe(OH)2 = | 5.212078 E-05 | 1.472280 E-03 | 0.0034 |
| IH = | 4.563954 E-05 | 1.289202 E-03 | 0.0030 |
| H2 = | 3.644405 E-05 | 1.029452 E-03 | 0.0024 |
| CO = | 2.167808 E-05 | 6.123510 E-04 | 0.0014 |
| BO2 = | 1.621773 E-05 | 4.581101 E-04 | 0.0011 |
| O = | 1.581501 E-05 | 4.467342 E-04 | 0.0010 |
| B2O3 = | 8.534221 E-06 | 2.410702 E-04 | 0.0006 |
| I2 = | 3.008815 E-06 | 8.499141 E-05 | 0.0002 |
| H = | 6.371418 E-07 | 1.799765 E-05 | 0.0000 |
| INO = | 1.913026 E-08 | 5.403816 E-07 | 0.0000 |
| FeO = | 2.516110 E-09 | 7.107376 E-08 | 0.0000 |
| BN = | 2.009885 E-09 | 5.677417 E-08 | 0.0000 |
| CH4 = | 6.224420 E-10 | 1.758242 E-08 | 0.0000 |
| BO = | 2.860448 E-10 | 8.080042 E-09 | 0.0000 |
| BH2 = | 1.557267 E-10 | 4.398885 E-09 | 0.0000 |
| NH3 = | 3.254162 E-11 | 9.192185 E-10 | 0.0000 |
| FeO(l) = | 2.309416 E-11 | 6.523517 E-10 | 0.0000 |
| BN(s) = | 2.226474 E-11 | 6.289227 E-10 | 0.0000 |
| CH3OH = | 1.978657 E-11 | 5.589205 E-10 | 0.0000 |
| FeO(s) = | 1.794080 E-11 | 5.067824 E-10 | 0.0000 |
| N = | 2.027103 E-12 | 5.726054 E-11 | 0.0000 |
| B2O3(l) = | 1.818844 E-12 | 5.137776 E-11 | 0.0000 |
| NH2 = | 1.334578 E-12 | 3.769845 E-11 | 0.0000 |
| CHNO = | 1.463563 E-13 | 4.134195 E-12 | 0.0000 |
| B2O3(s) = | 1.358794 E-13 | 3.838250 E-12 | 0.0000 |
| BHO2(s) = | 1.322294 E-13 | 3.735147 E-12 | 0.0000 |
| ICN = | 4.104490 E-14 | 1.159415 E-12 | 0.0000 |
| CNO = | 4.673131 E-16 | 1.320041 E-14 | 0.0000 |
| HCN = | 4.105060 E-17 | 1.159576 E-15 | 0.0000 |

Parameters at the nozzle exit:

---

- Total enthalpy of combustion prod. = -8761.42 kJ/kg
- Temperature at nozzle exit = 974.3 K
- Pressure at nozzle throat = 0.1 MPa
- Mole number of gaseous products = 42.510 mol/kg expl.
- Total mole number of products = 42.513 mol/kg expl.
- Volume of gaseous products (at SATP) = 1053.79 L/kg expl.
- Mass of gaseous products = 999.5 g/kg expl.
- Mass of condensed products = 0.6 g/kg expl.
- Mean molecular mass of gaseous prod. = 23.511 g
- Mean molecular mass of all products = 23.523 g
- Specific gas constant = 353.431 J/kg K
- Specific heat capacity at p=const. (Cp) = 1815.28 J/kgK
- Specific heat capacity at V=const. (Cv) = 1461.85 J/molK
- Specific heat ratio (Cp/Cv) = 1.2418

Characteristic parameters at the nozzle exit:

.....

- Specific impulse = 213.41 s
- Exhaust (or nozzle exit) velocity = 2093.6 m/s
- Characteristic exhaust velocity (c*) = 1285.8 m/s
- Thrust coefficient (Cf) = 1.628
- Nozzle area expansion ratio (Ae/At) = 8.36
- Pressure ratio (pc/pe) = 70.000

- Sound velocity at nozzle exit = 643.22 m/s
- Mach number at nozzle exit = 3.255

Composition of combustion products at the nozzle exit:

| Products | mol/mol | mol/kg | Mol % |
|---|---|---|---|
| H2O = | 1.097454 E00 | 3.100031 E01 | 72.9201 |
| O2 = | 1.956912 E-01 | 5.527782 E00 | 13.0027 |
| CO2 = | 1.548348 E-01 | 4.373692 E00 | 10.2880 |
| N2 = | 3.247645 E-02 | 9.173778 E-01 | 2.1579 |
| B(OH)3 = | 2.309581 E-02 | 6.523983 E-01 | 1.5346 |
| I = | 1.146471 E-03 | 3.238491 E-02 | 0.0762 |
| I2 = | 1.995806 E-04 | 5.637647 E-03 | 0.0133 |
| Fe3O4(s) = | 8.594179 E-05 | 2.427639 E-03 | 0.0057 |
| BHO2 = | 1.798207 E-05 | 5.079480 E-04 | 0.0012 |
| NO = | 5.237684 E-06 | 1.479514 E-04 | 0.0003 |
| IH = | 1.317100 E-06 | 3.720474 E-05 | 0.0001 |
| OH = | 2.477836 E-07 | 6.999262 E-06 | 0.0000 |
| B2O3(l) = | 3.467221 E-09 | 9.794024 E-08 | 0.0000 |
| INO = | 2.924281 E-10 | 8.260356 E-09 | 0.0000 |
| H2 = | 1.107293 E-10 | 3.127822 E-09 | 0.0000 |
| FeO(s) = | 2.511043 E-11 | 7.093062 E-10 | 0.0000 |
| O = | 2.402153 E-11 | 6.785474 E-10 | 0.0000 |
| FeO(l) = | 2.114545 E-11 | 5.973055 E-10 | 0.0000 |
| CO = | 1.107983 E-11 | 3.129771 E-10 | 0.0000 |
| Fe(OH)2 = | 5.636742 E-12 | 1.592237 E-10 | 0.0000 |
| BO2 = | 3.758494 E-12 | 1.061679 E-10 | 0.0000 |
| B2O3(s) = | 2.807707 E-12 | 7.931064 E-11 | 0.0000 |
| BHO2(s) = | 1.362133 E-12 | 3.847682 E-11 | 0.0000 |
| B2O3 = | 8.563672 E-13 | 2.419021 E-11 | 0.0000 |
| BN = | 7.806624 E-13 | 2.205174 E-11 | 0.0000 |
| BH2 = | 7.378504 E-13 | 2.084241 E-11 | 0.0000 |
| CH4 = | 6.632066 E-13 | 1.873391 E-11 | 0.0000 |
| CH3OH = | 5.749311 E-13 | 1.624035 E-11 | 0.0000 |
| ICN = | 4.412018 E-13 | 1.246284 E-11 | 0.0000 |
| HCN = | 4.370157 E-13 | 1.234459 E-11 | 0.0000 |
| CNO = | 3.652780 E-13 | 1.031818 E-11 | 0.0000 |
| BN(s) = | 3.573028 E-13 | 1.009290 E-11 | 0.0000 |
| CHNO = | 2.348781 E-13 | 6.634714 E-12 | 0.0000 |
| N = | 2.184649 E-13 | 6.171081 E-12 | 0.0000 |
| NH2 = | 2.158243 E-13 | 6.096492 E-12 | 0.0000 |
| BO = | 2.036389 E-13 | 5.752284 E-12 | 0.0000 |
| FeO = | 1.969877 E-13 | 5.564404 E-12 | 0.0000 |
| NH3 = | 1.258305 E-13 | 3.554394 E-12 | 0.0000 |
| H = | 8.846954 E-15 | 2.499041 E-13 | 0.0000 |

Notes:
- DataBase: C:\Users\student\Dropbox\EXPLO5\Database\2018-06 ionic liquids db_5.xls
- Activity: Model 1: Condensed products form pure phase (Default).