Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Information

Article: Thermodynamics and reaction mechanism of urea decomposition

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A The extended Arrhenius expression

Like many simulation software packages, e. g. CHEMKIN or CANTERA, we also use an extended Arrhenius expression for the description of the rate of a reaction (see Eq. 5 in the manuscript)

$$r_k = A_k T^{\beta_k} \exp\left(-\frac{E_{\mathrm{a},k}}{RT}\right) \prod_{S_i \in R_k} c_i^{\tilde{\nu}_{ik}} \quad . \tag{A.1}$$

This formulation differs from the normal Arrhenius expression through the additional term T^{β_k}. Often it is just stated that this is an additional fit factor to account for temperature dependencies of the pre-exponential factor. However, we want to give a physical justification why this term is necessary for elementary-step kinetics.

Suppose we have a reversible elementary-step reaction. Then we can write the rates of the forward and of the reverse reactions as

$$r_\mathrm{f} = k_\mathrm{f} \prod_{S_i \in R} c_i^{\nu_i'} \tag{A.2}$$

and

$$r_\mathrm{r} = k_\mathrm{r} \prod_{S_i \in R} c_i^{\nu_i''} \tag{A.3}$$

respectively, with some (temperature-dependent) rate coefficients k_f and k_r as well as stoichiometric coefficients ν_i' for reactants and ν_i'' for products. Both rates are equal in case of equilibrium, thus

$$\frac{k_\mathrm{f}}{k_\mathrm{r}} = \frac{\prod_{S_i \in R} c_i^{\nu_i''}}{\prod_{S_i \in R} c_i^{\nu_i'}} = \prod_{S_i \in R} c_i^{\nu_i} \tag{A.4}$$

with $\nu_i = \nu_i'' - \nu_i'$.

If we further assume ideal mixtures, we can convert concentrations into activity factors a_i by

$$c_i = \begin{cases} a_i \frac{p^\ominus}{RT} & \text{for gas-phase species } S_i \in P_\mathrm{gas}, \\ a_i c_i^\ominus & \text{for condensed species } S_i \in P_\mathrm{cond}. \end{cases} \tag{A.5}$$

With

$$\Delta\nu_\mathrm{gas} = \sum_{S_i \in P_\mathrm{gas}} \nu_i \tag{A.6}$$

and

$$C_\mathrm{cond} = \prod_{S_i \in P_\mathrm{cond}} c_i^{\ominus\,\nu_i} \tag{A.7}$$

we get

$$\frac{k_\mathrm{f}}{k_\mathrm{r}} = \prod_{S_i \in R} a_i^{\nu_i} \cdot \left(\frac{p^\ominus}{RT}\right)^{\Delta\nu_\mathrm{gas}} \cdot C_\mathrm{cond} = K_p \cdot \left(\frac{p^\ominus}{RT}\right)^{\Delta\nu_\mathrm{gas}} \cdot C_\mathrm{cond} \quad . \tag{A.8}$$

Here,

$$K_p(T) = \exp\left(-\frac{\Delta_\mathrm{R} G(T)}{RT}\right) \tag{A.9}$$

is the equilibrium constant of the reaction, which relates to the change of Gibbs free energy. Since $G = H - TS$, we can state for the temperature dependency of the rate coefficients:

$$\frac{k_\mathrm{f}(T)}{k_\mathrm{r}(T)} = C_\mathrm{cond} \cdot \left(\frac{p^\ominus}{RT}\right)^{\Delta\nu_\mathrm{gas}} \cdot \exp\left(-\frac{\Delta_\mathrm{R} H(T)}{RT}\right) \cdot \exp\left(\frac{\Delta_\mathrm{R} S(T)}{R}\right) \quad . \tag{A.10}$$

Due to symmetry, it makes sense to assume the same mathematical structure for the temperature dependency of the rate coefficients as for the right-hand side of Eq. A.10, which is the extended Arrhenius expression.

$$k_{\mathrm{f/r}}(T) = A_\mathrm{f/r} \cdot T^{\beta_\mathrm{f/r}} \cdot \exp\left(-\frac{E_\mathrm{a,f/r}}{RT}\right) \tag{A.11}$$

A temperature exponent will appear as soon as the molarity of gas-phase species changes by the reaction. Therefore, this term shall not be neglected in multi-phase reactions.

Moreover, even in reactions that proceed in homogeneous phase there is a contribution to the temperature exponent due to heat capacity. Enthalpy and entropy are themselves functions of temperature. The first coefficient of the Taylor series of the temperature dependency of enthalpy, i. e. the derivative of enthalpy with respect to temperature, is the heat capacity C_p. If we neglect higher-order terms, we get

$$\Delta_\mathrm{R} H(T) = \Delta_\mathrm{R} H^\ominus + \Delta_\mathrm{R} C_p \cdot (T - T^\ominus) \tag{A.12}$$

and

$$\Delta_\mathrm{R} S(T) = \Delta_\mathrm{R} S^\ominus + \Delta_\mathrm{R} C_p \cdot \ln\left(\frac{T}{T^\ominus}\right) \quad . \tag{A.13}$$

Inserting these into Eq. A.10 gives

$$\begin{aligned} \frac{k_\mathrm{f}(T)}{k_\mathrm{r}(T)} = \quad & C_\mathrm{cond} \cdot \left(\frac{p^\ominus}{RT}\right)^{\Delta\nu_\mathrm{gas}} \cdot \exp\left(-\frac{\Delta_\mathrm{R} H^\ominus - \Delta_\mathrm{R} C_p T^\ominus}{RT}\right) \\ & \cdot \exp\left(-\frac{\Delta_\mathrm{R} C_p}{R}\right) \cdot \exp\left(\frac{\Delta_\mathrm{R} S^\ominus}{R}\right) \cdot \left(\frac{T}{T^\ominus}\right)^{\frac{\Delta_\mathrm{R} C_p}{R}} \quad . \end{aligned} \tag{A.14}$$

By comparison of coefficients with Eq. A.11 we get

$$\beta_\mathrm{f} - \beta_\mathrm{r} = -\Delta\nu_\mathrm{gas} + \frac{\Delta_\mathrm{R} C_p}{R} \quad . \tag{A.15}$$

This term can become large in case of phase changes, e. g. in case of water condensation $\Delta_\mathrm{R} C_p \approx 5R$. However, often this term is neglected for homogeneous reactions, as we also did for the liquid phase reactions in this manuscript. Another advantage of this extended Arrhenius expression is that the parameters of adsorption models from kinetic gas theory (Eq. 11 in the manuscript) can be treated with the same formalism when

$$A_k = \alpha_\mathrm{c} \sqrt{\frac{R}{2\pi M_i}} \quad , \tag{A.16}$$

$$\beta_k = \frac{1}{2} \quad \text{, and} \tag{A.17}$$

$$E_{\mathrm{a},k} = 0 \quad . \tag{A.18}$$

B Thermodynamic data

This section lists the coefficients of the NASA polynomials of all species in DETCHEM format. There are two groups of 7 coefficients, first for high temperature ($T > 1000$ K), then for low temperature.

```
H2NCN(s)                C   1N   2H   2     G   300.000  2000.000   800.000    1
 3.80231648E+00 3.14630087E-03-1.06315727E-06 1.66185438E-10-9.79891962E-15    2
 1.42849502E+04 1.57501632E+00 2.25901199E+00 1.00510475E-02-1.33514567E-05    3
 1.00920479E-08-3.00880408E-12 1.45903166E+04 8.91631960E+00                   4
H2O                     H   2O   10   0     G   200.000  6000.000  1000.000    1
 2.67703890E+00 2.97318160E-03-7.73768890E-07 9.44335140E-11-4.26899910E-15    2
-2.98858940E+04 6.88255000E+00 4.19863520E+00-2.03640170E-03 6.52034160E-06    3
-5.48792690E-09 1.77196800E-12-3.02937260E+04-8.49009010E-01                   4
H2O(l)                  H   2O   100  000  0L   273.150   600.0                1
 7.25575005E+01-6.62445402E-01 2.56198746E-03-4.36591923E-06 2.78178981E-09    2
-4.18865499E+04-2.88280137E+02 7.25575005E+01-6.62445402E-01 2.56198746E-03    3
-4.36591923E-06 2.78178981E-09-4.18865499E+04-2.88280137E+02                   4
HCN(g)                  C   1N   1H   1     G   300.000  2000.000   800.000    1
 3.80231648E+00 3.14630087E-03-1.06315727E-06 1.66185438E-10-9.79891962E-15    2
 1.42849502E+04 1.57501632E+00 2.25901199E+00 1.00510475E-02-1.33514567E-05    3
 1.00920479E-08-3.00880408E-12 1.45903166E+04 8.91631960E+00                   4
HNCO                    C   1N   1H   1O   1G   200.000  6000.000  1000.000    1
 5.30045051E+00 4.02250821E-03-1.40962280E-06 2.23855342E-10-1.32499966E-14    2
-1.61995274E+04-3.11770684E+00 2.24009031E+00 1.45600497E-02-1.54352330E-05    3
 8.55535028E-09-1.79631611E-12-1.54589951E+04 1.21663775E+01                   4
HNCO(aq)                C   1N   1H   1O   1L   313.000   500.000              1
 5.42104492E+00 3.87779945E-03-1.35533061E-06 2.15908655E-10-1.28546607E-14    2
-2.03499148E+04-1.83045774E+01 5.42104492E+00 3.87779945E-03-1.35533061E-06    3
 2.15908655E-10-1.28546607E-14-2.03499148E+04-1.83045774E+01                   4
HNCO(l)                 C   1N   1H   1O   1L   300.000  1500.000              1
 1.17416801E+01-2.21709747E-02 3.86833525E-05-2.61489306E-08 6.24089818E-12    2
-2.06264086E+04-4.51279792E+01 1.17416801E+01-2.21709747E-02 3.86833525E-05    3
-2.61489306E-08 6.24089818E-12-2.06264086E+04-4.51279792E+01                   4
N2                J 3/77N   20   00   00   0G   200.000  6000.000  1000.000    1
 2.95257637E+00 1.39690040E-03-4.92631603E-07 7.86010195E-11-4.60755204E-15    2
-9.23948688E+02 5.87188762E+00 3.53100528E+00-1.23660988E-04-5.02999433E-07    3
 2.43530612E-09-1.40881235E-12-1.04697628E+03 2.96747038E+00                   4
NH(x)                   N   1H   1          G   300.000  2000.000  1100.000    1
 2.11000000E+00 2.63000000E-03-1.28000000E-06 3.09400000E-10-2.83200000E-01    2
 4.42468612E+04 1.74100441E+00 3.53000000E+00-2.38000000E-04 4.58500000E-07    3
 3.04800000E-17-1.25100000E-20 4.42468612E+04 1.74100441E+00                   4
NH3                     H   3N   10   0     G   300.000  1500.000              1
 2.09566674E+00 6.14750045E-03-2.00328925E-06 3.01334626E-10-1.71227204E-14    2
-6.30945436E+03 9.59574081E+00 4.46075151E+00-5.68781763E-03 2.11411484E-05    3
-2.02849980E-08 6.89500555E-12-6.70753514E+03-1.34450793E+00                   4
NH3(aq)                 H   3N   10   0     L   273.000   373.000              1
 5.34407604E+00 5.53852966E-03-1.97421300E-06 3.00835751E-10-1.71199316E-14    2
-9.55184403E+03-1.78383952E+01 5.34407604E+00 5.53852966E-03-1.97421300E-06    3
 3.00835751E-10-1.71199316E-14-9.55184403E+03-1.78383952E+01                   4
NH3(l)                  H   3N   10   0     L   200.000   400.000              1
 9.47974387E+00-2.17989318E-02 3.80821042E-05-2.48154987E-08 5.73360060E-12    2
-1.03928295E+04-3.74317361E+01 9.47974387E+00-2.17989318E-02 3.80821042E-05    3
-2.48154987E-08 5.73360060E-12-1.03928295E+04-3.74317361E+01                   4
ammd(s)                 C   3N   4H   4O   2S   300.000  1500.000   500.000    1
 2.51995250E-01 7.21681024E-02-6.83783230E-05 3.71582288E-08-8.78187782E-12    2
-6.20277191E+04-2.28345276E+00 2.51995250E-01 7.21681024E-02-6.83783230E-05    3
 3.71582288E-08-8.78187782E-12-6.20277191E+04-2.28345276E+00                   4
```

```
ammn(s)                 C   3N   5H   5O   1S   300.000  1500.000   500.000    1
 2.51995144E-01 7.21681029E-02-6.83783240E-05 3.71582296E-08-8.78187803E-12    2
-3.88271739E+04-2.28345229E+00 2.51995144E-01 7.21681029E-02-6.83783240E-05    3
 3.71582296E-08-8.78187803E-12-3.88271739E+04-2.28345229E+00                   4
biu(g)                  C   2N   3H   5O   2G   100.000  1500.000   500.000    1
-3.37348672E-01 7.03835430E-02-8.94699561E-05 6.77723865E-08-2.20019943E-11    2
-5.49538013E+04 2.69795128E+01-3.37348672E-01 7.03835430E-02-8.94699561E-05    3
 6.77723865E-08-2.20019943E-11-5.49538013E+04 2.69795128E+01                   4
biu(l)                  C   2N   3H   5O   2L   100.000  1500.000   500.000    1
 1.11855734E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-6.79267938E+04-3.92774872E+01 1.11855734E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-6.79267938E+04-3.92774872E+01                   4
biu(s)                  C   2N   3H   5O   2S   100.000  1500.000   500.000    1
 1.57917656E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-7.25034957E+04-7.23953678E+01 1.57917656E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-7.25034957E+04-7.23953678E+01                   4
cya(g)                  C   3N   3H   3O   3G   300.000  1000.000  1000.000    1
 1.89308355E+00 5.05144383E-02-2.40545731E-05 1.17998036E-13-5.38094067E-17    2
-7.04405495E+04 1.60465366E+01 1.89308355E+00 5.05144383E-02-2.40545731E-05    3
 1.17998036E-13-5.38094067E-17-7.04405495E+04 1.60465366E+01                   4
cya(s)                  C   3N   3H   3O   3S   300.000  1000.000  1000.000    1
 1.71915339E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-8.96983399E+04-9.27710260E+01 1.71915339E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-8.96983399E+04-9.27710260E+01                   4
melem(s)                C   6N  10H   6     S   300.000  1500.000   500.000    1
 1.30100000E+00 6.40000000E-02-5.17700000E-05 2.27700000E-08-4.54200000E-12    2
-1.85013486E+04-7.90422994E+00 1.30100000E+00 6.40000000E-02-5.17700000E-05    3
 2.27700000E-08-4.54200000E-12-1.85013486E+04-7.90422994E+00                   4
triu(s)                 C   3N   4H   6O   3S   100.000  1500.000   500.000    1
 1.57917656E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-8.99722705E+04-4.67850220E+01 1.57917656E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-8.99722705E+04-4.67850220E+01                   4
urea(aq)                C   1N   2H   4O   1L   300.000  500.00                  1
 5.20808968E+00 8.75549199E-03-3.77147176E-06 6.08811502E-10-3.25671974E-14    2
-4.10431486E+04-1.74687703E+01 5.20808968E+00 8.75549199E-03-3.77147176E-06    3
 6.08811502E-10-3.25671974E-14-4.10431486E+04-1.74687703E+01                   4
urea(g)                 C   1N   2H   4O   1G   200.000  6000.000  1000.000    1
 1.03465230E+01 8.95410779E-03-3.10367689E-06 4.89573387E-10-2.88531892E-14    2
-3.20127628E+04-2.69745331E+01-2.10707501E-01 4.36948607E-02-4.60607638E-05    3
 2.36547939E-08-4.42050926E-12-2.94198537E+04 2.60661959E+01                   4
urea(l)                 C   1N   2H   4O   1L     0.000  1000.000   500.000    1
 1.11861920E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-4.17120034E+04-4.67960457E+01 1.11861920E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-4.17120034E+04-4.67960457E+01                   4
urea(s)                 C   1N   2H   4O   1S     0.000  1000.000   500.000    1
 1.11861920E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-4.34584551E+04-5.10992409E+01 1.11861920E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-4.34584551E+04-5.10992409E+01                   4
```

C Reaction mechanism

The listing shows the mechanism input for DETCHEM[MPTR].

```
<SPECIES>
  <GASPHASE>
     H2O NH3 CO2 HNCO urea(g) cya(g) HCN(g) N2
  </GASPHASE>
  <PHASE liquid>
     DCSLMAX=20
     urea(l)  1320  # name, density in kg/m^3
     HNCO(l)  1140
   NH3(l)    700
   biu(l)   1470
   triu(l)  1547
  </PHASE>
  <PHASE aq>
     H2O(l)    998
   urea(aq) 1100
   NH3(aq)   700
   HNCO(aq) 1140
  </PHASE>
  <PHASE solid>
     ammn(s)  2220
     ammd(s)  1573
   melem(s) 1717
   H2NCN(s) 1140
   NH(x)    1140
  </PHASE>
  <PHASE urea_s>
     urea(s)  1320
  </PHASE>
  <PHASE biu_s>
   biu(s)   1470
  </PHASE>
  <PHASE triu_s>
   triu(s)  1547
  </PHASE>
  <PHASE cya_s>
     cya(s)   2500
  </PHASE>
</SPECIES>

<MECHANISM>
  <HOMOGENEOUS>
    <GLOBAL>
         3 ammd(s) > 2 ammn(s) + H2NCN(s) + 2 CO2
         <ARRHENIUS>
         ammd(s)  1
             A/cm_units = 1e10
             Ea/kJ_mol  = 165.67
     </ARRHENIUS>
     </GLOBAL>

     <GLOBAL>
         ammn(s) > HNCO + 2 H2NCN(s)
         <ARRHENIUS>
```

```
        A/cm_units = 5.0e9
        Ea/kJ_mol  = 165.67
 </ARRHENIUS>
 </GLOBAL>

 <GLOBAL>
     ammn(s) + 3 H2NCN(s) > melem(s) + H2O(l) + NH3
     <ARRHENIUS>
         A/cm_units = 8.0e13
         Ea/kJ_mol  = 140.67
   </ARRHENIUS>
 </GLOBAL>

 <GLOBAL>
     melem(s)  > 6 HCN(g) + 2 N2
     <ARRHENIUS>
         A/cm_units = 6.0e6
         Ea/kJ_mol  = 165.67
   </ARRHENIUS>
 </GLOBAL>

 <GLOBAL>
     H2NCN(s) > NH(x) + HCN(g)
     <ARRHENIUS>
         A/cm_units = 2.0e5
         Ea/kJ_mol  = 105.67
   </ARRHENIUS>
 </GLOBAL>

 <GLOBAL>
     3 NH(x) > NH3 + N2
     <ARRHENIUS>
         A/cm_units = 1.0e5
         Ea/kJ_mol  = 50.67
   </ARRHENIUS>
 </GLOBAL>

<REACTION>
   urea(l) + HNCO(l) = biu(s)
   A/SIunits = 1e-4
   Ea/kJ_mol = 0
</REACTION>

<REACTION>
   urea(l) + HNCO(l) = biu(l)
   A/SIunits = 1e-4
   Ea/kJ_mol = 0
</REACTION>

<REACTION>
    biu(l) + HNCO(l) = triu(s)
    A/SIunits = 1e-4
    Ea/kJ_mol = 0
</REACTION>

<REACTION>
```

```
        triu(s) > cya(s) + NH3
        A/SIunits  = 1.2e2
        Ea/kJ_mol  = 45
    </REACTION>

    <REACTION>
        triu(s) > ammd(s) + H2O
        A/SIunits  = 0.3e2
        Ea/kJ_mol  = 45
    </REACTION>
</HOMOGENEOUS>

  <INTERPHASE>
     <REACTION>
        cya(s) > cya(g)
      A/SIunits =  3e4
        Ea/kJ_mol  = 141.3
     </REACTION>

 <REACTION> # (neu ST)
        urea(l) + urea(l) > biu(l) + NH3
      A/SIunits =  3.5e0
        Ea/kJ_mol  = 99
     </REACTION>

     <REACTION> # neu ST
      biu(l) + urea(l) > triu(s) + NH3
    A/SIunits =  2e2
    Ea/kJ_mol  = 116.5
   </REACTION>

     <REACTION>
        H2O = H2O(l)
        A/SIunits = 0.086
        beta=0.5
     </REACTION>

   <REACTION>
      NH3 = NH3(l)
      A/SIunits = 0.088
      beta=0.5
   </REACTION>

   <REACTION>
        NH3 = NH3(aq)
        A/SIunits = 0.088
        beta=0.5
     </REACTION>

   <REACTION>
      NH3(aq) = NH3(l)
      A/SIunits = 0.088
      beta=0.5
   </REACTION>

   <REACTION>
```

```
        urea(g) = urea(l)
        A/SIunits = 0.047
        beta=0.5
      </REACTION>

    <REACTION>
        urea(aq) = urea(s)
        A/SIunits = 0.047
      beta=0.5
      </REACTION>

    <REACTION>
        urea(aq) = urea(l)
        A/SIunits = 0.047
      beta=0.5
      </REACTION>

    <REACTION>
      HNCO = HNCO(l)
      A/SIunits = 0.055
      beta=0.5
    </REACTION>

    <REACTION>
      HNCO = HNCO(aq)
      A/SIunits = 0.055
      beta=0.5
    </REACTION>

    <REACTION>
      HNCO(aq) = HNCO(l)
      A/SIunits = 0.055
      beta=0.5
    </REACTION>

    <REACTION>
        urea(l) = urea(s)
        A/SIunits = 1e-6
      </REACTION>

    <REACTION>
        biu(l) = biu(s)
        A/SIunits = 1e-6
      </REACTION>
  </INTERPHASE>
</MECHANISM>
```

D Simulation results for TG experiments

The figures in this supplemental information show a comparison of all TG experiments as listed in Table 1 with their respective numerical simulation. The experimental data are shown by symbols. Lines represent simulation results. In addition to the total mass of substance in the crucible, the numerically predicted composition is shown.

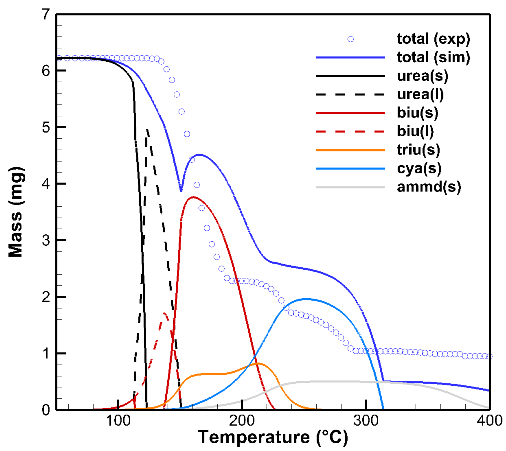

Fig. 1 TG of urea, plate crucible, initial weight 6.23 mg, ramp 2 K/min

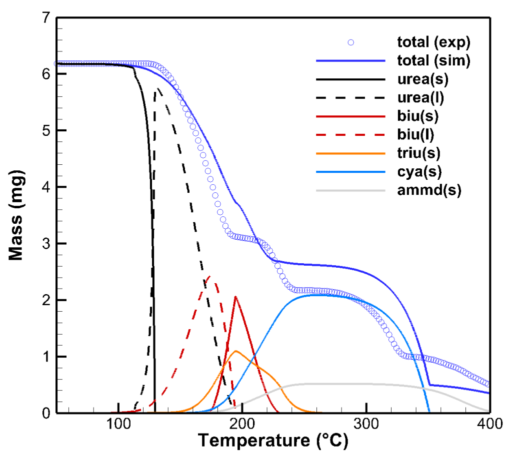

Fig. 2 TG of urea, cylinder crucible, initial weight 6.18 mg, ramp 2 K/min

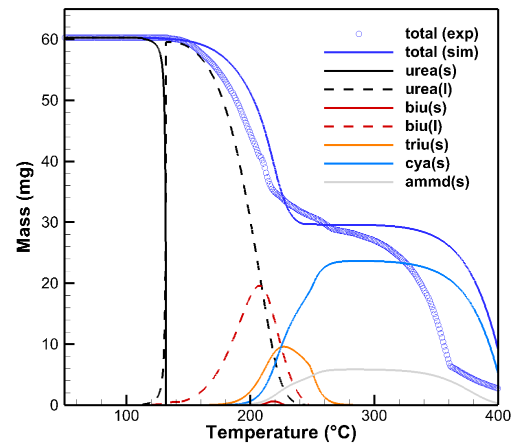

Fig. 3 TG of urea, cylinder crucible, initial weight 60.3 mg, ramp 2 K/min

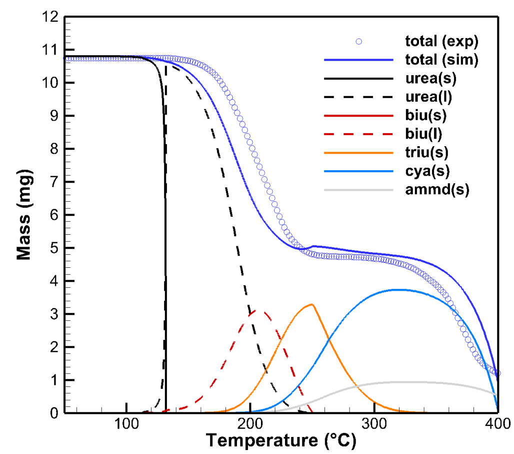

Fig. 4 TG of urea, cylinder crucible, initial weight 10.8 mg, ramp 10 K/min

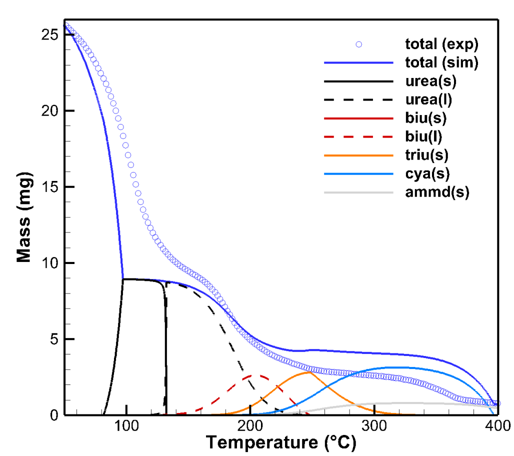

Fig. 5 TG of 32.5 wt-% urea-water solution, cylinder crucible, initial weight 27.5 mg, ramp 10 K/min

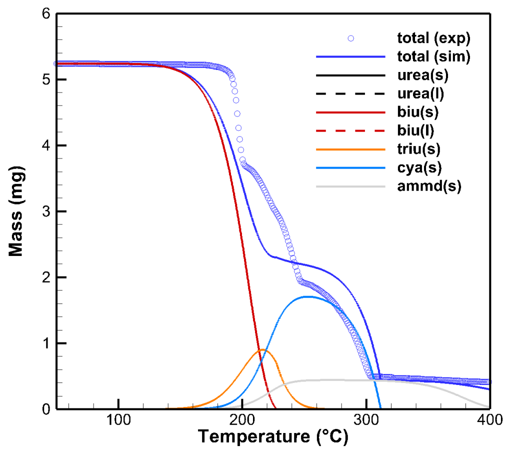

Fig. 6 TG of biuret, plate crucible, initial weight 5.24 mg, ramp 2 K/min

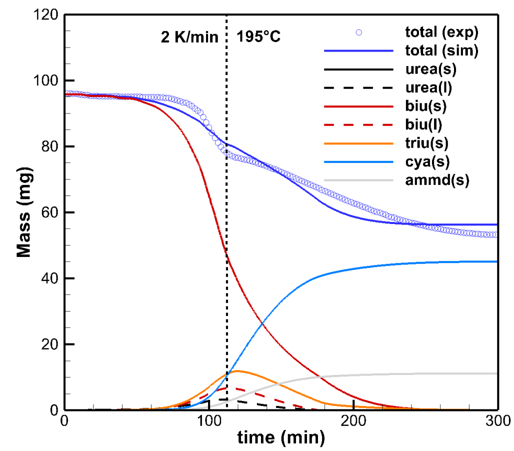

Fig. 9 TG of biuret, cylinder crucible, initial weight 95.8 mg, ramp 2 K/min stopped at 195 °C

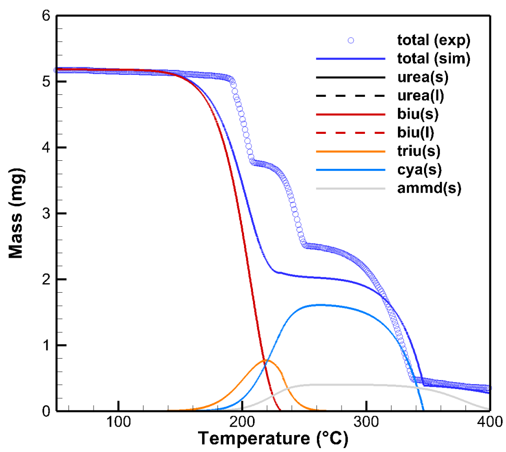

Fig. 7 TG of biuret, cylinder crucible, initial weight 5.18 mg, ramp 2 K/min

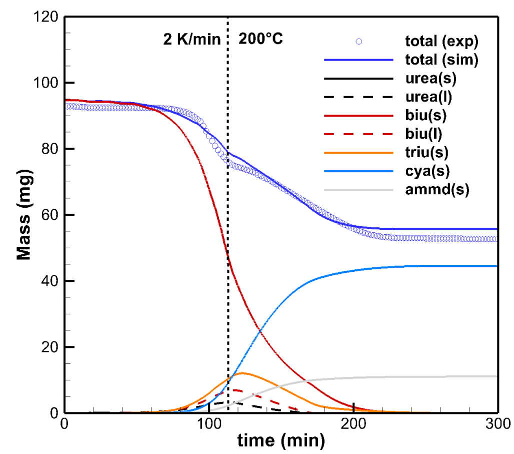

Fig. 10 TG of biuret, cylinder crucible, initial weight 94.6 mg, ramp 2 K/min stopped at 200 °C

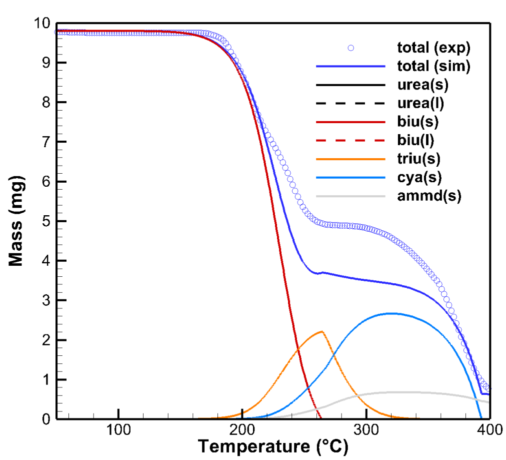

Fig. 8 TG of biuret, cylinder crucible, initial weight 9.8 mg, ramp 10 K/min

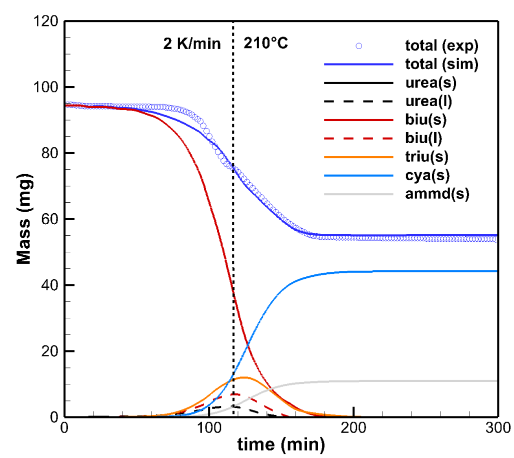

Fig. 11 TG of biuret, cylinder crucible, initial weight 94.4 mg, ramp 2 K/min stopped at 210 °C

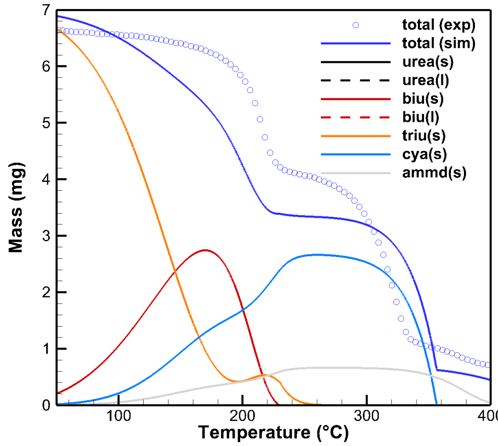

Fig. 12 TG of triuret, cylinder crucible, initial weight 6.98 mg, ramp 2 K/min

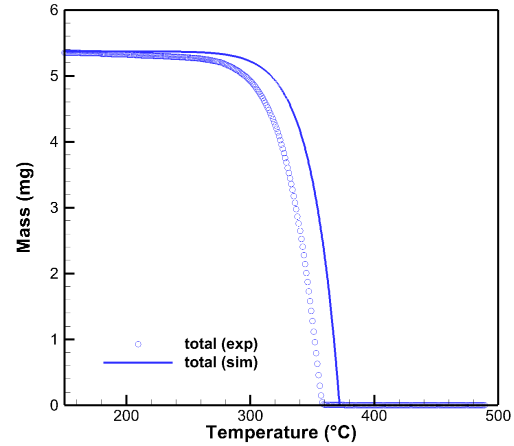

Fig. 15 TG of cyanuric acid, cylinder crucible, initial weight 5.37 mg, ramp 2 K/min

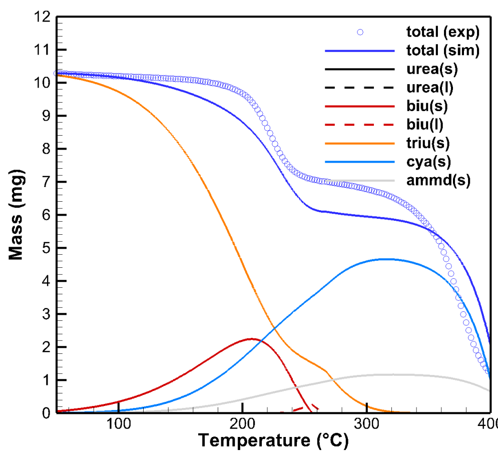

Fig. 13 TG of triuret, cylinder crucible, initial weight 10.31 mg, ramp 10 K/min

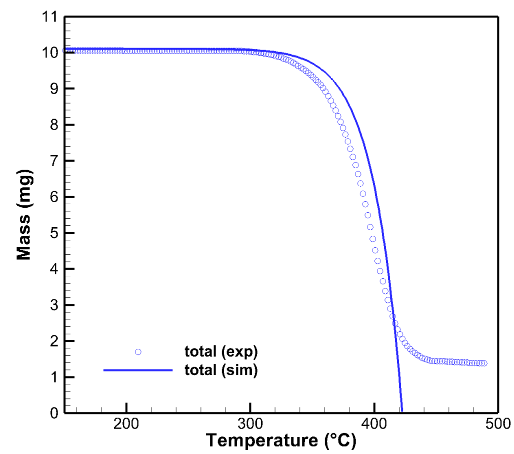

Fig. 16 TG of cyanuric acid, cylinder crucible, initial weight 10.1 mg, ramp 10 K/min

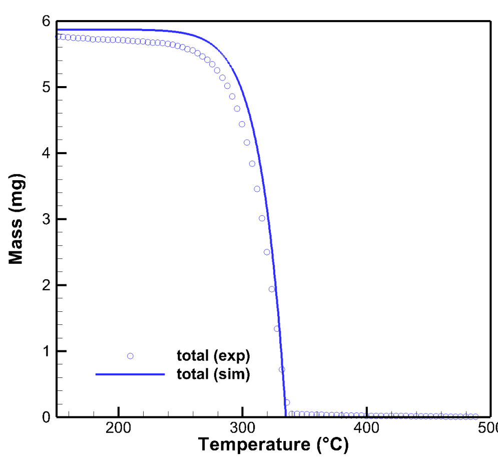

Fig. 14 TG of cyanuric acid, plate crucible, initial weight 5.87 mg, ramp 2 K/min

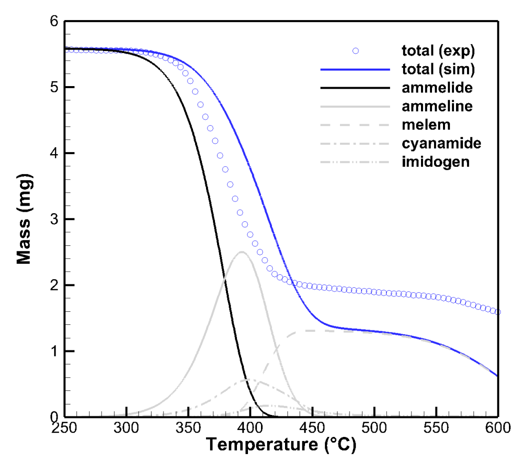

Fig. 17 TG of ammelide, plate crucible, initial weight 5.58 mg, ramp 2 K/min

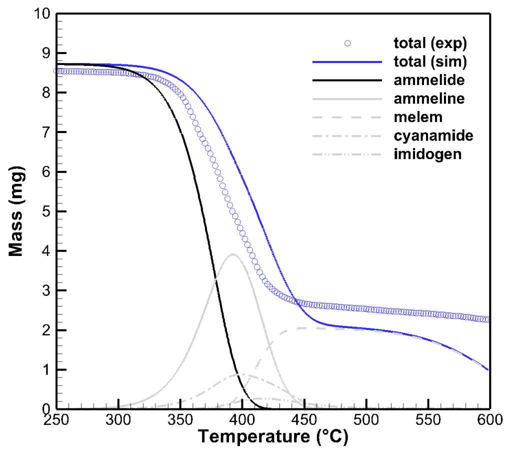

Fig. 18 TG of ammelide, cylinder crucible, initial weight 8.72 mg, ramp 2 K/min

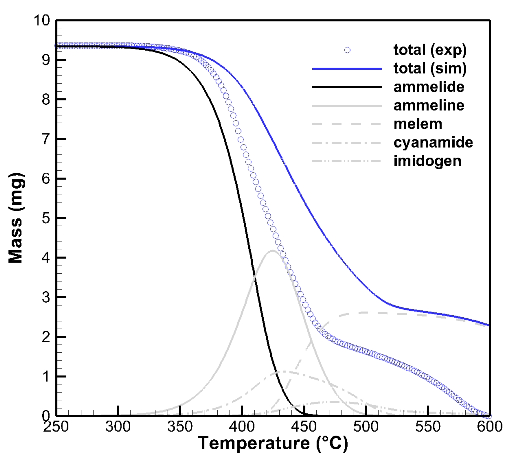

Fig. 19 TG of ammelide, cylinder crucible, initial weight 9.34 mg, ramp 10 K/min