Supplementary information: List of chemical reactions included in the model

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ABSTRACT: This supplementary data lists all the reactions included in the model. The same reaction data is also provided in CHEMKIN format.

REACTION RATE FORMAT

The rates of two-body reactions generally take the form of a sum of Arrhenius expressions

$$k_{II} = \sum_{i=1}^{N} A_i T^{b_i} e^{-E_i/(RT)}$$

where N is the number of elements in the sum and A_i, b_i and E_i are the Arrhenius parameters (pre-exponential factor, temperature exponent and activation energy, respectively. However, for most reactions, $N = 1$ and only one set of Arrhenius parameters is needed.

The rates of three-body reactions are given as

$$k_{III} = P_r A T^b e^{-E/(RT)}$$

where A , b and E are, again, the Arrhenius parameters and P_r is a gas-specific pre-exponential factor. The default value of P_r is 1.0, unless specified otherwise

LIST OF REACTIONS

All reactions included in the model, together with their rates, are listed in the table below:

Reaction	A	b	E
2O + M ↔ O2 + M	$1.2 \cdot 10^{17}$	-1.0	0.0
	Third body efficiencies: $P_{H2} = 2.4$, $P_{H2O} = 15.4$, $P_{Ar} = 0.83$		
O + H + M ↔ OH + M	$5.0 \cdot 10^{17}$	-1	0.0
	Third body efficiencies: $P_{H2} = 2.0$, $P_{H2O} = 6.0$, $P_{Ar} = 0.7$		
O + H_2 ↔ H + OH	$3.870 \cdot 10^{4}$	2.7	6260
O + HO_2 ↔ OH + O_2	$2.0 \cdot 10^{13}$	0.0	0.0
O + H_2O_2 ↔ OH + HO_2	$9.63 \cdot 10^{6}$	2.0	4000
H + O_2 + M ↔ HO_2 + M	$2.8 \cdot 10^{18}$	-0.86	0.0
	Third body efficiencies: $P_{O2} = 0.0$, $P_{H2O} = 0.0$, $P_{Ar} = 0.0$		
H + $2O_2$ ↔ HO_2 + O_2	$2.08 \cdot 10^{19}$	-1.24	0.0
H + O_2 + H2O ↔ HO_2 + H_2O	$11.26 \cdot 10^{18}$	-0.76	0.0
H + O_2 + N2 ↔ HO_2 + N_2	$2.6 \cdot 10^{19}$	-1.24	0.0
H + O_2 + AR ↔ HO_2 + Ar	$7.0 \cdot 10^{17}$	-0.8	0.0
H + O_2 ↔ O + OH	$2.65 \cdot 10^{16}$	-0.6707	17041

$2H + M \leftrightarrow H_2 + M$	$1.0 \cdot 10^{18}$	-1.0	0.0
	Third body efficiencies: $P_{H2} = 0.0$, $P_{H2O} = 0.0$, $P_{Ar} = 0.0$		
$2H + H_2 \leftrightarrow 2H_2$	$9.0 \cdot 10^{16}$	-0.6	0.0
$2H + H_2O \leftrightarrow H_2 + H_2O$	$6.0 \cdot 10^{19}$	-1.25	0.0
$H + OH + M \leftrightarrow H_2O + M$	$2.2 \cdot 10^{22}$	-2.0	0.0
	Third body efficiencies: $P_{H2} = 0.73$, $P_{H2O} = 3.65$, $P_{Ar} = 0.38$		
$H + HO_2 \leftrightarrow O + H_2O$	$3.97 \cdot 10^{12}$	0.0	671
$H + HO_2 \leftrightarrow O_2 + H_2$	$4.48 \cdot 10^{13}$	0.0	1068
$H + HO_2 \leftrightarrow 2OH$	$8.4 \cdot 10^{13}$	0.0	635
$H + H_2O_2 \leftrightarrow HO_2 + H_2$	$1.21 \cdot 10^{7}$	2.0	5200
$H + H_2O_2 \leftrightarrow OH + H_2O$	$1.0 \cdot 10^{13}$	0.0	3600
$OH + H_2 \leftrightarrow H + H_2O$	$2.16 \cdot 10^{8}$	1.51	3430
$2OH + M \leftrightarrow H_2O + M$	$7.4 \cdot 10^{3}$	-0.37	0.0
	Third body efficiencies: $P_{H2} = 2.0$, $P_{H2O} = 6.0$, $P_{Ar} = 0.7$		
$OH + H_2O_2 \leftrightarrow HO2 + H_2O$	$2.0 \cdot 10^{12}$	0.0	427
	$1.7 \cdot 10^{18}$	0.0	29410
$2HO_2 \leftrightarrow O_2 + H2O_2$	$1.3 \cdot 10^{11}$	0.0	-1630
	$4.2 \cdot 10^{14}$	0.0	12000