The Basic Sulphur Chemical Mechanism of MECCA

KPP version: `2.2.1_rs5`

MECCA version: `2.5n`

Date: June 16, 2011.

Selected reactions:
“`Tr && G && !C && !Cl && !Br && !I && !Hg`”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	31
Aqueous phase:	0
All species:	31

Number of reactions in selected mechanism:

Gas phase (Gnnn):	44
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	13
Heterogeneous (HETnnn):	0
Equilibria (EQnn):	0
Isotope exchange (IEXnnn):	0
Dummy (Dnn):	0
All equations:	57

Further information can be found in the article “Technical Note: The new comprehensive atmospheric chemistry module MECCA” by R. Sander et al. (Atmos. Chem. Phys. **5**, 445-450, 2005), available at `http://www.atmos-chem-phys.net/5/445`.

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.3E-11*EXP(55./temp)`	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.E-34*((temp/300.)**(-2.4))*cair`	Sander et al. (2006)
G1002a	StTrG	$O_3 + O(^1D) \rightarrow 2\ O_2$	`1.2E-10`	Sander et al. (2006)*
G1003a	StTrG	$O_3 + O(^3P) \rightarrow 2\ O_2$	`8.E-12*EXP(-2060./temp)`	Sander et al. (2006)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,4.4E-32,1.3,4.7E-11, 0.2,0.6)`	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + O_2$	`1.7E-12*EXP(-940./temp)`	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	`2.8E-12*EXP(-1800./temp)`	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$	`1.E-14*EXP(-490./temp)`	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	`4.8E-11*EXP(250./temp)`	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	`k_HO2_HO2`	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	`1.63E-10*EXP(60./temp)`	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`1.8E-12`	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`2.15E-11*EXP(110./temp)`	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	`3.E-12*EXP(-1500./temp)`	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`	Sander et al. (2006)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`	Sander et al. (2006)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(2.7E-27*EXP(11000./temp))`	Sander et al. (2006)*
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	`3.5E-12*EXP(250./temp)`	Sander et al. (2006)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	`k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0., 0.6)`	Sander et al. (2006)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	`k_NO2_HO2`	Sander et al. (2006)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	`3.5E-12`	Sander et al. (2006)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	`k_HNO3_OH`	Sander et al. (2006)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`	Sander et al. (2006)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	`1.3E-12*EXP(380./temp)`	Sander et al. (2006)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	`1.85E-20*EXP(2.82*log(temp)-987./temp)`	Atkinson (2003)*
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	`2.9E-12*EXP(-345./temp)`	Sander et al. (2006)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	`4.1E-13*EXP(750./temp)`	Sander et al. (2006)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	`2.8E-12*EXP(300./temp)`	Sander et al. (2006)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	`1.3E-12`	Atkinson et al. (2006)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
`G4106a`	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	`9.5E-14*EXP(390./temp)/(1.+1./26.2*EXP(1130./temp))`	Sander et al. (2006)
`G4106b`	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$	`9.5E-14*EXP(390./temp)/(1.+26.2*EXP(-1130./temp))`	Sander et al. (2006)
`G4107`	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	`k_CH3OOH_OH`	Sander et al. (2006)*
`G4108`	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*log(temp)+636./temp)`	Sivakumaran et al. (2003)
`G4109`	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Sander et al. (2006)*
`G4110`	StTrG	$CO + OH \rightarrow H + CO_2$	`(1.57E-13+cair*3.54E-33)`	McCabe et al. (2001)
`G9200`	StTrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	`k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0.,0.6)`	Sander et al. (2006)
`G9400a`	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	`1.13E-11*EXP(-253./temp)`	Atkinson et al. (2004)*
`G9400b`	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	`k_DMS_OH`	Atkinson et al. (2004)*
`G9401`	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2004)
`G9402`	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`	Hynes and Wine (1996)
`G9403`	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	`1.9E13*EXP(-8661./temp)`	Barone et al. (1995)
`G9404`	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	`3.E-13`	Barone et al. (1995)
`G9405`	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	`5.E-11`	Barone et al. (1995)

*Notes:

Rate coefficients for three-body reactions are defined via the function `k_3rd`(T, M, k_0^{300}, n, $k_{\rm inf}^{300}$, m, $f_{\rm c}$). In the code, the temperature T is called `temp` and the concentration of "air molecules" M is called `cair`. Using the auxiliary variables $k_0(T)$, $k_{\rm inf}(T)$, and $k_{\rm ratio}$, `k_3rd` is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^n \quad (1)$$

$$k_{\rm inf}(T) = k_{\rm inf}^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^m \quad (2)$$

$$k_{\rm ratio} = \frac{k_0(T)M}{k_{\rm inf}(T)} \quad (3)$$

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\rm ratio}} \times f_{\rm c}^{\left(\frac{1}{1+(\log_{10}(k_{\rm ratio}))^2}\right)} \quad (4)$$

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^n \quad (5)$$

$$k_{\rm inf}(T) = k_{\rm inf}^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^m \quad (6)$$

$$k_{\rm ratio} = \frac{k_0(T)M}{k_{\rm inf}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_{\rm c}) \quad (8)$$

$$\texttt{k\_3rd\_iupac} = \frac{k_0(T)M}{1+k_{\rm ratio}} \times f_{\rm c}^{\left(\frac{1}{1+(\log_{10}(k_{\rm ratio})/N)^2}\right)} \quad (9)$$

G1002a: The path leading to 2 O(^{3}P) + O_2 results in a null cycle regarding odd oxygen and is neglected.

G2110: The rate coefficient is: `k_HO2_HO2` = `(1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp) *cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

G3109: The rate coefficient is: `k_NO3_NO2` = `k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6)`.

G3110: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3203: The rate coefficient is: `k_NO2_HO2` = `k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

G3206: The rate coefficient is: `k_HNO3_OH` = `2.4E-14 * EXP(460./temp) + 1./ ( 1./ (6.5E-34 * EXP(1335./temp)*cair) + 1./ (2.7E-17 * EXP(2199./temp)) )`

G3207: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G4103: Sander et al. (2006) recommend a zero product yield for HCHO.

G4107: The rate coefficient is: `k_CH3OOH_OH` = `3.8E-12*EXP(200./temp)`.

G4109: The same temperature dependence assumed as for CH_3CHO+NO_3.

G9400b: Addition path. The rate coefficient is: `k_DMS_OH` = `1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
`J1000`	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	`jx(ip_O2)`	see note
`J1001a`	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	`jx(ip_O1D)`	see note
`J1001b`	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	`jx(ip_O3P)`	see note
`J2101`	StTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	`jx(ip_H2O2)`	see note
`J3101`	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	`jx(ip_NO2)`	see note
`J3103a`	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	`jx(ip_NO2O)`	see note
`J3103b`	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	`jx(ip_NOO2)`	see note
`J3104a`	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	`jx(ip_N2O5)`	see note
`J3201`	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	`jx(ip_HNO3)`	see note
`J3202`	StTrGNJ	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	`jx(ip_HNO4)`	see note
`J4100`	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	`jx(ip_CH3OOH)`	see note
`J4101a`	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	`jx(ip_COH2)`	see note
`J4101b`	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	`jx(ip_CHOH)`	see note

*Notes: J-values are calculated with an external module and then supplied to the MECCA chemistry

Table 3: Henry's law coefficients

substance	$\frac{k_\mathrm{H}^\ominus}{\mathrm{M/atm}}$	$\frac{-\Delta_\mathrm{soln}H/R}{\mathrm{K}}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^{1}	4300.	Hanson et al. (1992)
HO_2	3.9×10^{3}	5900.	Hanson et al. (1992)
H_2O_2	$1.\times10^{5}$	6338.	Lind and Kok (1994)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO_3	2.	2000.	Thomas et al. (1993)
HNO_3	$2.45\times10^{6}/1.5\times10^{1}$	8694.	Brimblecombe and Clegg (1989)*
HNO_4	1.2×10^{4}	6900.	Régimbal and Mozurkewich (1997)
CH_3O_2	6.	5600.	Jacob (1986)*
CH_3OOH	3.0×10^{2}	5322.	Lind and Kok (1994)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1.\times10^{11}$	0.	see note
DMSO	$5.\times10^{4}$	6425.	De Bruyn et al. (1994)*

*Notes:

The temperature dependence of the Henry constants is:

$$K_\mathrm{H} = K_\mathrm{H}^\ominus \times \exp\left(\frac{-\Delta_\mathrm{soln}H}{R}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)$$

where $\Delta_\mathrm{soln}H$ = molar enthalpy of dissolution [J/mol] and $R = 8.314$ J/(mol K).

NO_2: The temperature dependence is from Chameides (1984).

HNO_3: Calculated using the acidity constant from Davis and de Bruin (1964).

CH_3O_2: This value was estimated by Jacob (1986).

H_2SO_4: To account for the very high Henry's law coefficient of H_2SO_4, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{\text{K}}$	reference
O_2	0.01	2000.	see note
O_3	0.002	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO_2	0.5	0.	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
NO	5.0×10^{-5}	0.	Saastad et al. (1993)*
NO_2	0.0015	0.	Ponche et al. (1993)*
NO_3	0.04	0.	Rudich et al. (1996)*
N_2O_5	0.1	0.	DeMore et al. (1997)*
HNO_3	0.5	0.	Abbatt and Waschewsky (1998)*
HNO_4	0.1	0.	DeMore et al. (1997)*
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
CO_2	0.01	2000.	see note
SO_2	0.11	0.	DeMore et al. (1997)
H_2SO_4	0.65	0.	Pöschl et al. (1998)*
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMSO	0.048	2578.	De Bruyn et al. (1994)

*Notes:

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\begin{aligned}\frac{\alpha}{1-\alpha} &= \exp\left(\frac{-\Delta_{\text{obs}}G}{RT}\right)\\ &= \exp\left(\frac{-\Delta_{\text{obs}}H}{RT}+\frac{\Delta_{\text{obs}}S}{R}\right)\end{aligned}$$

where $\Delta_{\text{obs}}G$ is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and $\Delta_{\text{obs}}H$ and $\Delta_{\text{obs}}S$ are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\text{obs}}H}{R}\times\frac{1}{T}+\frac{-\Delta_{\text{obs}}S}{R}$$

and further:

$$\mathrm{d}\ln\left(\frac{\alpha}{1-\alpha}\right)\Big/\mathrm{d}\left(\frac{1}{T}\right) = \frac{-\Delta_{\text{obs}}H}{R}$$

If no data were available, a value of $\alpha = 0.01$, $\alpha = 0.1$, or $\alpha = 0.5$, and a temperature dependence of $-\Delta_{\text{obs}}H/R = 2000$ K has been assumed.

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

NO: Value measured between 193 and 243 K.

NO_2: Value measured at 298 K.

NO_3: Value is a lower limit, measured at 273 K.

N_2O_5: Value for sulfuric acid, measured between 195 and 300 K.

HNO_3: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

HCHO: Value measured between 260 and 270 K.

CO_2: Estimate.

H_2SO_4: Value measured at 303 K.

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