

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 (Gnn): 44

Aqueous phase (Annn): 0

Henry (Hnn): 0

Photolysis (Jnn): 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_H02_H02	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_N03_N02	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_N03_N02/(2.7E-27*EXP(11000./temp))$	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_N02_H02	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_HN03_OH	Sander et al. (2006)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	$k_N02_H02/(2.1E-27*EXP(10900./temp))$	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	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{HCHO} + 2 \text{HO}_2$	$9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1. + 1./26.2 * \text{EXP}(1130./\text{temp}))$	Sander et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1. + 26.2 * \text{EXP}(-1130./\text{temp}))$	Sander et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH	Sander et al. (2006)*
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E-}18 * \text{EXP}(2.03 * \log(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E-}13 * \text{EXP}(-1900./\text{temp})$	Sander et al. (2006)*
G4110	StTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E-}13 + \text{cair} * 3.54\text{E-}33)$	McCabe et al. (2001)
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	k_3rd(temp, cair, 3.3E-31, 4.3, 1.6E-12, 0., 0.6)	Sander et al. (2006)
G9400a	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E-}11 * \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E-}13 * \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3\text{O}_2 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.9\text{E}13 * \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	5.E-11	Barone et al. (1995)

*Notes:

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

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

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

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

$$\text{k_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}}))^2} \right)} \quad (4)$$

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:

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

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

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

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

$$\text{k_3rd_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2} \right)} \quad (9)$$

G1002a: The path leading to $2 \text{ O}(^3\text{P}) + \text{O}_2$ 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 $\text{CH}_3\text{CHO} + \text{NO}_3$.

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	$\text{O}_2 + h\nu \rightarrow \text{O}(^3\text{P}) + \text{O}(^3\text{P})$	jx(ip_02)	see note
J1001a	StTrGJ	$\text{O}_3 + h\nu \rightarrow \text{O}(^1\text{D})$	jx(ip_01D)	see note
J1001b	StTrGJ	$\text{O}_3 + h\nu \rightarrow \text{O}(^3\text{P})$	jx(ip_03P)	see note
J2101	StTrGJ	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2 \text{OH}$	jx(ip_H202)	see note
J3101	StTrGNJ	$\text{NO}_2 + h\nu \rightarrow \text{NO} + \text{O}(^3\text{P})$	jx(ip_N02)	see note
J3103a	StTrGNJ	$\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{O}(^3\text{P})$	jx(ip_N020)	see note
J3103b	StTrGNJ	$\text{NO}_3 + h\nu \rightarrow \text{NO}$	jx(ip_N002)	see note
J3104a	StTrGNJ	$\text{N}_2\text{O}_5 + h\nu \rightarrow \text{NO}_2 + \text{NO}_3$	jx(ip_N205)	see note
J3201	StTrGNJ	$\text{HNO}_3 + h\nu \rightarrow \text{NO}_2 + \text{OH}$	jx(ip_HN03)	see note
J3202	StTrGNJ	$\text{HNO}_4 + h\nu \rightarrow .667 \text{NO}_2 + .667 \text{HO}_2 + .333 \text{NO}_3 + .333 \text{OH}$	jx(ip_HN04)	see note
J4100	StTrGJ	$\text{CH}_3\text{OOH} + h\nu \rightarrow \text{HCHO} + \text{OH} + \text{HO}_2$	jx(ip_CH300H)	see note
J4101a	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H}_2 + \text{CO}$	jx(ip_COH2)	see note
J4101b	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H} + \text{CO} + \text{HO}_2$	jx(ip_CH0H)	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	k_H^\ominus M/atm	$-\Delta_{\text{soln}}H/R$ 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 ₂ O ₂	$1. \times 10^5$	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	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO ₄	1.2×10^4	6900.	Régimbal and Mozurkewich (1997)
CH ₃ O ₂	6.	5600.	Jacob (1986)*
CH ₃ OOH	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 ₂ SO ₄	$1. \times 10^{11}$	0.	see note
DMSO	$5. \times 10^4$	6425.	De Bruyn et al. (1994)*

*Notes:

The temperature dependence of the Henry constants is:

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

where $\Delta_{\text{soln}}H$ = molar enthalpy of dissolution [J/mol]and $R = 8.314 \text{ J}/(\text{mol K})$.NO₂: The temperature dependence is from Chameides (1984).HNO₃: Calculated using the acidity constant from Davis and de Bruin (1964).CH₃O₂: This value was estimated by Jacob (1986).H₂SO₄: To account for the very high Henry’s law coefficient of H₂SO₄, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	α^\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 ₂ O 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 ₂ O 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 ₃ O ₂	0.01	2000.	see note
CH ₃ OOH	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 ₂ SO ₄	0.65	0.	Pöschl et al. (1998)*
CH ₃ SO ₃ H	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:

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

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.

O₂: Estimate.

O₃: Value measured at 292 K.

OH: Value measured at 293 K.

NO: Value measured between 193 and 243 K.

NO₂: Value measured at 298 K.

NO₃: Value is a lower limit, measured at 273 K.

N₂O₅: Value for sulfuric acid, measured between 195 and 300 K.

HNO₃: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO₄: Value measured at 200 K for water ice.

CH₃O₂: Estimate.

HCHO: Value measured between 260 and 270 K.

CO₂: Estimate.

H₂SO₄: Value measured at 303 K.

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