Supplement B – Chemistry

Isoprene chemistry and emissions

The isoprene chemistry scheme used in the MATCH-model is somewhat more condensed, i.e., uses fewer model species and reactions (7 species, 26 reactions) than the EMEP MSC-W scheme (currently, EmChem09: 19 species, 32 reactions; Simpson et al., 2012). Both are, however, very small compared to more explicit chemical mechanisms, such as, e.g., the MCM scheme (http://mcm.leeds.ac.uk/) with hundreds of species and reactions for the isoprene chemistry.

The EMEP MSC-W isoprene scheme is based on the isoprene chemistry scheme by Paulson and Seinfeld (1992) (with a few reactions omitted, as described by Simpson et al., 1993); the scheme has been updated with new reaction rate constants and some other changes of the chemical mechanism during 2008-2009 (Simpson et al., 2012).

The MATCH model isoprene scheme was constructed in 1998 (Langner et al., 1998) and is based on the Carter 1-product scheme (Carter, 1996). The MATCH isoprene scheme was updated simultaneously as the EMEP scheme (EmChem09) taking into account the same new reaction rate data.

Both the MATCH and EMEP MSC-W model isoprene schemes were chosen to be computationally efficient and still model ozone formation well (compared to larger chemical mechanisms). The compact MATCH isoprene scheme has been shown to yield comparable ozone concentrations as the somewhat larger EMEP MSC-W scheme (Langner et al., 1998) and has been successfully used in many studies focused on ozone (e.g., van Loon et al., 2007).

The isoprene *emission* scheme in the MATCH-SALSA model is different from the completely revised biogenic emission module in the EMEP MSC-W model (Simpson et al., 2012). The emissions of isoprene in the MATCH and EMEP MSC-W models are compared in Langner et al. (2012); the total European isoprene emissions are about twice as large in the EMEP MSC-W model as in the MATCH model.

The MATCH SOA chemistry is presently under development. The latest version of MATCH includes a new biogenic emission model, including isoprene and terpene emissions. In the current MATCH-SALSA version, SOA formation from terpene emissions (α-pinene) is taken into account. In future versions of MATCH-SALSA, SOA formation from isoprene will be included as well.

MATCH-SALSA chemical mechanism

The chemical reactions and rates used in the MATCH-SALSA model are found in Table 1 (except for particulate ammonium species). The following particulate nitrogen-species are included in MATCH-SALSA: ammonium sulfate [$(NH_4)_2SO_4$], ammonium nitrate [NH_4NO_3] and coarse mode nitrate.

These species are all treated outside the SALSA-module and the ammonium chemistry scheme and gas-particle partitioning are very simplified:

NH_3(g) reacts instantaneously (and irreversibly) with available sulfate and form ammonium sulfate $(NH_4)_2SO_4$, which is distributed over different particle sizes according to the sulfate distribution in MATCH-SALSA.

If there is excess NH_3(g) available, ammonium nitrate can be formed via the reaction:

$NH_3(g) + HNO_3(g) \leftrightarrow NH_4NO_3(p)$.

The ammonium nitrate is assumed to be in equilibrium and the dissociation constant of NH_4NO_3 is dependent on relative humidity and temperature, using the equations and parameters from Mozurkewich (1993). Ammonium nitrate is distributed over different particle sizes according to the available aerosol surface area.

Table 1. Gas phase chemical reactions and heterogeneous reactions in the MATCH model and the corresponding reaction rates. The KPP, kinetic pre-processor (Damian et al., 2002), is used to produce the Fortran code for the chemical solver. Text within {}-brackets are comments or compounds in the reactions which are not explicitly included in the chemical mechanism.

Chemical reaction	**Rate**
{Inorganic chemistry}	
{ 1.} O {+ O2 + M} = O3	KOO2;
{ 7.} O1D {+ M} = O	KO1DtoO;
{ 8.} O1D + H2O = 2 OH	2.2e-10;
{ 11.} O3 + NO = NO2 {+O2}	ARR(1.4E-12, -1310.);
{ 12.} O3 + NO2 = NO3 {+O2}	ARR(1.4E-13, -2470.);
{ 13.} O3 + OH = HO2 {+O2}	ARR(1.7E-12, -940.);
{ 14.} O3 + HO2 = OH {+2O2}	KO3HO2;
{ 15.} NO + NO3 = 2 NO2	ARR(1.8E-11, 110.);
{ 17.} NO + HO2 = NO2 + OH	ARR(3.6E-12, 270.);
{ 19.} NO2 + NO3 = NO + NO2	ARR(4.5E-14, -1260.);
{ 30.} OH + HO2 = H2O	ARR(4.8E-11, 250.);
{ 31.} OH + H2O2 = HO2 {+H2O}	ARR(2.9E-12, -160.);
{ 33.} OH + H2 = HO2 {+H2O}	ARR(7.7E-12, -2100.);
{ 35.} OH + HNO3 = NO3 {+H2O}	KMT3_OH_HNO3;
{ 36.} 2 HO2 = H2O2	FH2O*ARR(2.2E-13, 600.);
{ 37.} 2 HO2 + M = H2O2	FH2O*ARR(1.9E-33, 980.);
OH + HONO = NO2	ARR(2.5e-12, -260.0);
OH + HO2NO2 = NO2 {+ H2O + O2}	ARR(3.2e-13, 690.0);
{Sulfur chemistry}	
{ 39.} OH + SO2 = HO2 + H2SO4	KSO2OH;
{Methane chemistry}	
{ 59.} OH + CH4 = CH3O2	KOHCH4;
{ 70.} OH + CO = HO2	KOHCO;

{ 60.} CH3O2 + NO = HCHO + HO2 + NO2	ARR(2.3e-12, 360.0);
{ 61.} 2 CH3O2 = 2 HCHO + 2 HO2	ARR(7.4E-13, -520.);
{ 62.} 2 CH3O2 = CH3OH + HCHO	KCH3O2x2b ;
{ 63.} OH + CH3OH = HO2 + HCHO {+H2O}	KOHCH3OH ;
{ 65.} HO2 + CH3O2 = 0.9 CH3O2H + 0.1 HCHO	ARR(3.8E-13, 780.);
{67&68} CH3O2H + OH = 0.4 HCHO + 0.4 OH + 0.6 CH3O2 {+0.6 H2O}	ARR(5.3E-12, 190.);
{ 66.} OH + HCHO = CO + HO2 {+H2O}	KOHHCHO;
{ 69.} NO3 + HCHO = HNO3 + CO + HO2	ARR(2.0e-12, -2440.0);
{Ethane chemistry}	
{ 71.} OH + C2H6 = C2H5O2	ARR(6.9E-12, -1000.);
{ 72.} C2H5O2 + NO = HO2 + CH3CHO + NO2	ARR(2.55e-12, 380.);
{ 74.} C2H5O2 + HO2 = C2H5OOH	ARR(3.8E-13, 900.);
{76A.} C2H5OOH + OH = CH3CHO + OH	8.01e-12; {MCM; highly uncertain rate, IUPAC gives only lower limit k(C2H5OOH + OH) > 6e-12 at 298K, but this also includes 76B}
{76B.} C2H5OOH + OH = C2H5O2	KRC92 ;
{ 75.} OH + CH3CHO = 0.95 CH3COO2 + 0.05 CH3O2 + 0.05 CO	ARR(4.4E-12, 365.);
{ 79.} CH3COO2 + NO = NO2 + CH3O2 {+CO2}	ARR(7.5e-12, 290.0);
{ 80.} CH3O2 + CH3COO2 = 0.9 HO2 + HCHO + 0.9 CH3O2 + 0.1 CH3COOH	ARR(2.0e-12, 500.);
{ 94.} 2 CH3COO2 = 2 CH3O2	ARR(2.9E-12, 500.);
{88&89} CH3COO2 + HO2 = 0.41 CH3COO2H + 0.15 O3 + 0.44 OH + 0.44 CH3O2 + 0.15 CH3COOH	ARR(5.2E-13, 980.); {highly uncertain rate}
{ 90.} CH3COO2H + OH = CH3COO2	KRC92 ;
{Ethanol chemistry}	
{ 64.} OH + C2H5OH = CH3CHO + HO2	KOHC2H5OH ;
{n-butane chemistry}	
{ 81.} OH + NC4H10 = SECC4H9O2	KOHNC4H10 ;
{ 83.} NO + SECC4H9O2 = NO2 + 0.65 HO2 + 0.65 CH3COC2H5 + 0.35 CH3CHO + 0.35 C2H5O2	KRO2NO;
{108.} SECC4H9O2 + HO2 = SECC4H9O2H	0.625*KHO2RO2;
{ 86.} OH + CH3COC2H5 = CH3COCHO2CH3	KOHMEK;
{105.} CH3COCHO2CH3 + NO = NO2 + CH3COO2 + CH3CHO	KRO2NO;
{104.} CH3COCHO2CH3 + HO2 = CH3COCHO2HCH3	0.625*KHO2RO2;
{107.} CH3COCHO2HCH3 + OH = CH3COCHO2CH3	ARR(1.9e-12, 190.);
SECC4H9O2H + OH = SECC4H9O2	KRC92;
SECC4H9O2H + OH = OH + CH3COC2H5	2.15e-11; {MCM}
{Ethene chemistry}	
{110.} CH2O2CH2OH + NO = NO2 + 2 HCHO + HO2	KRO2NO;

{113.} CH2O2CH2OH + HO2 = CH2OOHCH2OH	1.2e-11 ; {IUPAC – b[2005] (298K)}
CH2OOHCH2OH + OH = CH3CHO + OH	1.38e-11; {MCM-rate, but product in MCM is HOCH2CHO}
CH2OOHCH2OH + OH = CH2O2CH2OH	KRC92;
{112.} C2H4 + O3 = 1.14 HCHO + 0.63 CO + 0.13 HO2 + 0.13 OH + 0.14H2O2 + 0.23 HCOOH	ARR(9.1E-15, -2580.); {IUPAC – b rate, MCM products}
{Propene chemistry}	
{123.} O3 + C3H6 = 0.545 HCHO + 0.545 CH3CHO + 0.56 CO + 0.36 OH + 0.28 HO2 + 0.09 H2O2 + 0.1 CH4 + 0.28 CH3O2 + 0.075 HCOOH + 0.075 CH3COOH	ARR(5.5E-15, -1880.); {products based on MCM}
{126.} NO + CH3CHO2CH2OH = NO2 + CH3CHO + HCHO + HO2	KRO2NO;
{122.} CH3CHO2CH2OH + HO2 = CH3CHOOHCH2OH	0.52*KHO2RO2;
CH3CHOOHCH2OH + OH = ACETOL + OH	2.44e-11;
ACETOL + OH =MGLYOX + HO2	ARR(1.6e-12, 305.) ; {IUPAC - b, uncertain rate}
CH3CHOOHCH2OH + OH = CH3CHO2CH2OH	KRC92;
{o-xylene chemistry}	
{234.} OXYLENE + OH = OXYO2	1.36E-11;
{235.} OXYO2H + OH = OXYO2	4.2E-11; {Based on MCM 55% of OXYO2H reacts at 7.62e-11, but the other OXYO2Hs do not return to OXYO2!}
{219.} MAL + OH = MALO2	5.58E-11;
{220.} MALO2 + NO = NO2 + HO2 + MGLYOX + GLYOX	KRO2NO;
{ 85.} MALO2 + HO2 = MALO2H	0.706*KHO2RO2;
{223.} MALO2H + OH = MALO2	ARR(1.9e-12, 190.); {MCM}
{221.} OH + GLYOX = HO2 + 2 CO	KOHGLYOX;
{222.} OH + MGLYOX = CH3COO2 + CO	ARR(1.9e-12, 575.);
{Isoprene chemistry, version recommended by IVL, Sep 1997; A few rates updated!}	
C5H8 + O3 = 0.6 HCHO + 0.65 ISOPROD + 0.27 OH + 0.07 HO2 + 0.07 CO + 0.2 XO2 + 0.2 CH3COO2 + 0.15 CH3CHO + 0.39 HCOOH	ARR(1.03E-14, -1995.)
C5H8 + OH = ISRO2 + 0.079 XO2	ARR(2.7E-11, 390.);
C5H8 + NO3 = ISONRO2	ARR(3.15E-12, -450.);
ISRO2 + NO = 0.088 ONIT + 0.912 NO2 + 0.912 HO2 + 0.912 ISOPROD + 0.629 HCHO	ARR(4.20E-12, 180.);
ISRO2 + HO2 = C2H5OOH	ARR(7.70E-14, 1301.);

ISRO2 + CH3COO2 = ISOPROD + 0.5 HO2 + 0.5 CH3O2 + 0.5 CH3COOH	ARR(8.40E-14, 220.);
ISRO2 + CH3O2 = ISOPROD + 0.5 HCHO + 0.5 HO2	ARR(3.40E-14, 220.);
C5H8 + O = 0.75 ISOPROD + 0.25 CH3COO2 + 0.25 HCHO + 0.25 CH3O2	3.6E-11;
ISONRO2 + NO = 1.2 NO2 + 0.8 CH3CHO + 0.8 ONIT + 0.8 HO2 + 0.2 ISOPROD	ARR(4.20E-12, 180.);
ISONRO2 + HO2 = ONIT	ARR(7.70E-14, 1301.);
ISONRO2 + CH3COO2 = CH3CHO + ONIT + 0.5 HO2 + 0.5 CH3O2 + 0.5 CH3COOH	ARR(8.40E-14, 220.);
ISONRO2 + CH3O2 = CH3CHO + ONIT + 0.5 HCHO + 0.5 HO2	ARR(3.40E-14, 220.);
ISOPROD + OH = 0.5 CH3COO2 + 0.5 IPRO2 + 0.2 XO2	3.36E-11;
IPRO2 + NO = NO2 + HO2 + 0.59 CO + 0.55 CH3CHO + 0.25 HCHO + 0.08 GLYOX + 0.34 MGLYOX + 0.63 CH3COC2H5	ARR(4.20E-12, 180.);
IPRO2 + HO2 = C2H5OOH	ARR(7.70E-14, 1301.);
IPRO2 + CH3COO2 = 0.5 HO2 + 0.5 CH3O2 + 0.5 CH3COOH + 0.5 CH3CHO + 0.5 CH3COC2H5	ARR(8.40E-14, 220.);
IPRO2 + CH3O2 = 0.5 HCHO + 0.5 HO2 + 0.5 CH3CHO + 0.5 CH3COC2H5	ARR(3.40E-14, 220.);
ISOPROD + O3 = 0.268 OH + 0.1 HO2 + 0.114 CH3COO2 + 0.054 CH3O2 + 0.07 XO2 + 0.155 CO + 0.146 HCHO + 0.02 CH3CHO + 0.01 GLYOX + 0.85 MGLYOX + 0.09 CH3COC2H5 + 0.462 HCOOH	7.11E-18;
ISOPROD + NO3 = 0.075 CH3COO2 + 0.075 HNO3 + 0.643 CO + 0.282 HCHO + 0.925 ONIT + 0.282 CH3CHO + 0.925 HO2 + 0.925 XO2	1.0E-15;
XO2 + HO2 = C2H5OOH	ARR(7.7E-14, 1300.);
XO2 + CH3O2 = HCHO + HO2	ARR(1.7E-14, 220.);
XO2 + CH3COO2 = CH3O2	ARR(4.2E-14, 220.);
XO2 + XO2 = M	ARR(3.6E-16, 220.);
XO2 + NO = NO2	ARR(4.2E-12, 180.);
ONIT + OH = NO2 + 0.843 SECC4H9O2	ARR(1.55E-11, -540.);
N2O5 + H2O = 2 HNO3	KN2O5H2O;
{TROE TYPE REACTIONS}	
{ 5.} O + NO {+ M} = NO2	KONO;
{ 20.} NO2 + NO3 = N2O5	KNO2NO3;
{ 29.} N2O5 = NO2 + NO3	KN2O5;
{ 21.} NO2 + OH = HNO3	KNO2OH;
{ 77.} CH3COO2 + NO2 = PAN	KPANFOR;
{ 78.} PAN = CH3COO2 + NO2	KPANDIS;
{109.} C2H4 + OH = CH2O2CH2OH	KC2H4OH;

{125.} OH + C3H6 = CH3CHO2CH2OH	KOHC3H6;
{ 22.} NO2 + HO2 = HO2NO2	KNO2HO2;
{ 23.} HO2NO2 = NO2 + HO2	KHO2NO2DIS;
OH + NO = HONO	KOHNO;
{Heterogeneous reactions}	
{ 45.} HNO3 = NITRATE	R_HNO3_to_NITRATE
{ 43.} CH3O2H = AEROSOL	R_CH3O2H_to_AEROSOL;
{ 44.} N2O5 = 2 HNO3	R_N2O5_to_HNO3; {heterogeneous reaction, immediate evaporation of HNO3 assumed}
{SOA formation reactions, simplified version stopping after oxidation step for parameterised use in MATCH-SALSA}	
{Terpenes} APINENE + O3 = TERPPEROXY + O3	ARR(6.3e-16,-580.0) ; {MCM, IUPAC recommendation 2007}
APINENE + OH = TERPPEROXY + OH	ARR(1.2e-11,444.0) ;
APINENE + NO3 = TERPPEROXY + NO3	ARR(1.2e-12,490.0) ;

ARR(A, B) = A * EXP(B/T) – Arrhenius type reaction rate
KOO2: Rate from IUPAC - a
KO1DtoO = 1.8E-11*[N2]*EXP(107.0/T) + 3.2E-11*O2*EXP(67.0/T);
KO3HO2: Rate from IUPAC - a
KMT3_OH_HNO3: Rate from IUPAC (http://iupac.pole-ether.fr/htdocs/datasheets/pdf/NOx10_HO_HONO2.pdf using the Lamb et al., 1984 mechanism with the elementary rate constants from (Brown et al., 1999; NASA, 2000 – as referred to by IUPAC)
FH2O = 1.+1.4E-21*[H2O]*EXP(2200./T)
KSO2OH: Rate from IUPAC - a
KOHCH4 =1.85E-20*$T^{2.82}$*EXP(-987.0/T);
KOHCO = 1.44E-13 + [M]*3.43E-33;
KCH3O2x2b = 1.03E-13*EXP(365./T) - 7.4E-13*EXP(-520./T);
KOHCH3OH = 6.38E-18*T^2*EXP(144.0/T) ;
KOHHCHO = 1.25E-17* T^2*EXP(615.0/T);
KRC92 = 1.9E-12*EXP(190./T) ;
KOHC2H5OH = 6.7E-18*T^2*EXP(511.0/T);
KRO2NO = 2.54E-12*EXP(360.0/T);
KHO2RO2 =2.91E-13*EXP(1300.0/T);
KOHNC4H10 = 2.03E-17*T^2*EXP(78.0/T);
KOHMEK = 2.53E-18*T^2*EXP(503.0/T);
KOHGLYOX = 6.6E-18*T^2*EXP(820.0/T);
KN2O5H2O = 2.5E-22+1.8E-39*[H2O];
KONO: Pressure dependent rate from MCM [citing IUPAC2001] (k_0=1.0E-31*(T/300)$^{-1.6}$*[M], k_∞=3.0E-11*(T/300)$^{0.3}$, F_c=0.85)
KNO2NO3: Pressure dependent rate from IUPAC - a
KN2O5: Pressure dependent rate from IUPAC - a
KNO2OH: Pressure dependent rate from MCM [citing IUPAC2002] (k_0=3.3E-30*(T/300)$^{-3.0}$*[M], k_∞=4.1E-11, F_c=0.4)
KPANFOR: Pressure dependent rate from IUPAC - b
KPANDIS: Pressure dependent rate from IUPAC - b
KC2H4OH: Pressure dependent rate from IUPAC - b
KOHC3H6: Pressure dependent rate from IUPAC - b
KNO2HO2: Pressure dependent rate from IUPAC - a
KHO2NO2DIS: Pressure dependent rate from IUPAC - a
KOHNO: Pressure dependent rate from MCM [citing IUPAC2001] (k_0=7.4E-31*(T/300)$^{-2.4}$*[M], k_∞=3.3E-11*(T/300)$^{-0.3}$, F_c= EXP(-T/1420.)
R_HNO3_to_NITRATE = 5.E-6*[M]/2.55E19;
R_CH3O2H_to_AEROSOL = 5.E-6*[M]/2.55E19;
R_N2O5_to_HNO3 = RH>0.9: 1.E-4*[M]/2.55E19; RH<=0.9: 1.E-5*[M]/2.55E19

Table 2. Photolysis reactions in the MATCH model.

{Photolysis reactions}	**Rate**
{ 1.} O3 + hv = O1D	JO3_1 ;
{ 2.} O3 + hv = O	JO3_3 ;
{ 3.} NO2 + hv = NO + O	JNO2 ;
{ 4.} NO3 + hv = NO2 + O	JNO3a ;
{ 5.} NO3 + hv = NO	JNO3b ;
{ 6.} N2O5 + hv = NO2 + NO3	JN2O5 ;
{ 7.} H2O2 + hv = 2 OH	JH2O2 ;
{ 8.} HNO3 + hv = NO2 + OH	JHNO3 ;
{ 9.} HCHO + hv = 2 HO2 + CO	JHCHOa ;
{10.} HCHO + hv = H2 + CO	JHCHOb ;
{11.} CH3CHO + hv = CH3O2 + HO2 + CO	JCH3CHO ;
{12.} CH3COC2H5 + hv = CH3COO2 + C2H5O2	JCH3COC2H5 ;
{14.} GLYOX + hv = CO + HCHO	JGLYOX ;
{15.} CH3O2H + hv = OH + HCHO + HO2	JCH3O2H;
{16.} MGLYOX + hv = CO + CH3COO2 + HO2	JMGLYOX;
{17.} C2H5OOH + hv = OH + CH3CHO + HO2	JCH3O2H;
{18.} CH3COO2H + hv = OH + CH3O2	JCH3O2H;
{20.} CH3COCHO2HCH3 + hv = OH + CH3CHO + CH3COO2	JCH3O2H;
{21.} SECC4H9O2H + hv = OH + 0.65 HO2 + 0.65 CH3COC2H5 + 0.35 CH3CHO + 0.35 C2H5O2	JCH3O2H;
{22.} CH2OOHCH2OH + hv = OH + HO2 + 1.56 HCHO + 0.22 CH3CHO	JCH3O2H;
{23.} CH3CHOOHCH2OH + hv = CH3CHO + HCHO + HO2 + OH	JCH3O2H;
{24.} OXYO2H + hv = OH + MGLYOX + MAL + HO2	JCH3O2H;
{25.} MALO2H + hv = OH + MGLYOX + GLYOX + HO2	JCH3O2H;
{ivl} ONIT + hv = HO2 + NO2 + 0.2 CH3CHO + 0.8 CH3COC2H5	JONIT ;
HO2NO2 + hv = OH + NO3	JHO2NO2_1 ;
HO2NO2 + hv = HO2 + NO2	JHO2NO2_2 ;
HONO + hv = OH + NO	JHONO ;
ACETOL + hv = CH3COO2 + HCHO + HO2	JCH3COC2H5 ; {same J-expression for MEK and ACETOL in MCM}

The photolysis rates are pre-calculated with the Phodis model (Kylling et al., 1995), using absorption cross-sections and quantum yields according to CODATA and IUPAC evaluations (DeMore et al, 1997, Sander et al., 2000, Atkinson et al., 1997). Clear-sky photolysis rates are tabulated for model atmospheres for

different seasons at varying latitudes, surface albedos and heights above ground. Below clouds the photolysis rates are scaled by the ratio of the actual global radiation (with clouds) to the clear sky global radiation (Langner et al., 1998).

Table 3. Aqueous phase chemical reactions in the MATCH model, and the corresponding reaction rates. Text within {}-brackets are comments or compounds in the reactions which are not explicitly included in the chemical mechanism.

Chemical reaction	**Rate**
{Sulfur chemistry}	
{wet1a} SO2(aq) + O3(aq) = SULFATE	KSO2O3wet ;
{wet1b} $HSO3^-$(aq) + O3(aq) = SULFATE	KSO2O3wet ;
{wet2} SO2(aq) + H2O2(aq) = SULFATE	KSO2H2O2wet ;
{wet3a} SO2(aq) = SULFATE	KSO2catalysedwet ; {catalysed oxidation by O2}
{wet3b} $HSO3^-$(aq) = SULFATE	KSO2catalysedwet ; {catalysed oxidation by O2}

KSO2O3wet = $1.81E4*[H^+]^{-0.4}$ mol^{-1} l;
KSO2H2O2wet = 8.31E5 mol^{-1} l;
KSO2catalysedwet = 5.6e-6 s^{-1};

References

Atkinson, R., D. L. Baulch, R. A. Cox, R. F. Hampson Jr., J.A. Kerr, and J. Troe: Evaluated kinetics, photochemical and heterogeneous data for atmospheric chemistry, Supplement V, J. Phys. Chem. Ref. Data, 26, 521-1011, 1997.

Atkinson, R, Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J. Evaluated kinetic and photochemical data for atmospheric chemistry: volume I - gas phase reactions of Ox, HOx, NOx, and SOx, species. Atmos. Chem. Phys., 4, 1461-1738, 2004; and http://iupac.pole-ether.fr/

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and IUPAC Subcommittee: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II – gas phase reactions of organic species, Atmos. Chem. Phys., 6, 3625-4055, doi:10.5194/acp-6-3625-2006, 2006; and http://iupac.pole-ether.fr/

Brown, S. S., Talukdar, R. K. and Ravishankara, A. R.: J. Phys. Chem. A 103, 3031, 1999.

Carter, W. P. L.: Condensed atmospheric photooxidation mechanism for isoprene, Atmos. Environ. 30, 4275-4290, 1996.

Damian, V., Sandu, A., Damian, M., Potra, F. Carmichael, G.R.: The kinetic preprocessor KPP - a software environment for solving chemical kinetics, Comput. Chem. Eng., 26, 1567-1579, 2002.

DeMore, W. B., S. P. Sander, D. M. Golden, R. F. Hampson, M. J. Kurylo, C.J. Howard, A. R. Ravishankara, C. E. Kolb, and M. J. Molina, 1997, Chemical kinetics and photochemical data for use in stratospheric modeling, Evaluation 12, Jet Propul. Lab., Pasadena, California. JPL Publication 97-4

IUPAC - a: Atkinson et al., 2004 (see above), rates as on http://iupac.pole-ether.fr/htdocs/summary/vol1_summary.pdf (accessed 2014-10-27).

IUPAC - b: Atkinson et al., 2006 (see above), rates as on http://iupac.pole-ether.fr/htdocs/summary/vol2_summary.pdf (accessed 2014-10-27).

Kylling, A., Bais, A. F., Blumthaler, M., Schreder, J., Zerefos, C. S., and Kosmidis, E.: Effect of aerosols on solar UV irradiances during the Photochemical Activity and Solar Radiation campaign, J. Geophys. Res., 103, 26051–26060, doi:10.1029/98JD02350, 1998.

Lamb, J. J., Mozurkewich, M. and Benson, S. W.: J. Phys. Chem. 88, 6441, 1984.

Langner, J., Bergström, R., and Pleijel, H.: European Scale Modeling of Sulfur, Oxidised Nitrogen and Photochemical Oxidants, Model Development and Evaluation for the 1994 Growing Season, SMHI RMK 82, SMHI 60176 Norrköping, Sweden, 1998.

Langner, J., Engardt, M., Baklanov, A., Christensen, J. H., Gauss, M., Geels, C., Hedegaard, G. B., Nuterman, R., Simpson, D., Soares, J., Sofiev, M., Wind, P., and Zakey, A.: A multi-model study of impacts of climate change on surface ozone in Europe, Atmos. Chem. Phys., 12, 10423-10440, doi:10.5194/acp-12-10423-2012, 2012.

MCM: The chemical mechanistic information was taken from the Master Chemical Mechanism, MCM v3.2 (Jenkin et al., Atmos. Environ., 31, 81, 1997; Saunders et al., Atmos. Chem. Phys., 3, 161, 2003; Jenkin et al., Atmos. Chem. Phys., 3, 181, 2003; Bloss et al., Atmos. Chem. Phys., 5, 641, 2005), via website: http://mcm.leeds.ac.uk/MCM.

Mozurkewich, M.: The dissociation constant of ammonium nitrate and its dependence on temperature, relative humidity and particle size, Atmos. Environ., 27A, 261–270, 1993.

Paulson, S. E. and Seinfeld, J. H.: Development and evaluation of a photooxidation mechanism for isoprene, J. Geophys. Res., 95, 1871-1881, 1992.

Sander, S. P., R. R. Friedl, W. B. DeMore, D. M. Golden, M. J. Kurylo, R. F. Hampson, R. E. Huie, G. K. Moortgat, A. R. Ravishankara, C. E. Kolb, and M. J. Molina, 2000, Chemical kinetics and photochemical data for use in stratospheric modeling, Evaluation 13, Jet Propul. Lab., Pasadena, California. JPL Publication 00-3.

Simpson, D., Andersson-Sköld, Y., and Jenkin, M. E., Updating the chemical scheme for the EMEP MSC-W oxidant model: current status, EMEP MSC-W Note 2/93, 1993.

Simpson, D., Benedictow, A., Berge, H., Bergström, R., Emberson, L. D., Fagerli, H., Flechard, C. R., Hayman, G. D., Gauss, M., Jonson, J. E., Jenkin, M. E., Nyíri, A., Richter, C., Semeena, V. S., Tsyro, S., Tuovinen, J.-P., Valdebenito, A., and Wind, P.: The EMEP MSC-W chemical transport model – technical description, Atmos. Chem. Phys., 12, 7825–7865, doi:10.5194/acp-12-7825-2012, 2012.

van Loon, M., Vautard, R., Schaap, M., Bergström, R., Bessagnet, B., Brandt, J., Builtjes, P.J.H., Christensen, J. H., Cuvelier, K., Graf, A., Jonson, J.E., Krol, M., Langner, J., Roberts, P., Rouil, L., Stern, R., Tarrasón, L., Thunis, P., Vignati, E., White, L., Wind, P.: Evaluation of long-term ozone simulations from seven regional air quality models and their ensemble average, Atmos. Environ. 41, 2083-2097, 2007.Korhola et al., Geosci. Model Dev., 7, 161-174, doi:10.5194/gmd-7-161-2014, 2014.