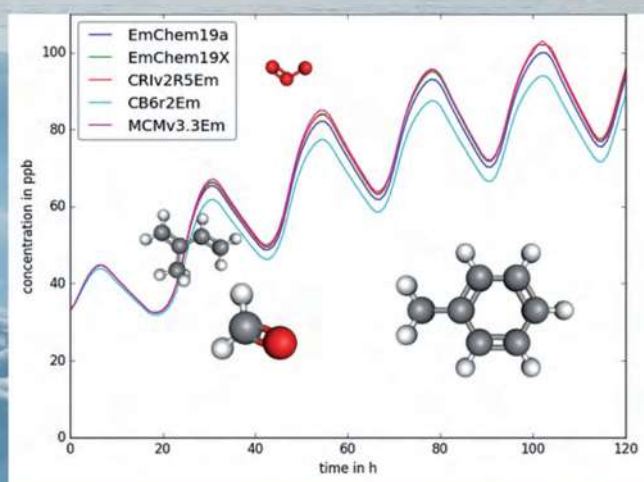


Update and comparison of atmospheric chemistry mechanisms for the EMEP MSC-W model system

– EmChem19a, EmChem19X, CRIv2R5Em, CB6r2Em, and MCMv3.3Em

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December 2022

ISSN 1504-6206

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1. Introduction

Atmospheric chemical transport models (CTMs), which simulate the emissions, transport, chemistry and deposition of pollutants, are essential tools for understanding air quality, and for assisting policymakers in setting environmental goals and emissions targets. CTMs are typically advanced 3-dimensional (3-D) models that can be used on different geographical scales and resolutions — simulations with ten million grid-cells, or more, are not unusual. The models account for transport (advection, diffusion) between the cells. Within each cell the chemistry is simulated, with chemical mechanisms of varying complexities. An important CTM in terms of policy within Europe, and the Convention on Long-Range Transboundary Air Pollution (CLRTAP; www.unece.org/env/lrtap/welcome.html), is that used by the Meteorological Synthesising Centre-West of the European Monitoring and Evaluation Programme (EMEP MSC-W). The EMEP MSC-W model (in the following denoted the EMEP model), described in detail in [Simpson et al. \(2012\)](#) and subsequent articles and EMEP reports (e.g. [Stadtler et al. 2018](#), [Simpson et al. 2022](#), and references therein), is a 3-D Eulerian model whose main aim is to support the CLRTAP and policymakers in their efforts to design effective emissions control strategies ([Amann et al. 2011](#)). The EMEP model has been available as open-source code (www.emep.int) since 2008, and it has since been run by several institutes across Europe (e.g. [Solberg et al. 2008](#), [Jeričević et al. 2010](#), [Vieno et al. 2010](#), [Ots et al. 2016](#), [Gašparac et al. 2020](#), [van der Swaluw et al. 2021](#)).

The EMEP model was designed to be very CPU efficient ([Skålin et al. 1995](#)); a crucial part of this is the use of a highly efficient numerical solver, TWOSTEP ([Verwer 1994](#), [Verwer and Simpson 1995](#)), for integrating the set of ordinary differential equations that describe the chemical reaction kinetics. The Fortran code for the numerical integration is generated by a chemical pre-processor — GenChem.py ([Simpson et al. 2020a](#)) — which makes it easy to modify, and add new, chemical mechanisms for the model. As well as GenChem.py, the so-called GenChem system includes a box-model, boxChem, which allows rapid testing of chemical mechanisms in stand-alone code. boxChem make use of the same chemical mechanisms as produced by GenChem, but also offers the possibility of running very large chemical mechanisms such the MCM scheme which are impossible to run in CTM mode (Ch. 2.5, 3).

The chemical scheme used as default in the EMEP model, EmChem19a¹ (Ch. 2.1), was developed in 2018–2019 as part of the study reported here. EmChem19a can trace its origins to work done by [Hesstvedt et al. \(1978\)](#), [Hov \(1983\)](#) and [Eliassen et al. \(1982\)](#). During

¹EmChem19r, introduced in [Simpson et al. \(2021\)](#) is simply a variation of EmChem19a which tracks residential emissions rather than the wood and fossil fuel tracking used in EmChem19a. We use the term EmChem19a here for both variants.

the 1990s the EMEP chemistry was thoroughly revised with updated rate-coefficients for all reactions, addition of a substantial $\text{HO}_2 + \text{RO}_2$ chemistry, and an extensive isoprene chemistry based upon the Paulson and Seinfeld (1992) mechanism (Simpson et al. 1993, Simpson 1995). Kuhn et al. (1998) compared the EMEP and eight other chemical mechanisms with box-model simulations covering remote and moderately polluted simulations over a 5-day period. EMEP was found to be among the schemes producing the highest ozone concentrations, although with similar results to that of the most extensive chemical mechanism, the IVL scheme (over 1800 reactions among 714 species, Andersson-Sköld et al. 1992, Andersson-Sköld 1995). The comparison with the IVL scheme was pursued further by Andersson-Sköld and Simpson (1999), who also added more polluted cases (including a London plume) to the comparison. They concluded that overall the EMEP chemistry gave a description of ozone formation, and the effects of emission control measures, which was in good agreement with that given by the much more comprehensive IVL chemistry.

With the increased computing power it has become feasible to run CTMs with much larger chemistry schemes than could be used in the 1990s. The Master Chemical Mechanism (MCM; v3.3.1 Jenkin et al. 2015), with over 5 800 chemical species and more than 17 000 reactions, is still too large for 3-D modelling on large scales with the EMEP CTM, but it can easily be used in box-model setups such as boxChem, and is useful as a benchmark for EmChem type mechanisms and other reduced chemistry schemes. During recent years the CRI (Common Representative Intermediates) schemes of Jenkin et al. (2008), Watson et al. (2008), and different versions of the Carbon Bond (CB5, CB6) mechanism (e.g. Yarwood et al. 2010b) have been introduced in the EMEP model. The CRI mechanism is still too large for the regular source-receptor calculations with the EMEP policy model but it has been used in research projects including global scale simulations to investigate impacts of mixtures of biogenic VOCs on formation of secondary organic aerosol (McFiggans et al. 2019).

In this report we document the chemical mechanisms which are currently implemented in the EMEP and/or boxChem systems (Ch. 2), compare these mechanisms (including MCMv3.3Em) in a series of box-model tests (Ch. 3), and then in a series of European and global scale simulations (Ch. 4-5). Chapter 6 discusses some of the reasons for the differences in results between the mechanisms. Ch. 7 presents a brief illustration of another important aspect of these mechanisms – the computer time needed to run the EMEP model. In the Conclusions (Ch.8), we summarise the results and identify some prospects for future activities.

It should be noted that this report has presented only a brief overview of the many tests which have been conducted in the design of the new EmChem schemes. The focus here has been the gas-phase chemistry, with some consideration of the inorganic particle chemistry. Much work remains to be done to evaluate the impact of these chemical mechanisms on secondary organic aerosols, but that issue is far more complex and unconstrained in terms of both chemistry and emissions than for the gas-phase compounds (e.g. Ng et al. 2006, Kroll and Seinfeld 2008, Hallquist et al. 2009, Jimenez et al. 2009, Bergström et al. 2012, Denier van der Gon et al. 2015, Hodzic et al. 2016, Simpson et al. 2020b), and will be the subject of further investigations.

2. Chemical mechanisms

The five mechanisms described in this report, namely EmChem19a, EmChem19X, CRIv2R5Em, CB6r2Em, and MCMv3.3Em, are discussed below. Except for MCMv3.3Em, listings for these mechanisms (as well as various rate coefficient data) can be found in Appendices G-J. All mechanisms, and the boxChem model used below, are made available as ascii files as part of the GenChem system (Simpson et al. 2020a, <https://github.com/metno/genchem>).

The EmChem19X scheme was developed as an updated and extended gas-phase chemistry mechanism for the EMEP model. The scheme was built starting from the EmChem16 scheme by first checking and updating all reaction rates to the latest IUPAC recommendations. Then extensions were made for different parts of the chemistry, using boxChem, the box model of the GenChem system (Simpson et al. 2020a). The MCMv3.3.1 scheme was initially used as the benchmark model, and during the development of the EmChem19X scheme, updates were also made to the GenChem-version of the MCM (and CRI) scheme(s), eventually leading to the MCMv3.3Em (and CRIv2R5Em versions), described in Ch. 2.5 (and Ch. 2.3). The goal was to have a new EmChem mechanism capable of reproducing MCM results as well as possible for a number of important atmospheric chemical components for varying conditions, while still being small enough to be usable for regular EMEP model simulations.

The final EmChem19X scheme was substantially larger than EmChem16 and, in order to have a faster scheme for operational EMEP applications, a substantially reduced scheme — EmChem19a — was constructed from EmChem19X. EmChem19a was also optimized (tuned) to get reasonably good agreement with MCM, but the limitations in size meant that e.g. the night time radicals are in somewhat less good agreement with MCM. The tuning of the mechanisms to agree as well as possible with MCM, while still keeping them reasonably small, included the neglect of some species that e.g. have low “net” reactivity, replacement of some species with others that have similar reactivities, and for some reactions (notably in the aromatic chemistry) neglect of some radical products to balance the effects of other neglected or changed products.

2.1. EmChem19a

The new EMEP default mechanism, EmChem19a, is an updated version of the EmChem09 scheme (Simpson et al. 2012) and the EmChem16 scheme (Simpson et al. 2017), themselves based upon the earlier EMEP mechanisms tracing back to Eliassen et al. (1982). The basic idea of the EmChem19a mechanism, as with earlier EMEP chemistry mechanisms, is that a limited set of representative volatile organic compounds (VOC) are used as surrogates for the large number of different VOCs actually emitted to the atmosphere. The aim is to balance complexity/realism against computational runtime. To this end, EmChem19a typically uses 12–14 different VOCs to represent anthropogenic non-methane VOC emissions; e.g. n-butane (nC4H10) represents most of the alkanes with more than three carbon atoms, but also a few other species with similar potential ozone creation potentials (POCPs, c.f. Derwent and Jenkin 1991, Andersson-Sköld et al. 1992, Jenkin et al. 2017). An example of how the emission surrogates can be set is given in Appendix D, Table D.1.

The full EmChem19a mechanism is presented in Appendix G, Table G.1. Chemical reaction rate coefficients have been updated (compared to EmChem16) to be in line with new IUPAC recommendations (updates until June 2019) (IUPAC 2019, Atkinson et al. 2004, 2006) and a number of additional reactions, and a few new chemical species, have been included. The most important differences to EmChem09 and EmChem16 are:

- Benzene and Toluene are added to the scheme. This was done for two reasons — the ability to model the concentrations of these important gas-phase species and possible improvements in the description of secondary organic aerosol formation from aromatic VOCs.
- The rate coefficients and/or products of more than 40 reactions were changed/updated compared to EmChem09/EmChem16, including a number of reactions between peroxy radicals and nitrate radicals.
- A revised treatment of peroxy + peroxy radical reactions was introduced, making use of the total RO₂ pool as a reactant.
- The isoprene chemistry was revised (see below).
- A sesquiterpene species was added, though this is treated as immediately forming secondary organic aerosol, without affecting the gas-phase chemistry.
- Two other new species were added: 2,3-butanedione (BIACET) and sec-butyl nitrate (sC4H9NO3). Earlier EmChem schemes only had organic nitrates originating from the isoprene chemistry.
- A few reactions and chemical species, were removed from the scheme, or simplified compared to EmChem16.

The isoprene chemistry in EmChem19a is very similar to the scheme introduced in EmChem16 (Simpson et al. 2017). It is based on the CheT2 scheme by Squire et al. (2015). Some modifications were made in EmChem19a compared to CheT2: reaction rate coefficients are

based on the recommendations from IUPAC (or MCMv3.3.1 for reactions not available from IUPAC). The peroxy + peroxy radical reactions for the isoprene peroxy radical (ISRO2 in EmChem) make use of the total RO₂ pool in EmChem19a, and the MACRO2 + RO₂ reactions are neglected in EmChem19a.

A small gas-phase mechanism for monoterpenes (MT) is included in EmChem19a, as in EmChem16. The MT scheme is an adapted version of the MOZART-4 MT chemistry (Emmons et al. 2010), which uses both methacrolein (MACR) and methyl vinyl ketone (MVK) as surrogates for monoterpene oxidation products, chosen to avoid adding more compounds to the MOZART mechanism. Since EmChem19a uses MACR to represent both methacrolein and methyl vinyl ketone, the MVK in the MT scheme is replaced by MACR in EmChem19a. A further simplification of the MT chemistry, compared to EmChem16, is that the standard EmChem19a scheme use a single surrogate MT (APINENE; similar to Emmons et al. 2010), instead of the three MTs used in EmChem16. However, the two additional monoterpenes from EmChem16 (BPINENE and XTERP) can easily be added to EmChem19a via the GenChem system if desired.

2.2. EmChem19X

A more extended chemical mechanism — EmChem19X — has also been developed, which allows better fidelity to MCM, though at the expense of greater computational cost. EmChem19X is intended for use in research projects where these costs are not prohibitive. A large number of reactions and chemical species have been added in EmChem19X, including several additional peroxy acyl nitrates (PANs) and other multifunctional organic nitrates. EmChem19X includes six different PANs (EmChem19a has only two). EmChem19X also adds a number of nitrate-containing peroxy radicals, formed mainly in NO₃ reactions and OH reactions of organic nitrates and nitro-compounds.

The biggest difference to EmChem19a is that EmChem19X has a completely revised, much larger, aromatic chemistry. Just as for earlier EmChem schemes the aromatic chemistry is based on using o-xylene (OXYL) as the surrogate species. In EmChem19X the OXYL+OH reaction mainly forms a peroxy radical (OXYBIPERO2) but also some 2,3-dimethyl phenol (OXYLOL). In EmChem19a only a peroxy radical product (OXYO2) is considered. OXYLOL has a rather complicated chemistry in EmChem19X. The OXYBIPERO2 is also treated in a much more detailed way in EmChem19X than the OXYO2 of EmChem19a (although still simplified compared to MCMv3.3.1). The aromatic chemistry of EmChem19X has 22 additional chemical species compared to EmChem19a (including 7 new peroxy radicals and 3 aryloxy radicals). EmChem19X also adds some new products from the reactions of ethene, propene, methyl ethyl ketone, acetaldehyde and peroxyacetic acid; the updates are based on the MCMv3.3.1 scheme (Jenkin et al. 2015).

Updates have also been made for biogenic VOCs. The isoprene chemistry in EmChem19X is extended compared to EmChem19a; it is partly based on the CheT2mod scheme. The CheT2mod scheme was initially developed for the EMEP model in 2016 as an extended version of CheT2, adding methyl vinyl ketone (MVK) to the mechanism but it has so far not been used in operational versions of the model. Further updates were made to the isoprene mechanism for EmChem19X: a number of reactions have been added, or modified, (based

mainly on the MCMv3.3.1 mechanism). An important update is that the methacryloyl peroxy radical (MACO3) is added to the scheme, to allow MPAN formation to be treated as in MCM — the EmChem19X models MPAN in fairly good agreement with MCM in our box model simulations.

MVK is also added as a surrogate product in the monoterpene chemistry in EmChem19X, so that the MT scheme is very similar to the one in [Emmons et al. 2010](#); the main differences are that some rate coefficients have been updated to new IUPAC recommendations, and that a reaction between the TERPO2 peroxy radical and NO₃ radicals has been added in EmChem19.

Since the same emitted species are included in EmChem19X as in EmChem19a the same surrogate species are used to describe emitted VOC species included in the MCMv3.3.1 (Appendix D, Table D.1).

2.3. CRIv2R5Em

The CRIv2R5Em chemical mechanism is an EMEP adaptation of the Common Representative Intermediates (CRI) v2-R5 mechanism ([Watson et al. 2008](#)), which in turn is a reduced variant of the CRI v2 ([Jenkin et al. 2008](#)). The R5 reduction is based on using a subset of 22 different VOCs to represent all the different emitted non-methane VOCs, leading to a mechanism with ca 600 reactions and a total of 220 species.

The updates of this EMEP version (from a version based on CRIv2.1) were done before the release of CRI v2.2 (now available at <http://cri.york.ac.uk/>), so the CRIv2R5Em is thus not completely identical to the CRI v2.2, but similar.

The CRIv2R5Em includes a recently developed isoprene reaction scheme (CRI v2.2a) that describes the major HOx recycling routes (included in MCM v3.3.1) in a simplified way ([Jenkin et al. 2019](#)). A detailed description of the updated isoprene chemistry in CRI is given by [Jenkin et al. \(2019\)](#) and will not be repeated here, though the impacts of the CRI v2.2a isoprene revisions on the simulated global atmospheric composition have recently been tested with the STOCHEM-CRI model ([Khan et al. 2021](#)). It should be noted that the isoprene scheme of CRI v2.2a was optimised for warm conditions (ca. 300 K) typical of European ozone episode, or tropical, conditions.

The rate coefficients and products of other (non-isoprene) reactions in CRI v2-R5 have also been reviewed and updated to take into account new and revised IUPAC recommendations, and for some reactions revisions were made to be more in line with MCM v3.3.1. Some of the differences in CRIv2R5Em, compared to CRI v2.2a, include:

- Six reactions in CRIv2R5Em use the IUPAC recommended modified Arrhenius rate expressions (including a temperature dependent pre-exponential factor), which IUPAC recommends for a wider temperature range than the simpler Arrhenius expression used in CRIv2.2 (OH-reactions of CH₃OH, C₂H₅OH, HCHO, CH₄, C₂H₆, C₃H₈)
- Changed products of the glyoxal+OH reaction (using the MCMv3.3.1 products)
- Changed products for the α -pinene+O₃ reaction
- Changes in aldehyde+NO₃ reactions

- Introducing temperature dependence for the $\text{NO}_3 + \text{HCHO}$ reaction
 - Adding NO_3 reactions for glyoxal and methylglyoxal
- Changed the organic nitrate yields for three $\text{RO}_2 + \text{NO}$ reactions based on IUPAC recommendations from 2018
- A number of other rate expressions were updated to be in agreement with IUPAC recommendations
 - This includes rate coefficient updates for monoterpene oxidation reactions, acyl peroxy + HO_2 reactions and alkene + O_3 reactions
- A few species and reactions were removed from the scheme, due to the revisions/simplifications based mainly on comparisons with the MCMv3.3.1 mechanism
 - In total three advected species and two peroxy radicals were removed
- The total number of added reactions (17) is about the same as the number of removed reactions (14)
- The rate coefficients and/or products of about 44 reactions are different in CRIv2R5Em compared to CRIv2.2
 - This includes a multiphase description of sulfate formation from SO_2 in CRIv2R5Em, which is not formally represented in CRIv2.2 (see Sec. 2.7).

The standard CRI mechanism includes two monoterpene species — α -pinene and β -pinene (APINENE, BPINENE). In the EMEP version (CRIv2R5Em) it is possible to run the model with the monoterpene emissions treated as 100% α -pinene or including both α -pinene and β -pinene emissions. As a third option we have introduced an additional model species XTERP, which represents emissions of other monoterpenes — the gas-phase products of the XTERP chemistry are treated as identical to those of APINENE, but the initiation reaction rate coefficients for XTERP are modified to reflect the faster reactions of many other monoterpenes.

Different choices of emission surrogates for emitted VOCs have been tested with the CRIv2R5Em mechanism in the present study. [Watson et al. \(2008\)](#) included a limited set of emitted species in their most reduced (R5) mechanism. They used only a single, or two different, VOC species to represent each VOC group in the emission inventory; e.g., all emitted aromatic VOCs, except benzene and toluene, are modelled as o-xylene, and all alcohols and ethers are modelled as either methanol or ethanol (for details see [Watson et al. 2008](#)). We have used an adapted version of this simple surrogate scheme for the CRIv2R5Em in the model simulations presented in this paper — a table describing how the VOC species from MCMv3.3.1 are converted into the CRIv2R5Em surrogate species is included in Appendix D, Table D.2. Alternative surrogate choices can be made when running the boxChem or EMEP models.

2.4. CB6r2Em

The Carbon Bond 6 mechanism Revision 2 (CB6r2 — [Yarwood et al. 2010a,b](#), [Hildebrandt Ruiz and Yarwood 2013](#)) has been implemented in the EMEP model with a few adaptations — the most important being the use of EMEP photolysis rates in the 3-D model and MCM-style photolysis rates in the box model simulations. The treatment of the SO₂ chemistry has also been harmonized with the standard EMEP model (see Sec. 2.7). The formation of negative amounts of paraffinic carbon in some reactions in the original CB mechanisms in some reactions (to keep the number of carbon atoms balanced) has been replaced by the introduction of a “PARLOSS” species in the CB6r2Em adaption since the GenChem system can not handle negative production rates.

A key element in the CB6 mechanism, just as for earlier versions of the Carbon Bond Mechanism (e.g. [Gery et al. 1989](#), and references therein), is the usage of different “carbon bond” surrogates to represent different types of carbon bonds (or functional groups) for representing most of the VOC species in the atmosphere — e.g. PAR is used as a surrogate for a single-bonded carbon atom and OLE for the two double bonded carbon atoms in terminal alkenes. In CB6 there are five such carbon bond “fragment” species (PAR, OLE, IOLE, ALDX, KET). In addition to this, the CB6 uses a number of organic species as surrogates for sets of different VOC-species, e.g. TOL for toluene and other monoalkylbenzene species, and XYL for xylenes and other di- and tri-alkylbenzenes (in both cases combined with additional PAR unit(s)).

A few important VOC species are treated explicitly in CB6 and are not used as surrogates for other species. This includes: methane, ethane, propane, acetylene, isoprene, benzene, methanol, ethanol, acetone, glyoxal, methylglyoxal, glycolaldehyde, formic acid and acetic acid. We have mapped the other emitted VOC species to the CB6r2Em species/surrogates based on [Yarwood et al. \(2005\)](#) but extended to include the new species in CB6. The mapping matrix for converting emitted VOC species included in the MCMv3.3.1 to CB6r2Em is included in Appendix D, Table D.3.

CB6r2Em includes a number of additional inorganic reactions compared to CRIv2R5Em and the EmChem19 schemes — for example a number of reactions of O(³P) and OH, HO₂, H₂O₂ and NO₃; and NO₃-reactions with NO₃ and O₃. Some of the reaction rate expressions in CB6r2Em also differ from those in the other mechanisms; the differences are relatively large for the formation and dissociation reactions of peroxyntic acid (HO₂NO₂) and for the OH + NO₂ and O(³P) + NO₂ reactions.

An important new feature in CB6r2 compared to earlier CB mechanisms is a modification of the treatment of organic nitrates ([Hildebrandt Ruiz and Yarwood 2013](#)). CB6r2 introduces a particle bound organic nitrate (NTR2) that only undergoes hydrolysis (to form HNO₃) and thereby acts as a sink for NO_x.

Finally, it should be noted that a new version of CB6 — CB6r5 — has been released ([Yarwood et al. 2020](#)), which includes updated reaction rates for many reactions, to be in agreement with more recent recommendations from IUPAC. This version was not available at the time of our implementation, but will hopefully be included in future testing.

2.5. MCMv3.3Em

A slightly revised/updated version of the ‘Master Chemical Mechanism’ v3.3.1 (Jenkin et al. 2015) has been included in the GenChem system. Our implementation of the MCM mechanism has over 5800 species and over 17000 reactions, which means that it is too large for usage in the 3-D EMEP model but it can be run in box models and the ESX system. For the present work it is used as a reference model in the box model simulations.

The GenChem version of MCM is denoted MCMv3.3Em. The differences to the official MCMv3.3.1 are mainly updates of some reaction rate coefficients to be in agreement with IUPAC recommendations from 2015–2018; the inorganic reaction rate expressions were also reviewed and updated to be in line with the IUPAC recommendations. A summary of the updates/differences compared to the official MCM version is given in Appendix A.

2.6. Photolysis treatment

The calculation of photolysis rates in the EMEP CTM is based on precalculated (tabulated) rates for 17 different photo-dissociation reactions for clear-sky and two different cloud types (Jonson et al. 2001, Simpson et al. 2012), based on the PHODIS mechanism of Kylling et al. (1995, 1998). For photolysis reactions that are not included in the EMEP database the photo-dissociation rates are set using the reaction with the most closely matched zenith angle dependence in the MCMv3.3.1, scaled to get the same clear-sky photolysis rate at a solar zenith angle of 56° . In the box model simulations a somewhat simpler treatment of photolysis was used. Only clear sky simulations were performed and the photolysis rates were calculated using the same methodology as in the MCMv3.3.1 model (Saunders et al. 2003, <http://mcm.leeds.ac.uk/MCMv3.3.1/parameters/photolysis.htm>).

2.7. Box vs 3-D model simulations – differences

A number of simplifications are made in the chemical schemes as used in boxChem as opposed to when used in the full EMEP CTM. In the boxChem simulations, the formation of sulfate, initiated by gas-phase oxidation of SO_2 by OH, is treated identically with all chemistry mechanisms in the box-model simulations presented in this study. The same OH-oxidation rate expression was used with all mechanisms (pressure and temperature dependent rate, as recommended by IUPAC 2017–11–01); see Table 3.1 and G.3. No aqueous phase oxidation of SO_2 is included in the boxChem simulations.

Ammonium chemistry is not included in the boxChem simulations presented here, and particulate nitrate formation is only included as simple first-order reactions for HNO_3 and N_2O_5 with the rate constants $k=6\times 10^{-6} \text{ s}^{-1}$ and $k=4\times 10^{-4} \text{ s}^{-1}$, respectively. The dummy

inorganic nitrate species is referred to as simply NITRATE in the box model tests to be presented in Sect. 3.

In the full 3-D model, the treatment of sulfate formation from aqueous and gas phase oxidation of SO₂, by O₃(aq), H₂O₂(aq), O₂(aq) and OH(g), is treated as in [Simpson et al. \(2012\)](#), which largely follows [Jonson et al. \(2000\)](#). The same treatment of sulfate is used for all chemistry schemes in the present study when used in the 3-D model — this means that the gas-phase oxidation of SO₂ in the CB6r2Em and CRIV2R5Em is not treated as in the original CB6 and CRI models. Heterogeneous reactions of N₂O₅, NO₃, HNO₃ and HO₂ are also treated in the same way with all gas phase chemistry schemes, based upon work presented in [Stadtler et al. \(2018\)](#). As discussed there, the reaction rate of a species *X* with aerosol of accumulation mode and larger can be approximated by the expression:

$$k_X = \frac{c_X \cdot \gamma_X}{4} S_a \quad (2.1)$$

where c_X is the mean molecular velocity of the species *X*, γ_X represents the reaction probability and S_a the surface area density of reacting aerosol. Table 2.1 (in conjunction with [Stadtler et al. 2018](#)) lists the reactions and γ values used in the EMEP model for these four species. As seen in Table 2.1, these surface-area based gas-aerosol reactions are only used for the production of coarse-mode nitrate (NO_{3,c}). For inorganic fine particulate nitrate (NH₄NO₃) and ammonium sulfate formation, the EMEP model uses the MARS, EQSAM or ISORROPIA equilibrium modules ([Binkowski and Shankar 1995](#), [Metzger and Lelieveld 2007](#), [Fountoukis and Nenes 2007](#)). To be consistent with older EMEP model versions very simple loss reactions are also included for H₂O₂ and CH₃OOH to represent heterogeneous losses in a crude way (both species are lost with a constant rate $k=1 \times 10^{-5} \text{ s}^{-1}$).

Table 2.1: Main aerosol-uptake reactions in EMEP model

Reaction	γ
N ₂ O ₅ $\longrightarrow$ 2 HNO ₃	‘Smix’ hydrolysis method
HNO ₃ + sea-salt _c $\longrightarrow$ NO _{3,c}	0.01
HNO ₃ + dust _c $\longrightarrow$ NO _{3,c}	0.1
HO ₂ + PM $\longrightarrow$ $\frac{1}{2}$ H ₂ O	0.2
NO ₃ + PM $\longrightarrow$ NO _{3,c}	0.001

Notes: Subscript *c* denotes coarse mode; PM denotes particulate matter. See [Simpson et al. \(2015\)](#), [Stadtler et al. \(2018\)](#) for more details.

3. Box model simulations

The different gas-phase chemistry schemes were compared and evaluated against the reference MCMv3.3Em mechanism in box-model simulations, performed using boxChem, the box model of the GenChem system (Simpson et al. 2020a). In order to simplify the comparison some parts of the set-up were harmonized — this included photolysis rates, which were calculated using solar zenith angle dependent parameterisations from MCM (Saunders et al. 2003) for all model schemes, and simplified handling of deposition and aerosol uptake losses (Ch. 2.7).

Here we present the final set of boxChem simulations, which used the box model conditions described in Table 3.1. For simplicity cloud free conditions were assumed and temperature, pressure, mixing height (used as box-height), and all emission rates (except those for isoprene) were kept constant during the 5-day long simulations. Isoprene emissions were only included during daytime (to roughly simulate biogenic emissions). No exchange with the surrounding atmosphere was included.

In the MCMv3.3Em simulations the VOC-emissions were split into 101 different model species as specified in Table B.1. The simplified VOC emission-splits used to represent the detailed MCM-split in the other chemistry schemes are given in Table B.2 (for EmChem19a, EmChem19X and CRIv2R5Em) and Table B.3 (for CB6r2Em). The distribution of the different VOC-species on the limited number of model VOCs in the EmChem schemes are partly based on estimated Photochemical Ozone Creation Potentials (POCP) from Derwent et al. (1998), Altenstedt and Pleijel (2000) and Jenkin et al. (2017). For CRIv2R5Em the VOC-split is based on the CRI v2-R5 reduced mechanism of Watson et al. (2008) (see Ch. 2.3). For CB6r2Em the split is mainly based on the surrogates used for CB05 by Yarwood et al. (2005) but extended with new surrogate species included in CB6.

Table 3.1: Box model set-up (for emissions, see Table 3.2)

Conditions		
Mixing height	1 km	
Pressure	760 torr	
Relative humidity	0.665	
Latitude	51.5°N	
Longitude	0.0	
Start date	21st June	
Start time	12:00	
Initial concentrations		
O ₃	33.0 ppb	
NO	0.4 ppb	
NO ₂	1.6 ppb	
CO	120 ppb	
CH ₄	1800 ppb	
M	2.463×10^{19} molecule cm ⁻³	
Deposition losses		
HNO ₃	2.0×10^{-5} s ⁻¹	
SO ₂	5.0×10^{-6} s ⁻¹	
NO ₂	1.5×10^{-6} s ⁻¹	
O ₃	5.0×10^{-6} s ⁻¹	
Sulfur chemistry and nitrate formation (aerosol uptake)		
SO ₂ + O(³ P) → SO ₃	$4.0 \times 10^{-32} \exp(-1000/T) \times [M]$	cm ³ molecule ⁻¹ s ⁻¹
SO ₂ + OH → HSO ₃	KMT12box	See Table G.3
HSO ₃ + O ₂ → SO ₃ + HO ₂	$1.3 \times 10^{-12} \exp(-330/T)$	cm ³ molecule ⁻¹ s ⁻¹
SO ₃ → sulfate	$1.2 \times 10^{-15} \times [\text{H}_2\text{O}]$ s ⁻¹	
HNO ₃ → nitrate	6.0×10^{-6} s ⁻¹	
N ₂ O ₅ → 2 nitrate	4.0×10^{-4} s ⁻¹	

A number of different emission variations were tested to investigate model responses to different NO_x-to-VOC concentrations and to different amounts of isoprene. In addition to a base-case, which features emissions of NO_x, anthropogenic VOC (AVOC) and biogenic VOC (isoprene, C₅H₈) we have combined low-NO_x (LNO_x), zero-biogenic (ZBio) and high-biogenic (HBio) emissions scenarios as summarised in Table 3.2.

Table 3.2: Box model emissions set-up (units: g km⁻² s⁻¹).

Run	NO _x	AVOC	C5H8	SO ₂	CO	NO _x / ΣVOC ^(a)	C5H8/ ΣVOC
Base	0.218	0.173	0.0343	0.147	0.486	1.05–1.26	0.17
BNO _x ZBio	b	b	0.0	b	b	b	0.0
BNO _x HBio	b	b	0.343	b	b	0.42–1.26	1.65
LNO _x ZBio	0.0218	b	0.0	b	b	b	0.0
LNO _x HBio	0.0218	b	0.343	b	b	0.042–0.126	b

Notes: (a) ΣVOC is the sum of isoprene (C5H8) and AVOC, and range in ratios (where given) gives day–night values. (b) as base-case

Here we show results from the simulations using the base case set-up, with emissions loosely based on estimated average emission rates for anthropogenic NO_x and VOC emissions, and biogenic isoprene emissions representative for the UK during the early 2000s. Anthropogenic emissions are similar to those used by Jenkin et al. (2008, 2017) and Watson et al. (2008). Biogenic emission amounts were also similar to those used by Jenkin et al. (2008) and Watson et al. (2008), but here we treat all biogenic emissions as isoprene. Simulations were performed with different temperatures — here we show results at 278K, 288K and 298K.

The main focus of the comparison is on concentrations of ozone, OH, NO₃-radicals and NO_x, but many other species were also compared and some additional plots are included in Appendix B. Time-series plots with results from the various emission scenarios (Table 3.2) are also shown in Appendix B. It should be noted that such 5-day simulations tend to exaggerate the differences in the chemical schemes compared to differences seen in 3-D simulations, but such comparisons are valuable in comparing and developing the gas-phase mechanisms.

3.1. Box model results — time-series plots

The base case simulation results are illustrated in Fig. 3.1 (and Fig. C.1). At 298 K there is a steady daytime ozone formation, with increasing O₃ levels for each day from about 40 ppb the first day to more than 90 ppb the fifth day (Fig. 3.1). Night-time NO₃ levels also increase from about 30 ppt the first night to peak values of about 90 ppt the last night. All five model schemes give similar results at 298K but the CB6r2Em produces somewhat less O₃ and NO_x (and more HNO₃, Fig. C.1) after the first day. Although the results with the different mechanisms are closer at the higher temperatures the CB6r2Em gives lower ozone and OH concentrations even at the highest temperatures (up to 303 K).

At the lower temperatures the concentrations develop in more complicated ways and the differences between the five model schemes are much larger, at least after the first 24 hours of simulation. CB6r2Em gives lower O₃ than the other schemes. OH and NO₃ are also

lowest in the CB6r2Em simulations. The other mechanisms overestimate OH (compared to MCMv3.3Em).

NO_x-concentrations are highest with CB6r2Em at 278 K, but at 298 K this scheme gives the lowest concentrations; the other schemes are relatively close to the MCMv3.3Em results, but (especially the EmChem19 schemes) tend to underestimate NO_x; this NO_x-underestimation at the lower temperatures is possibly connected to some overestimation of the OH radical concentrations, leading to slightly larger HNO₃ formation (Fig. C.1).

The differences between EmChem19a and EmChem19X are relatively small for the four components in Fig. 3.1 but large for night-time organic peroxy radical concentrations, which are much lower in EmChem19a (Fig. C.1) due to the simplified treatment of some NO₃ reactions in the smaller EmChem19a mechanism.

The CB6r2Em behaves differently than the other mechanisms for the peroxy radicals (Fig. C.1). The temperature dependence of the simulated concentrations of both HO₂ and total organic peroxy radicals (RO₂+RCO₃) is stronger in CB6r2Em. At low temperatures (273–283 K) the daytime total peroxy radical concentration in CB6r2Em becomes much lower than with the other schemes after one–two days of simulation — at high temperatures (298–303 K) CB6r2Em produces the highest total peroxy radical concentrations (both during day and night time).

Results from the BNOxZBio case (with zero isoprene, c.f. Table 3.2) are shown in Fig. C.2. This case leads to less ozone formation and lower NO₃ radical concentrations, especially at the lowest temperature simulation, but the differences between the different model schemes are similar to the base case, with CB6r2Em producing less ozone than the other mechanisms. The agreement between CRIV2R5Em and MCMv3.3Em tends to be slightly worse for O₃, NO₃ and NO_x at the lower temperatures in this purely “anthropogenic” emission case, but the agreement for OH (Fig. C.2) and HNO₃ is excellent. The EmChem19 schemes are relatively close to MCMv3.3Em for O₃ and NO₃ but tend to overestimate OH and underestimate NO_x at the mid-temperature 288 K.

Results from the BNOxHBio case (with high isoprene, c.f. Table 3.2) are shown in Fig. C.3. In these runs, the ozone formation is substantial with all model versions, even at 278 K. EmChem19X and CRIV2R5Em are both close to MCMv3.3Em but with slightly higher NO₃ concentrations for CRIV2R5Em at the higher temperatures. EmChem19a deviates slightly more, with somewhat lower O₃ and higher OH and NO₃ concentrations, but the agreement is still fairly good. As for the other cases, CB6r2Em produce less ozone and OH than the other schemes, and the differences to the other mechanisms are larger at 298 K than for the base case simulation, but smaller at 278 K. The CB6r2Em simulates clearly higher HNO₃ concentrations (except during the first day and daytime at high temperatures). For CB6r2Em the high HNO₃ concentration is primarily due to formation from organic nitrates, which is very different from the other mechanisms. A large fraction of the organic nitrates in CB6r2Em are considered as being particle phase nitrates (or are transformed into this form after oxidation) and this particle organic nitrate is an important sink for reactive nitrogen in CB6r2Em—its only loss reaction is conversion to nitric acid HNO₃. The EmChem19a mechanism also produces somewhat more HNO₃ than the MCMv3.3Em at 278 K and 288 K; in this case it seems to be due to the higher OH-concentrations formed in the EmChem19a simulations than with the other mechanisms.

Results from the LNOxZBio case (low NO_x, zero isoprene, c.f. Table 3.2) are shown in Fig. C.4. For this case, O₃ concentrations are very similar in MCMv3.3Em, CRIV2R5Em and EmChem19X at all three temperatures. EmChem19a is also fairly close, but with a slight

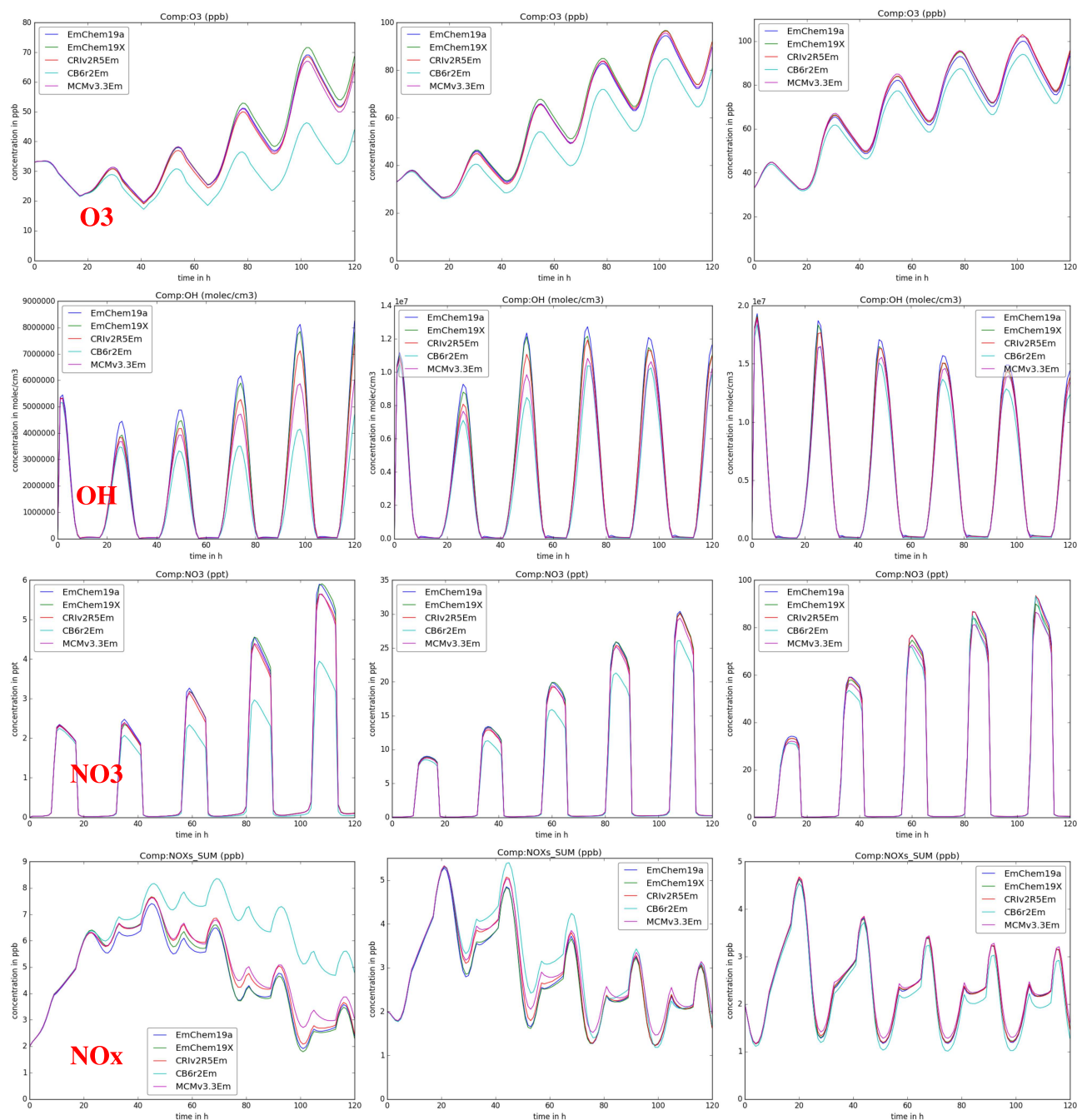


Figure 3.1: Model simulated O_3 , OH , NO_3 and NO_x at $T=278K$ (left), $288K$ (middle), and $298K$ (right). Base case model set-up

tendency to overestimate O_3 at the lower temperatures. $CB6r2Em$, however, gives clearly lower O_3 than the other four schemes at all temperatures. $EmChem19a$ has a tendency to overestimate the OH and NO_3 radical concentrations at all temperatures, while $EmChem19X$ and $CRIV2R5Em$ are closer to the $MCMv3.3Em$ levels; the $CB6r2Em$ scheme produce OH and NO_3 that are mostly in quite good agreement with $MCMv3.3Em$ but OH is lower at $298K$ and less NO_3 is produced for the nights 3–5 at the lower temperatures.

Results from the LNO_xHBio case (low NO_x , high isoprene, c.f. Table 3.2) are shown in Fig. C.5. This scenario also leads to relatively slow ozone formation, and OH and NO_3

radical levels are low. EmChem19X is in very good agreement with MCMv3.3Em for O_3 , OH, NO_3 and NO_x , while EmChem19a gives slightly more O_3 at 278 K and less at 298 K, and clearly higher NO_3 concentrations than MCMv3.3Em. CRIv2R5Em deviates somewhat more from MCMv3.3Em for this low- NO_x case than the previous case and produce a bit higher concentrations of O_3 , OH and NO_3 than EmChem19X. CB6r2Em gives substantially lower concentrations than the other schemes for these species, especially at the higher temperatures; at 298K the ozone concentration is about 25 ppb lower at the end of the 120 h simulation with CB6r2Em than with MCMv3.3Em; OH and NO_x concentrations are roughly a factor of two lower, and the peak NO_3 concentration on the last night of the simulation is about 1/7th of the MCMv3.3Em level.

For this case isoprene concentrations are significant also at night (Fig. C.6). RO_2 concentrations reach ~ 10 – 30 ppt at night with all model schemes except EmChem19a, which, due to its limitations in the night-time chemistry, does not produce as much RO_2 during night as the other mechanisms (Fig. C.5).

In order to summarise these results further, Table 3.3 provides the mean concentrations for some key species from day 3 of the T=298 K runs. Day 3 was chosen as a period where differences between mechanisms are significant, but before the box-model results become too far removed from those expected in CTM simulations. The T=298 K choice was simply to reflect the meteorology most associated with high ozone formation conditions. In general Table 3.3 confirms that the different mechanisms track MCM results to a reasonable degree (often within a few percent) for many species, but the level of agreement varies significantly from scenario to scenario. For example, EmChem19a captures mean day 3 OH to within 5% of MCM on the high ozone scenario BNO_xHBio, but shows one of the biggest discrepancies (26%) for OH in the low ozone LNO_xZBio case.

In general the CB6r2Em mechanism tends to deviate most from the MCMv3.3Em for several of the species investigated in the box model simulations. Ozone levels are lower with CB6r2Em and, at least for the box model scenarios with isoprene emissions and/or small NO_x emissions, the simulated levels of NO_x tends to be lower and HNO_3 higher with CB6r2Em. Clearly the CB6r2Em loses substantially more NO_x than the other mechanisms (especially under low- NO_x conditions), due to the formation of organic nitrates, and this leads to a much smaller ozone formation potential and less OH formation. This difference is not too surprising given that the EmChem19 and CRI schemes all derive from MCM-schemes to varying extents, whereas the CB6 mechanisms are created from quite different procedures and tested in very different environments (with e.g. a greater emphasis on comparisons with smog-chambers). Some of the differences in results may also stem from assumptions concerning emission surrogate choices and VOC mapping criteria and methods. Indeed, we can note that Kuhn et al. 1998 found significant discrepancies in concentrations from different modelling groups which claimed to run the same versions of an earlier carbon-bond scheme (CBM-IV). We can thus not claim that the MCM mechanism is more accurate than CB6, but rather both mechanisms have advantages and dis-advantages, and the differences between them reflect uncertainties in the underlying gas-phase chemistry and organic nitrate partitioning between gas and particle phase.

Table 3.3: Comparison of mean concentrations for day 3 of box-model simulations, for T=298 K

Poll	chem	unit	Base	BNOxHBio	BNOxZBio	LNOxHBio	LNOxZBio
O3	MCMv3.3Em	(ppb)	74.99	106.08	69.40	51.15	39.30
	CRIV2R5Em	(%)	-0.9	-0.4	-1.2	5.0	-0.2
	EmChem19a	(%)	-3.2	-4.9	-2.7	-5.1	0.4
	EmChem19X	(%)	-1.1	-1.1	-0.8	-0.3	-1.8
	CB6r2Em	(%)	-8.5	-13.9	-6.9	-26.9	-14.7
OH	MCMv3.3Em	(ppt)	0.21	0.19	0.21	0.05	0.08
	CRIV2R5Em	(%)	5.1	3.5	5.7	21.5	15.6
	EmChem19a	(%)	9.2	5.2	10.3	9.9	25.9
	EmChem19X	(%)	5.9	3.2	7.1	-0.6	8.1
	CB6r2Em	(%)	-5.6	-17.3	-3.2	-41.2	-11.9
HO2	MCMv3.3Em	(ppt)	10.13	17.63	8.64	16.60	9.99
	CRIV2R5Em	(%)	7.4	2.9	8.6	6.7	14.0
	EmChem19a	(%)	8.6	3.5	10.0	7.8	18.4
	EmChem19X	(%)	9.6	4.3	12.1	-0.0	5.2
	CB6r2Em	(%)	-2.3	-11.4	2.6	-6.1	7.7
NOx	MCMv3.3Em	(ppb)	2.23	2.13	2.32	0.48	0.46
	CRIV2R5Em	(%)	-2.8	-2.1	-2.7	2.2	-4.8
	EmChem19a	(%)	-3.5	-2.5	-4.3	-4.7	-5.4
	EmChem19X	(%)	-3.2	-1.3	-4.0	-0.0	-1.1
	CB6r2Em	(%)	-10.1	-17.3	-9.9	-37.1	-30.7
HNO3	MCMv3.3Em	(ppb)	3.21	3.05	3.24	0.19	0.27
	CRIV2R5Em	(%)	-0.4	-1.2	0.3	26.6	10.1
	EmChem19a	(%)	0.3	-3.4	0.7	-4.9	10.8
	EmChem19X	(%)	0.0	0.3	-0.1	1.5	4.0
	CB6r2Em	(%)	3.4	7.6	3.3	86.2	21.7
H2O2	MCMv3.3Em	(ppb)	1.65	5.05	1.20	7.14	2.75
	CRIV2R5Em	(%)	13.8	7.6	14.2	9.0	19.5
	EmChem19a	(%)	13.2	0.2	18.6	-0.6	26.3
	EmChem19X	(%)	17.6	6.7	23.6	-0.4	7.8
	CB6r2Em	(%)	4.4	-12.0	14.2	-8.3	23.2
Σ RO2	MCMv3.3Em	(ppt)	6.81	15.99	5.52	25.60	10.77
	CRIV2R5Em	(%)	-0.2	-0.2	-1.6	-5.8	-10.4
	EmChem19a	(%)	-14.6	-23.8	-12.5	-27.0	-23.7
	EmChem19X	(%)	-2.0	-3.1	-2.7	-4.2	-7.8
	CB6r2Em	(%)	33.8	45.8	24.0	18.7	0.5
Σ XO2	MCMv3.3Em	(ppt)	16.94	33.62	14.16	42.22	20.76
	CRIV2R5Em	(%)	4.4	1.4	4.6	-0.9	1.3
	EmChem19a	(%)	-0.7	-9.4	1.2	-13.4	-3.4
	EmChem19X	(%)	5.0	0.8	6.3	-2.6	-1.5
	CB6r2Em	(%)	12.2	15.8	10.9	8.9	4.0
HCHO	MCMv3.3Em	(ppb)	2.13	4.42	1.91	4.71	1.54
	CRIV2R5Em	(%)	0.1	-2.9	0.6	-5.8	-1.6
	EmChem19a	(%)	-0.7	-3.4	-0.7	-7.5	0.9
	EmChem19X	(%)	5.0	5.9	4.6	9.0	4.7
	CB6r2Em	(%)	-18.8	-20.9	-18.3	-27.8	-24.2
PAN	MCMv3.3Em	(ppb)	0.41	1.28	0.33	0.40	0.11
	CRIV2R5Em	(%)	41.0	14.9	48.2	13.1	38.1
	EmChem19a	(%)	26.3	3.9	31.9	0.8	37.2
	EmChem19X	(%)	31.3	12.3	36.6	7.2	25.1
	CB6r2Em	(%)	31.6	2.8	39.7	-34.8	8.6
Σ PANs	MCMv3.3Em	(ppb)	0.69	1.98	0.56	0.64	0.20
	CRIV2R5Em	(%)	-7.7	-11.4	-7.7	-15.2	-19.8
	EmChem19a	(%)	-22.8	-27.0	-22.4	-28.1	-26.9
	EmChem19X	(%)	-10.8	-7.1	-12.6	-8.1	-24.3
	CB6r2Em	(%)	2.4	-13.8	6.2	-36.7	-18.8
NITRATE	MCMv3.3Em	(μg m⁻³)	20.97	18.12	21.39	1.30	2.40
	CRIV2R5Em	(%)	2.1	5.2	1.2	9.0	5.7
	EmChem19a	(%)	3.4	10.9	2.9	2.7	17.0
	EmChem19X	(%)	1.4	0.9	1.6	0.9	7.5
	CB6r2Em	(%)	-3.8	-2.9	-4.8	26.3	3.3

Notes: MCM values (in bold font) given as concentrations, in ppb, ppt, or $\mu\text{g m}^{-3}$ as noted. Values for other chemical mechanisms give deviation from MCM values, as %. ΣRO2 is sum of RO2 and RCO2 species; ΣXO2 is sum of HO_2 + ΣRO2 ; ΣPANs is sum of all PAN-like species; NITRATE is a dummy inorganic nitrate species used for boxChem, see Sect. 2.7.

4. European scale model simulations

Model performance for Europe is of crucial importance for the EMEP model, due to the use of the model for policy applications within the UN-ECE Air Convention (www.unece.org/env/lrtap/welcome.html), and for real-time air pollution forecasts for Europe within the Copernicus Atmosphere Monitoring Service (CAMS; <https://atmosphere.copernicus.eu/>). In this analysis of the European scale model results (Ch. 4) we compare model results with EmChem19a, EmChem19X, CRIv2R5Em and CB6r2Em for ozone and the important radicals OH, NO₃, HO₂ and organic peroxy radicals RO₂. We evaluate the model results for ozone and nitrogen and sulfur containing species against measurements from the EMEP monitoring network in a similar way as the standard policy model is regularly evaluated (Ch. 4.3).

Model simulations were performed for an area covering Europe and the neighboring regions of Asia — the so called EECCA domain (e.g. Introduction, [Fagerli et al. 2015](#)), which in addition to Europe also includes the countries in the EECCA (Eastern European, Caucasus and Central Asia) block (for the Russian Federation the easternmost part of the country is not included).

Current EMEP calculations typically use a $0.1^\circ \times 0.1^\circ$ degree grid for European calculations (e.g. [Fagerli et al. 2020](#)), but the calculations performed here used an older polar-stereographic projection with a grid resolution of $50\text{km} \times 50\text{km}$ resolution at latitude 60°N . The grid has 132×159 points in the horizontal, and 20 vertical levels; the lowest level is about 90 m thick. Meteorological data were taken from the IFS model of ECMWF (IFSv40r1). The convective transport scheme available in the EMEP CTM was not used in the European scale simulations. Convection is neglected for pragmatic reasons; model results for simulations over the EECCA domain have been found to be somewhat worse with convection than without ([Simpson et al. 2012](#)).

Anthropogenic emission data for the European scale simulations were based upon an updated version of emissions described by [Kuenen et al. \(2014\)](#), including condensable organics in residential wood burning PM emissions (similar to [Denier van der Gon et al. 2015](#)). Biogenic emissions of isoprene and monoterpenes, as well as soil NO emissions and open biomass fire emissions, were set as described in [Simpson et al. \(2012\)](#). Boundary and initial concentrations (BIC) for ozone are based on climatological data from [Logan \(1998\)](#). For a number of other relatively long-lived components the BIC are set using simple prescribed functions of the day of the year and altitude, as described in [Simpson et al. \(2012, 2015\)](#) except that the background CH₄ concentration was updated to 1870 ppb.

It should be noted that there are numerous factors which control the differences in ozone,

OH, and other compounds in air quality simulations, including differences in reaction choices, pathways, and rates. Some of these factors are discussed further in Ch. 6. In this chapter (and Ch. 5 on global modelling) we do not attempt to compare all compounds, or explain differences, but rather illustrate the impact of the chemical mechanisms on some commonly produced outputs from the EMEP model.

4.1. Ozone and OH concentrations

Model simulated annual mean ozone concentrations from CRIv2R5Em are shown in Fig. 4.1(a), with differences from CRIv2R5Em shown in Fig. 4.1(b)–(d). These mean concentrations are somewhat higher with the EmChem19 schemes than with CRIv2R5Em — for most of Europe the difference is between 0.1–0.5 ppb(v). Consistent with the boxChem studies of Ch. 3, the CB6r2Em scheme gives clearly lower ozone concentrations than with CRIv2R5Em (Fig. 4.1(d)). The differences are largest over the Mediterranean Sea where the CB6r2Em simulation gives more than 2 ppb(v) lower annual mean O₃ than CRIv2R5Em.

Model simulated annual mean OH concentrations are shown in Fig. 4.2(a), with differences from CRIv2R5Em shown in Fig. 4.2(b)–(d). The EmChem19 schemes produce higher OH concentrations than the CRIv2R5Em and CB6r2Em schemes in most of the model domain, especially in regions with large monoterpene emissions; the relative differences are largest in the northern parts of Europe and in some other areas with especially large MT emissions. As discussed further in Ch. 6 the reason for the higher OH concentrations with Emchem19 in the regions with MT emissions is that these schemes produce a lot more HO₂ radicals from the MT chemistry. This leads to enhanced OH production mainly via the HO₂+OH and HO₂+O₃ reactions. However, EmChem19a gives lower OH concentrations than CRIv2R5Em in some urban areas (e.g. Athens, Baku, Istanbul, Milan and Moscow).

CB6r2Em produces lower OH concentrations than CRIv2R5Em. The largest relative differences are found in (urban) regions with large anthropogenic emissions and in northern areas with relatively large monoterpene emissions. The lower modelled OH concentrations with CB6r2Em are to a small extent due to differences in reaction rates for some pressure dependent inorganic reactions involving NO_x, but other factors are more important, as discussed in Ch. 6.

4.2. Ozone metrics

The large interest in ozone, due to its impacts on human health, damage to crops and other vegetation, and climate (in addition to its importance in atmospheric photochemistry), has led to a plethora of ozone indices being used for different purposes. In Table 4.1 EMEP model results are compared to measurements for eight different ozone metrics; three of these include data from the whole year: daily mean and daily maximum (hourly) concentrations, and the SOMO35 metrics; the other five metrics cover the summer half-year (Apr–Sep; M7, M12, MDA8, AOT40) or the growing season (W126). For O₃ concentrations the comparisons are

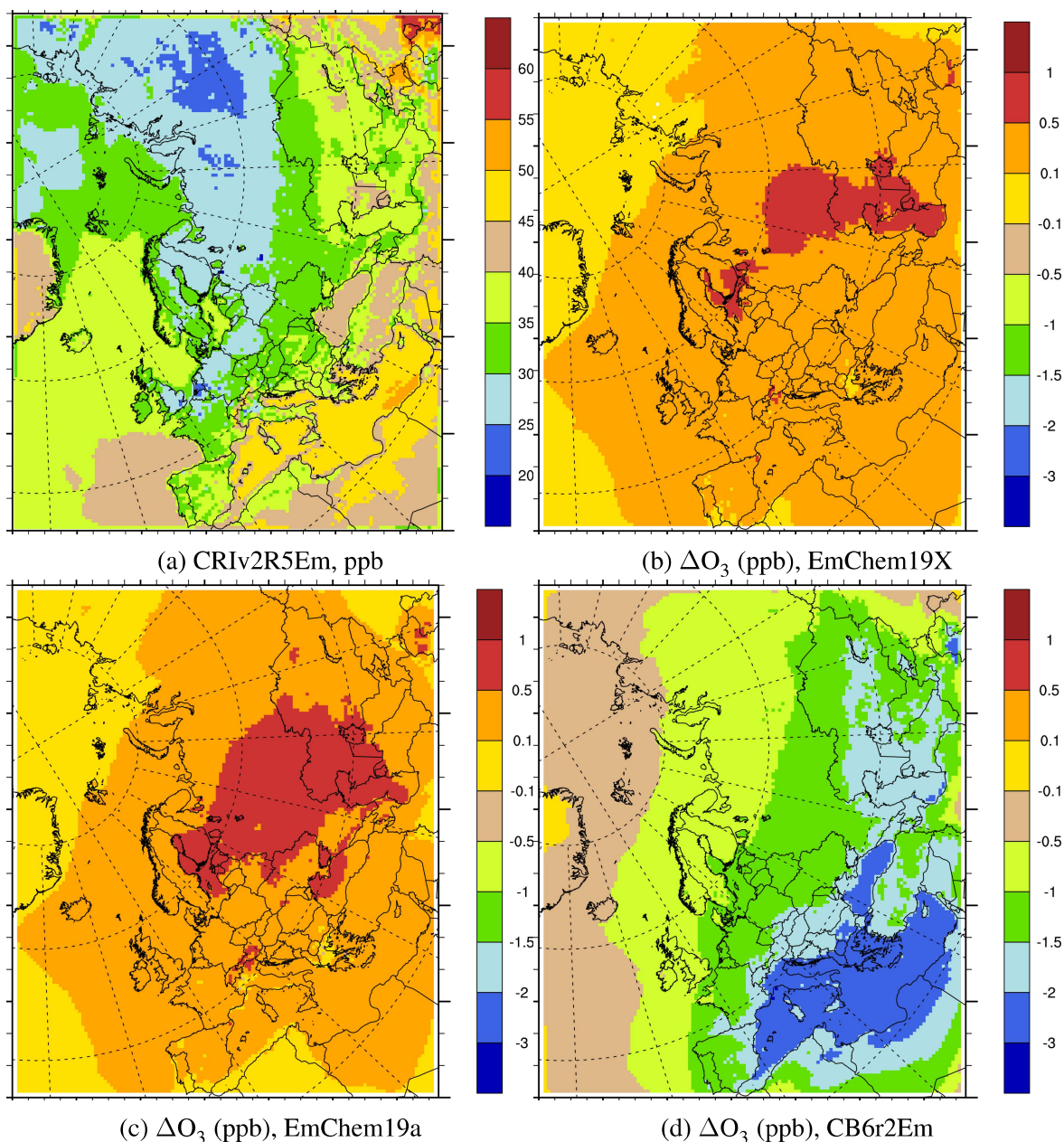


Figure 4.1: (a) Model simulated annual mean surface level O_3 concentrations for 2011 with CRIv2R5Em, and (b)–(d) differences to the CRIv2R5Em results from EmChem19X, EmChem19a, and CB6r2Em. (positive values indicating higher concentrations than CRIv2R5Em and negative lower). Unit: ppb(v)

based on hourly concentrations and 95 measurement sites were available and had sufficient data coverage to be included. All comparisons are based on only the hours for which measurements are available.

In general the simulations using the EmChem19a and EmChem19X schemes give very similar results for the ozone metrics in these model runs. CB6r2Em clearly gives lower ozone concentrations and with CRIv2R5Em the results are in between those of EmChem19 and CB6r2Em (but much closer to EmChem19 than to CB6r2Em). On average, the full-year daily mean ozone concentrations are overestimated with all chemistry schemes and CB6r2Em is closest to the measured mean. The mean of daily maximum ozone is underestimated with

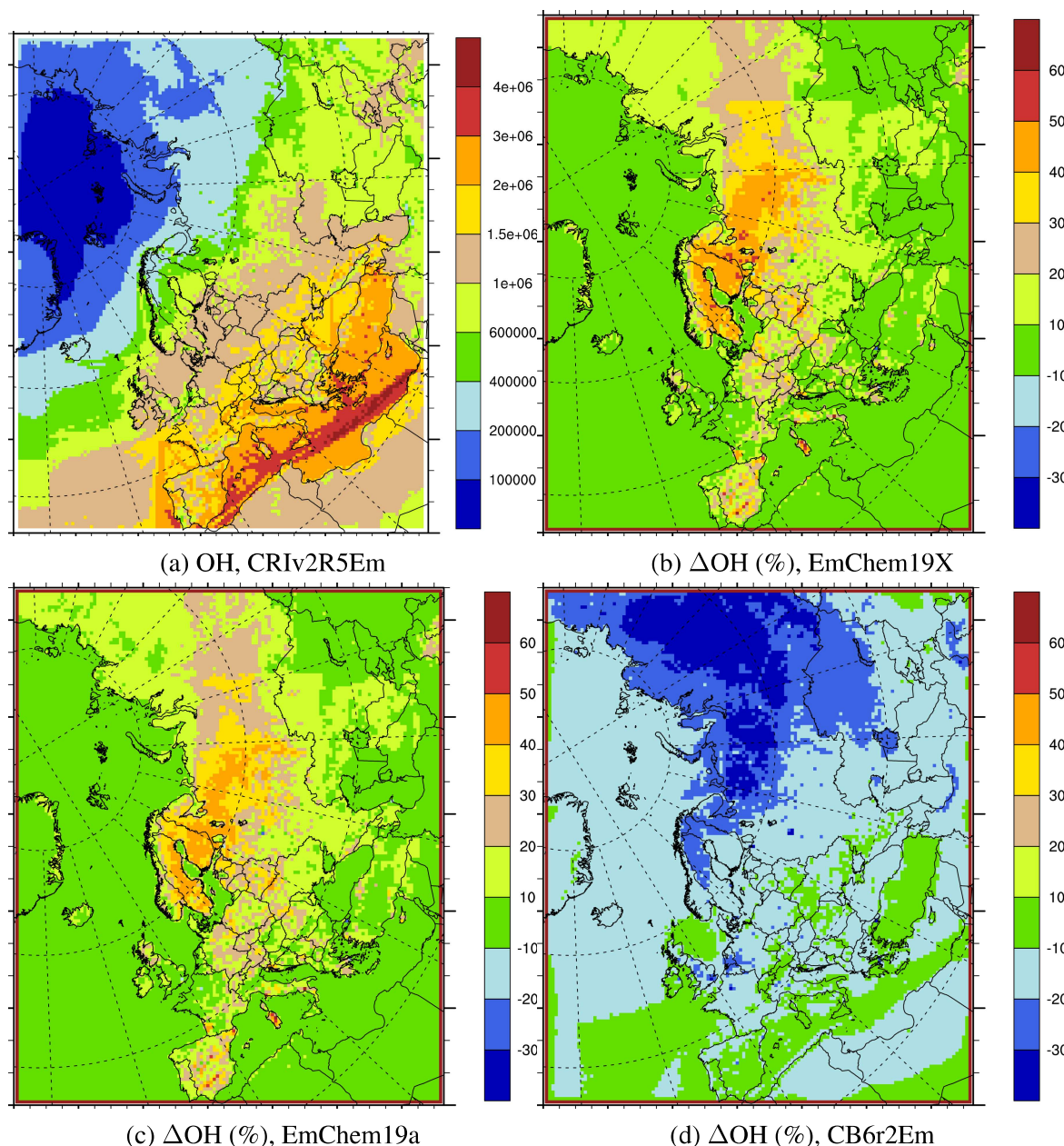


Figure 4.2: As Fig. 4.1 but for (a) OH concentrations (molec./cm³), and (b)–(d) gives relative changes (%) from the CRIv2R5Em case

all schemes but the EmChem19 schemes are relatively close to the measured level. For the 6-month M7 and M12 concentrations, CRIv2R5Em is closest to the measurements, while the EmChem19 schemes overestimate more, and CB6r2Em underestimates. The EmChem19 schemes and CRIv2R5Em are in good agreement with the measured level for the more complicated MDA8 metrics; CB6r2Em underestimates it by, on average, 2.6 ppb. The three accumulated ozone (exposure-related) metrics, SOMO35, AOT40 and W126, are underestimated with all schemes; SOMO35 by 9% with EmChem19, 13% with CRIv2R5Em and 32% with CB6r2Em; AOT40 by 22%(EmChem19), 26%(CRIv2R5Em) and 53%(CB6r2Em); W126 by 34%(EmChem19), 37%(CRIv2R5Em) and 56%(CB6r2Em). The W126 metric is clearly the most difficult to reproduce for the model — the correlation between the modelled and

Table 4.1: Regional background ozone concentrations in Europe, comparing EMEP chemical transport model results to measurements at European monitoring sites (at altitudes below 600 m a.s.l.). Units — Dmean, Dmax, M7, M12 and MDA8: ppb(v); SOMO35: ppb(v) days; AOT40 and W126 ppm(v) hours. Values in parenthesis are correlation coefficients (r) between the observed and model levels at the individual sites (“spatial” correlation coefficients). Results for selected measurement sites (including temporal correlation coefficients) are given in the Supplement (Tables E.1–E.3).

Ozone metric	# sites	Measured	EmChem19a	EmChem19X	CRIv2R5Em	CB6r2Em
Dmean	95	29.61	32.36 (0.720)	32.35 (0.718)	32.07 (0.715)	30.89 (0.724)
Dmax	95	39.22	38.56 (0.781)	38.56 (0.779)	38.23 (0.774)	36.77 (0.757)
M7 ^{a†}	87	38.07	39.32 (0.812)	39.34 (0.812)	38.84 (0.812)	36.76 (0.807)
M12 ^{b†}	87	37.65	39.06 (0.788)	39.07 (0.787)	38.57 (0.787)	36.49 (0.777)
MDA8 ^{c†‡}	85	41.56	41.68 (0.809)	41.71 (0.807)	41.21 (0.807)	38.97 (0.789)
SOMO35 ^{d†‡}	77	2041	1860 (0.785)	1863 (0.783)	1785 (0.778)	1397 (0.750)
AOT40 ^{e†}	86	8.57	6.65 (0.757)	6.72 (0.755)	6.32 (0.747)	4.01 (0.697)
W126 ^{f†}	83	5.45	3.58 (0.531)	3.61 (0.525)	3.43 (0.511)	2.42 (0.473)

Notes: ^a M7 is the 6-month mean (Apr.–Sep.) day time 7-h (09:00–16:00) ozone concentration (Heck et al. 1984); ^b M12 is the 6-month mean (Apr.–Sep.) day time 12-h (08:00–20:00) ozone concentration; ^c MDA8 is the 6-month (Apr.–Sep.) mean of the daily maximum 8-h moving average ozone concentration; ^d SOMO35 is the accumulated (yearly) sum of the daily maximum 8-hour moving average over 35 ppb; ^e AOT40 is the 6-month (Apr.–Sep.) accumulated amount of (hourly) ozone over the threshold value of 40 ppb during the hours 08:00–20:00; ^f W126 is a sigmoidal-weighted cumulative ozone exposure index (Lefohn et al. 1988); here calculated, as suggested by the U.S. EPA, as the maximum 3-month accumulated 12-h (08:00–20:00) W126 during March–October; note that this could be different 3-month periods for the model and measurements; [†] Only sites with > 50% data coverage for all months (Apr.–Sep., except W126:Mar.–Oct.) are included; [‡] All days with any 8-h averaging period containing more than two missing measurements are excluded.

measurement-derived W126 levels is rather mediocre (regardless of which chemistry scheme is used). Although not shown here, the two older EmChem schemes (EmChem09 and EmChem16) gave similar results to the EmChem19 schemes, but somewhat worse agreement with the measurements (except for the daily mean concentrations, which were slightly better with EmChem09).

4.3. Sulphur and nitrogen species

The modelled concentrations of sulphur and nitrogen compounds were evaluated against measurements done in 2011 within the EMEP monitoring network, using the same methods as for the standard evaluation of regular EMEP MSC-W model runs, published each year in the EMEP Status Reports (https://www.emep.int/mscw/mscw_publications.html). Table 4.2 gives the average model bias for the annual mean concentrations (relative to the measured concentrations) and the correlation (r) between observation and model for station yearly averages (thus showing the overall “spatial” correlation and not the temporal correlation between the model and measurements). The index of agreement (IOA) is also based on the yearly average concentrations. The differences in both bias and correlation coefficient are seen to be very small. The two EmChem19 schemes give almost identical statistics

in this evaluation and the CRIv2R5Em gives similar results (slightly more NO_x and less nitrates, and slightly less SO₄²⁻). CB6r2Em produces higher NO concentrations and slightly more SO₂ and less SO₄²⁻.

One reason for the similar statistics is that for sulphur, NO_x and NH_x components the spatial correlation of emissions and hence concentrations is strongly dependent on the emissions distribution across the model domain, and this is common to all mechanisms. Further, the treatment of sulphur components is essentially identical with all four mechanisms (in the EMEP versions) and the inorganic nitrogen chemistry was harmonized between the CRIv2R5Em and EmChem19 schemes (but not with CB6r2Em).

Table 4.2: Comparison of S and N gaseous and particulate components from the EECCA domain simulations. Table shows annual mean EMEP CTM results compared to measurements at sites in the EMEP monitoring network. Ns = number of sites; bias = mean deviation of the modelled concentration from the measured (in % of the measured concentration); corr. = “spatial” correlation coefficient (correlation between the modelled and measured yearly mean concentrations for the sites); IOA = index of agreement of spatial variations (Willmott 1981, 1982).

NO	Ns	bias	corr.(r)	IOA	SO₂	Ns	bias	corr.(r)	IOA
EmChem19a	34	-47%	0.83	0.80	EmChem19a	60	-15%	0.53	0.52
EmChem19X	34	-47%	0.83	0.80	EmChem19X	60	-15%	0.53	0.52
CRIV2R5Em	34	-47%	0.83	0.80	CRIV2R5Em	60	-15%	0.53	0.52
CB6r2Em	34	-44%	0.83	0.82	CB6r2Em	60	-14%	0.54	0.52
EmChem16	34	-49%	0.82	0.78	EmChem16	60	-16%	0.53	0.51
EmChem09	34	-45%	0.82	0.81	EmChem09	60	-14%	0.53	0.52
NO₂	Ns	bias	corr.(r)	IOA	SO₄²⁻	Ns	bias	corr.(r)	IOA
EmChem19a	71	-14%	0.83	0.90	EmChem19a	38	-36%	0.92	0.80
EmChem19X	71	-14%	0.83	0.90	EmChem19X	38	-37%	0.92	0.80
CRIV2R5Em	71	-14%	0.83	0.90	CRIV2R5Em	38	-37%	0.93	0.79
CB6r2Em	71	-14%	0.83	0.90	CB6r2Em	38	-39%	0.93	0.77
EmChem16	71	-18%	0.83	0.89	EmChem16	38	-35%	0.92	0.81
EmChem09	71	-14%	0.83	0.90	EmChem09	38	-38%	0.93	0.78
HNO₃+NO₃⁻	Ns	bias	corr.(r)	IOA	NH₃+NH₄⁺	Ns	bias	corr.(r)	IOA
EmChem19a	33	-6%	0.84	0.90	EmChem19a	33	4%	0.89	0.93
EmChem19X	33	-8%	0.84	0.90	EmChem19X	33	4%	0.89	0.93
CRIV2R5Em	33	-9%	0.84	0.89	CRIV2R5Em	33	4%	0.89	0.92
CB6r2Em	33	-7%	0.84	0.90	CB6r2Em	33	4%	0.89	0.92
EmChem16	33	-7%	0.84	0.90	EmChem16	33	4%	0.89	0.93
EmChem09	33	6%	0.86	0.92	EmChem09	33	6%	0.89	0.92
HNO₃	Ns	bias	corr.(r)	IOA	NH₃	Ns	bias	corr.(r)	IOA
EmChem19a	9	-50%	0.55	0.57	EmChem19a	8	44%	0.85	0.79
EmChem19X	9	-51%	0.56	0.56	EmChem19X	8	45%	0.86	0.79
CRIV2R5Em	9	-52%	0.56	0.56	CRIV2R5Em	8	47%	0.85	0.78
CB6r2Em	9	-50%	0.55	0.56	CB6r2Em	8	48%	0.86	0.78
EmChem16	9	-50%	0.56	0.57	EmChem16	8	44%	0.85	0.79
EmChem09	9	-46%	0.54	0.57	EmChem09	8	42%	0.86	0.80
NO₃⁻	Ns	bias	corr.(r)	IOA	NH₄⁺	Ns	bias	corr.(r)	IOA
EmChem19a	15	3%	0.98	0.99	EmChem19a	22	-14%	0.87	0.91
EmChem19X	15	1%	0.98	0.99	EmChem19X	22	-14%	0.87	0.91
CRIV2R5Em	15	1%	0.98	0.99	CRIV2R5Em	22	-15%	0.87	0.91
CB6r2Em	15	-1%	0.97	0.98	CB6r2Em	22	-17%	0.88	0.90
EmChem16	15	3%	0.98	0.99	EmChem16	22	-13%	0.87	0.92
EmChem09	15	18%	0.96	0.95	EmChem09	22	-7%	0.87	0.93

5. Global scale model simulations

5.1. Comparison of mechanisms

The EMEP model is also widely used at the global scale, for example as part of the work of the Task Force on Hemispheric Transport Air Pollution (e.g. [Jonson et al. 2018](#), [Tan et al. 2018](#)) or for studies of global crop damage due to ozone ([Mills et al. 2018a,b](#)). In this section we focus on a broader comparison of the different model schemes at the global scale, including more species and investigate how the results differ between various types of regions, with widely different emissions and climates. Comparisons to measured ozone concentrations at remote and regional background sites from the GAW network ([Schultz et al. 2015](#)) are also included (Ch. 5.2).

The EMEP model was run on the global scale with the four main chemical schemes, and also two modified schemes for sensitivity tests (CRIwMT19X, CB6wInorgCRI; see Ch. 6). A $1^\circ \times 1^\circ$ horizontal resolution was used, with 20 vertical levels (the lowest level being ca 90 m thick). The global simulations were performed for one year (2012). The setup of the model was essentially identical to that used in [Stadtler et al. \(2018\)](#) and [Mills et al. \(2018a\)](#). Global average model results for some important species are given in Table 5.1 and the annual mean ozone and OH concentrations and differences are shown in Figs. 5.1 and 5.2. We have also extracted average concentrations of many different inorganic and organic components and groups of species in various regions of the world with different emissions and climate characteristics. A selection of these regions are defined in Table 5.2, and Table 5.3 provides concentrations of some important species.

In the global simulations additional tracking was done of all reactions in the lowest model level involving the most important species (ozone, OH, NO_x, HO₂, RO₂, NO₃, organic nitrates and some others). The tracking counts the accumulated formation and losses of the different species via different reaction types. When combined with the accumulated dry deposition fluxes of ozone and NO₂ it is possible to get rough estimates of the mean fluxes of these two species between the first model level and higher levels. Using the results from the reaction-tracking e.g. the importance of different oxidation paths for formation of NO₂ or degradation of biogenic VOCs can be investigated and compared between the different chemistry mechanisms. This has been done for the global average and for eleven different regions around the world. These tracking simulations produced a very large amount of detailed results and here it is only possible to provide a limited selection. Most of it is discussed in Chapter 6.

Table 5.1 shows that global mean concentrations of many of the most interesting species are relatively similar with the EmChem19a, EmChem19X and CRIv2R5Em schemes, and indeed this is true in other regions as well (Table 5.3). Results with the CB6r2Em deviate more (at least for ozone and OH). Although the different mechanisms behave differently in different types of regions some general observations can be made. Firstly, CB6r2Em gives the lowest ozone concentrations everywhere; the simulated global average O_3 is 30.7 ppb with CB6r2Em, and about 33.4–33.6 ppb with CRIv2R5Em and the EmChem19 mechanisms. The largest differences between CB6r2Em and CRIv2R5Em are found in the tropical forest regions, with e.g. 7 ppb lower ozone with CB6r2Em over the Amazon (and > 10 ppb in central Africa). In the boreal region (e.g. Canada, or northern Scandinavia) differences between CB6r2Em and CRIv2R5Em are smaller, ca. 1–2 ppb. Secondly, the EmChem19 schemes give ozone concentrations quite close to CRIv2R5Em in the boreal region, somewhat higher (~ 1 –4 ppb) in parts of South America and Indonesia, and somewhat lower (~ 1 –4 ppb) concentrations in the Asian regions with large anthropogenic emissions (NE China and NE India) as well as in the SE USA (which has substantial isoprene emissions).

The ozone formation in the lowest model level is larger with the EmChem19 schemes than with CRIv2R5Em. This is, however, to some extent compensated by larger influx of ozone from higher levels in most regions in the CRIv2R5Em-simulation, indicating larger ozone formation in higher model levels. The net effect is relatively small differences in simulated ozone concentrations near the surface. The somewhat higher OH concentrations in EmChem19 in

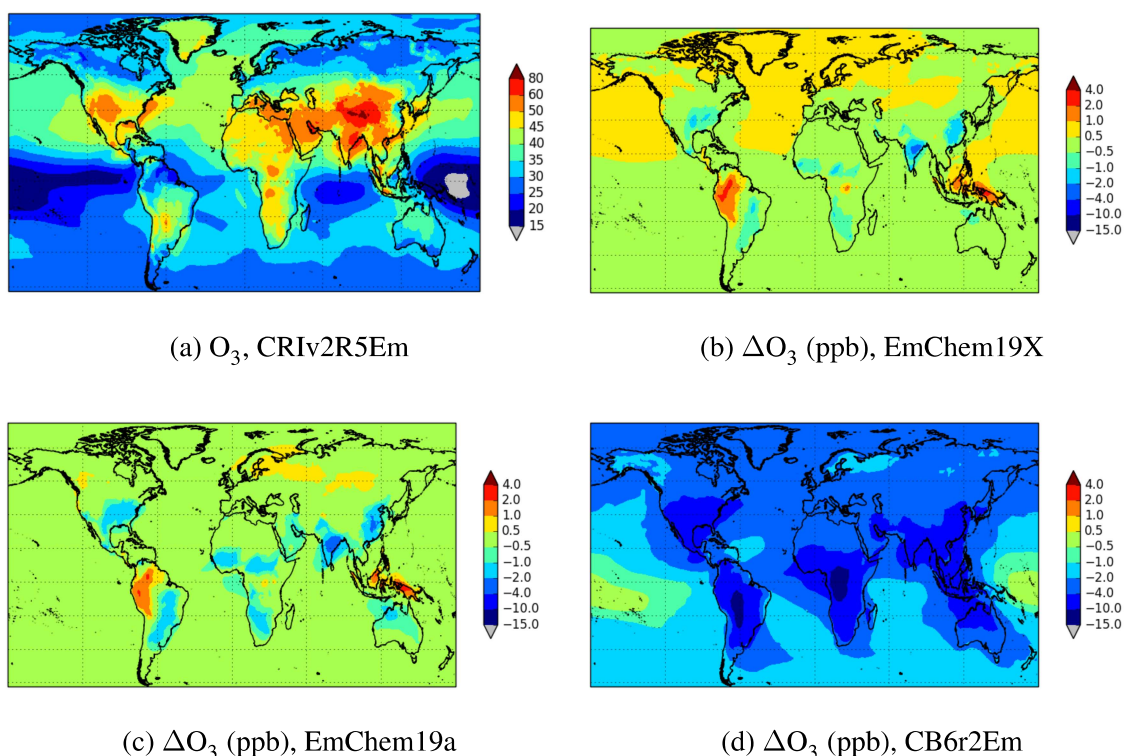


Figure 5.1: (a) Model simulated annual mean surface level ozone concentrations (ppb) for 2012 from the CRIv2R5Em model, and (b)–(d) concentration differences (ppb) to the CRIv2R5Em results from schemes EmChem19X, EmChem19a, and CB6r2Em. (Positive values indicate higher concentrations than CRIv2R5Em and negative lower).

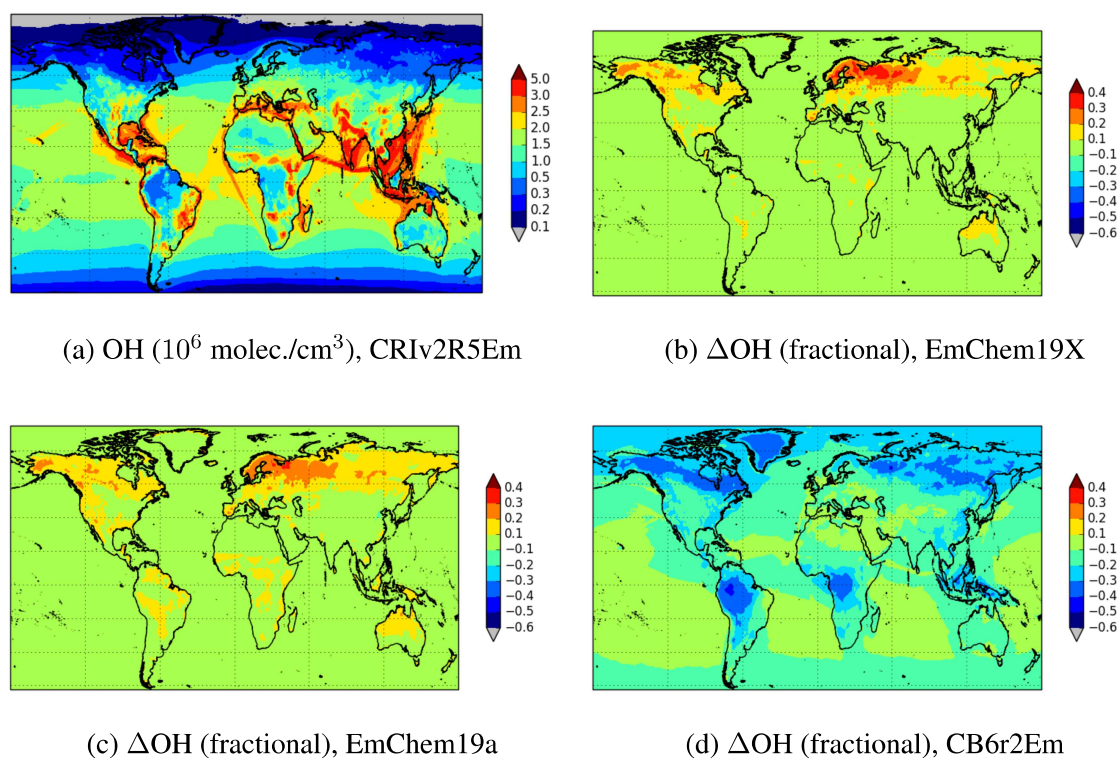


Figure 5.2: (a) Model simulated annual mean surface level OH concentrations (10^6 molec. cm⁻³) for 2012 from the CRIv2R5Em model, and (b)–(d) relative differences (as fractional changes) to the CRIv2R5Em results from schemes EmChem19X, EmChem19a, and CB6r2Em. (Positive values indicate higher concentrations than CRIv2R5Em and negative lower).

the lowest model level means that more VOC are consumed near the surface than with the CRIv2R5Em and this means that more VOC are available for ozone production in the higher levels in the CRI simulations. Indeed, the longer "reaction chains" of some of the initial reaction products in the CRI scheme, especially for the larger emitted species such as the monoterpenes, will generate ozone over longer reaction times than with the smaller surrogate species used in the EmChem19 schemes. The ozone production in the lowest model level is relatively similar in CB6r2Em as in CRIv2R5Em in many of the regions, however, in all regions the influx of ozone from higher levels is smaller with CB6r2Em than with CRIv2R5Em. The global average difference in influx between CRIv2R5Em and CB6r2Em is 13% and the largest differences, about 30%, are found in the tropical rainforest regions—the ozone formation capacity is lost more quickly in the CB6r2Em simulations than with CRIv2R5Em.

Considering OH (Fig. 5.2, Tables 5.2–5.3), concentrations are also clearly lower with CB6r2Em than with the other mechanisms in all regions. The modelled global average of surface OH concentration is 1.28×10^6 molecules cm⁻³ with CRIv2R5Em and about 1% higher with EmChem19X, 3% higher with EmChem19a and 12% lower with CB6r2Em. Less OH is formed with CB6r2Em than with the other mechanisms in all regions. The differences to CRIv2R5Em are largest in the tropical rain forest regions, but differences are also large in the boreal regions and SE Asia. In most regions the EmChem19 mechanisms produce somewhat more OH than CRIv2R5Em, but the (relative) differences are very large in northern

Table 5.1: Model calculated global average concentrations in the lowest model level (annual areal means). For the OH, HO₂, RO₂ and NO₃ radicals accumulated annual formation is also given.

	CRIv2R5Em	EmChem19X	EmChem19a	CB6r2Em
O₃ (ppb)	33.4	33.6	33.4	30.7
OH (10 ⁶ molecules cm ⁻³)	1.28	1.30	1.32	1.12
HO₂ (ppt)	4.7	5.2	5.3	4.7
H₂O₂ (ppt)	313	307	304	270
NO₃ (ppt)	2.4	2.5	2.6	2.7
NO (ppt)	53	56	57	59
NO₂ (ppb)	0.41	0.44	0.44	0.41
NO_x (ppb)	0.48	0.51	0.51	0.48
HNO₃ (ppt)	66	67	68	68
N₂O₅ (ppt)	2.5	2.5	2.6	1.8
HO₂NO₂ (ppt)	1.1	1.8	1.9	1.3
HONO (ppt)	0.6	0.6	0.6	0.5
PAN (ppt)	128	145	137	108
∑ PANs (ppt)	166	168	156	157
∑ Org-NO₃ (ppt)	74	44	51	76
total oxidised N (μg(N) m ⁻³)	0.56	0.56	0.56	0.56
fraction NO _x	0.480	0.506	0.509	0.485
fraction total PANs	0.169	0.174	0.160	0.160
fraction organic nitrate	0.073	0.045	0.050	0.076
fraction inorg. particle nitrate	0.199	0.199	0.202	0.202
fraction other oxidised N	0.079	0.076	0.079	0.077
∑ RO₂ (ppt)	8.8	7.7	7.4	9.5
∑ XO₂ (ppt)	13.6	13.0	12.7	14.1
Benzene (ppt)	40	40	39	45
isoprene (ppb)	0.32	0.31	0.31	0.38
HCHO (ppb)	0.52	0.55	0.53	0.44
∑ ROOH (ppb)	0.29	0.27	0.26	0.53

Notes: ∑ PANs, ∑ RO₂, ∑ RO₂ as in Table 3.3. ∑ Org-NO₃ is sum of total organic nitrates. ∑ ROOH is sum of organic hydroperoxides.

Europe, which seems to be mainly attributable to the differences in monoterpene chemistry (see Ch. 6.2).

The simulated global mean NO_x concentrations in the lowest model level are about 5–6% higher with the EmChem19 schemes than with the CRIv2R5Em and CB6r2Em mechanisms (Table 5.1). The global mean difference between CB6r2Em and CRIv2R5Em is small, but in most of the investigated (land) sub-regions CRIv2R5Em (e.g. Table 5.3) gives somewhat lower annual mean NO_x concentrations than CB6r2Em (though not in south-eastern USA or the Persian Gulf). The EmChem19 mechanisms give the highest NO_x concentrations in most regions and the differences are especially large in the tropical rain forest regions. Exceptions include the Moscow, northern Italy and north-eastern China regions, where the CB6r2Em simulation give similar or slightly higher annual mean NO_x concentrations — these regions are all strongly influenced by anthropogenic emissions and have fairly high NO_x/VOC emission ratios in the model simulations.

The model simulated annual mean near surface total concentrations of organic peroxy radicals (∑ RO₂ = RO₂+RCO₃) are clearly lower with the EmChem19 schemes than with CRIv2R5Em, however, the actual accumulated amount of peroxy radicals produced (and re-

acting) is higher in the EmChem19 simulations than with CRIV2R5Em in most of the studied regions. For example, about 20% more $\text{RO}_2 + \text{NO}$ reactions occur in the lowest model level with the EmChem19 schemes than with CRIV2R5Em as a global average (more in regions dominated by biogenic emission and less in regions with large anthropogenic emissions). (An explanation for this difference between concentrations and production is that different RO_2 and RCO_3 radicals may have strongly varying lifetimes, with CRIV2R5Em having some longer lived species that contribute to higher average concentrations.) The sum of all peroxy radicals ($\sum \text{XO}_2 = \text{HO}_2 + \text{RO}_2 + \text{RCO}_3$) is rather similar in the EmChem19 and CRIV2R5Em schemes except in the boreal regions where it is about twice as high with CRIV2R5Em. CB6r2Em, on the other hand, produces the same global mean concentration of HO_2 , but higher RO_2 concentrations than CRIV2R5Em both globally and in most regions; up to more than 40% more in the tropical rain forest regions, though about 30% lower in northerly (boreal) regions. The total number of $\text{RO}_2 + \text{NO}$ reactions in the lowest model level is somewhat higher with CB6r2Em than with the EmChem19 schemes in most regions (and about 26% higher than CRIV2R5Em globally). On average about 7% of the $\text{RO}_2 + \text{NO}$ reactions produce organic nitrates with the CRIV2R5Em and CB6r2Em; this fraction is about 4–5% with the EmChem19 mechanisms.

In most regions, the total concentration of oxidised nitrogen (NO_y) is similar with all the mechanisms (the main exception being the tropical forest regions, where the EmChem19 mechanisms give somewhat higher annual mean total NO_y than CRIV2R5Em and CB6r2Em) but there are differences in the distribution of NO_y between different types of compounds: the EmChem19 schemes tend to have larger fractions of NO_x and somewhat smaller fractions of PANs and/or other organic nitrates. Thus more NO_y is available for ozone formation in the EmChem19 simulations than with the other chemistry schemes, at least in the lowest model level.

Table 5.2: Regions used in Table 5.3

Region	Description
GLOB	Globe - i.e. full domain
AMAZ	The Amazon (Lat 8°S–5°N, Lon 51.5–73.5°W), wet (RH=0.85, prec=2142 mm) and hot (T=298 K), total VOC-emis. 23200 mg m ⁻² (isoprene 18200, MT 4220, AVOC 835), total NOx-emis. 1340 mg (NO ₂) m ⁻² , NOx/VOC=0.06, Hmix=406 m
CAN	Northern America, mainly Canada (Lat 49–69°N, Lon 61.5–162.5°W), intermediate precip (RH=0.76, prec=807 mm), cold (T=271 K), total VOC-emis. 1080 mg m ⁻² (isoprene 484, MT 439, AVOC 160), total NOx-emis. 174 mg (NO ₂) m ⁻² , NOx/VOC=0.15, Hmix=561 m
N-ITAL	Northern Italy (Lat 44–47°N, Lon 6.5–13.5°E), rel. large precip (RH=0.73, prec=1212 mm), intermediate temperature (T=282 K), total VOC-emissions 3640 mg m ⁻² (isoprene 345, monoterpenes 683, anthropogenic VOC 2610), total NOx-emissions 2750 mg (NO ₂) m ⁻² , NOx/VOC=0.76, Hmix=337 m
NE-CHIN	Northeastern China (Lat 30–41°N, Lon 111.5–122.5°E), intermediate precip (RH=0.61, prec=791 mm), intermediate temp (T=286 K), total VOC-emis. 12300 mg m ⁻² (isoprene 1650, MT 495, AVOC 10150), total NOx-emis. 19000 mg (NO ₂) m ⁻² , NOx/VOC=1.55, Hmix=612 m

Notes: meteorology and emissions estimates given for regions are annual averages over the given spatial domain (annual total for precipitation).

Table 5.3: Global and regional (see Table 5.2) average concentrations from the global model runs. Results are given for four base-schemes (CRIV2Em, EmChem19X, EmChem19a and CB6r2Em), and from two experimental schemes (CRIwMT19X, CB6wInorgCRI – see Ch.6).

Spec	Reg	CRIV2R5Em	CRIwMT19X	EmChem19X	EmChem19a	CB6r2Em	CB6wInorgCRI
O3	GLOB	33.4	33.7	33.6	33.4	30.7	31.2
-	AMAZ	29.2	30.7	30.2	29.8	22.1	22.3
-	CAN	32.1	32.5	32.6	32.4	29.8	30.3
-	N-ITAL	39.1	39.6	39.3	39.1	35.7	36.4
-	NE-CHIN	37.9	38.2	36.9	36.2	32.6	33.5
OH	GLOB	1.28	1.31	1.30	1.32	1.12	1.15
-	AMAZ	0.49	0.56	0.51	0.53	0.33	0.33
-	CAN	0.42	0.48	0.45	0.46	0.33	0.34
-	N-ITAL	2.00	2.21	2.12	2.15	1.76	1.82
-	NE-CHIN	1.61	1.67	1.53	1.53	1.24	1.30
HO2	GLOB	4.7	5.3	5.2	5.3	4.7	4.7
-	AMAZ	13.3	19.0	18.9	20.6	15.3	15.3
-	CAN	2.3	4.1	4.0	4.0	2.5	2.6
-	N-ITAL	3.3	4.7	4.4	4.4	3.0	3.1
-	NE-CHIN	3.0	3.5	3.0	3.0	2.3	2.3
NO3	GLOB	2.4	2.5	2.5	2.6	2.7	3.1
-	AMAZ	0.2	0.3	0.3	0.3	0.1	0.1
-	CAN	0.5	0.5	0.5	0.5	0.5	0.5
-	N-ITAL	4.0	4.2	4.2	4.3	4.0	4.6
-	NE-CHIN	7.0	7.2	6.9	6.9	7.0	7.9
NOx	GLOB	0.48	0.50	0.51	0.51	0.48	0.48
-	AMAZ	1.19	1.55	1.56	1.59	1.24	1.24
-	CAN	0.24	0.26	0.26	0.26	0.24	0.24
-	N-ITAL	5.79	5.75	5.93	5.93	6.08	6.07
-	NE-CHIN	22.88	22.76	23.50	23.61	24.54	24.47
H2O2	GLOB	313	327	307	304	270	273
-	AMAZ	771	914	790	710	489	490
-	CAN	78	97	89	86	66	66
-	N-ITAL	195	228	208	203	162	163
-	NE-CHIN	490	519	457	435	343	350
HNO3	GLOB	66	67	67	68	68	68
-	AMAZ	49	57	56	55	84	83
-	CAN	24	26	25	26	27	27
-	N-ITAL	353	362	362	367	354	350
-	NE-CHIN	1399	1417	1377	1379	1245	1253
Σ RO2	GLOB	8.8	7.8	7.7	7.4	9.5	9.6
-	AMAZ	37.6	30.1	28.8	26.5	53.3	53.6
-	CAN	16.0	5.3	5.5	5.0	11.3	11.4
-	N-ITAL	7.9	6.9	6.4	5.9	8.8	9.0
-	NE-CHIN	4.4	4.4	3.6	3.2	5.1	5.3
Σ XO2	GLOB	13.6	13.1	13.0	12.7	14.1	14.3
-	AMAZ	50.9	49.1	47.7	47.1	68.6	68.9
-	CAN	18.3	9.3	9.4	9.0	13.9	14.0
-	N-ITAL	11.2	11.6	10.8	10.3	11.8	12.1
-	NE-CHIN	7.4	7.8	6.7	6.2	7.4	7.6
HCHO	GLOB	0.52	0.54	0.55	0.53	0.44	0.45
-	AMAZ	4.88	5.15	5.33	4.90	3.82	3.82
-	CAN	0.29	0.33	0.35	0.32	0.28	0.28
-	N-ITAL	1.29	1.34	1.34	1.38	1.05	1.06
-	NE-CHIN	2.35	2.37	2.31	2.34	1.81	1.82
PAN	GLOB	128	150	145	137	108	111
-	AMAZ	351	456	445	347	200	201
-	CAN	255	333	338	320	227	233
-	N-ITAL	560	661	609	586	431	443
-	NE-CHIN	846	906	808	775	654	679
Σ PANs	GLOB	166	169	168	156	157	160
-	AMAZ	767	595	595	567	622	625
-	CAN	336	366	375	357	324	330
-	N-ITAL	716	743	706	644	592	607
-	NE-CHIN	987	1010	924	824	845	876
Σ Org-NO3	GLOB	74	64	44	51	76	77
-	AMAZ	444	387	461	552	539	541
-	CAN	63	51	24	30	61	62
-	N-ITAL	172	126	84	80	287	290
-	NE-CHIN	297	271	219	218	404	410
Σ ROOH	GLOB	0.29	0.28	0.27	0.26	0.53	0.52
-	AMAZ	1.70	1.68	1.29	1.31	5.44	5.44
-	CAN	0.15	0.14	0.14	0.13	0.47	0.46
-	N-ITAL	0.12	0.12	0.11	0.10	0.21	0.21
-	NE-CHIN	0.14	0.13	0.10	0.10	0.25	0.24

Notes: For definition of regions, see Table 5.2; Σ RO2 is sum of RO2 and RCO2 species; Σ XO2 is sum of HO₂ + Σ RO2; Σ PANs is sum of all PAN-like species. Units are ppb for O₃, PAN and Σ PANs, ppt for HO₂, NO₃, H₂O₂, Σ RO2 and Σ XO2, molecules cm⁻³ for OH.

5.2. Comparison with measurements from GAW sites

The global scale model results for surface level ozone were compared to hourly measurement data from a number of stations in the Global Atmosphere Watch Programme ([Schultz et al. 2015](#)). Only sites with altitude $\leq 600\text{m}$ were included and city sites were excluded. In total, data from 47 sites were included.

The geographical distribution of the sites is rather uneven, and many of the stations are coastal, or near-coastal, and/or located on islands, which may pose special challenges for model simulations of surface level ozone with coarse resolution models. Data were available from a number of sites in Europe, Canada, Antarctica, the Arctic, the south-western Pacific and Japan, and several islands in the North Atlantic, but data from Africa were limited to one site (Cape Point, at the southernmost tip of the continent) and only one rainforest site was included (Danum Valley on Borneo). With the exception of the site on Borneo and three sites on Japanese islands, no data from Asia were included.

A comparison of modelled and observed mean of daily maximum hourly ozone (MDmaxO₃) concentrations at the 47 sites is given as a scatter plot in Fig. 5.3, and with statistics for individual sites in Table F.1. For the scatter plots, results are given with all data included, but also with the two obvious outliers (which are Danum Valley, Borneo, and Tudor Hill, Bermuda) excluded. With the exceptions of the two outliers the correlation between modelled and measured mean ozone concentrations is excellent for all four model schemes, and indeed identical ($R=0.92$) across the four mechanisms. For the mean of daily maximum ozone concentrations (Fig. 5.3) the CB6r2Em simulation has the smallest bias (-0.7 ppb when outliers are excluded) while the other three model schemes have a small overestimate of about 2.3–2.6 ppb.

Model performance varies a lot from site to site (e.g. Table F.1 for MDmaxO₃), but the correlation between modelled and measured MDmaxO₃ is quite similar regardless of which chemistry scheme is used. All model versions have correlation coefficients (R) for MDmaxO₃ above 0.7 at 37–38 of the sites. For three coastal sites at the Arctic Ocean (Barrow/Alaska, Villum/Greenland, Alert/Nunavut) the model O₃ shows no correlation with the measurements, but this is mainly because these sites experience strong springtime arctic depletion events caused by halogen species which the model does not account for (e.g. [Oltmans et al. 2012](#)). The Zeppelin station is modelled rather well ($R > 0.75$), however, as are most of the Antarctic sites.

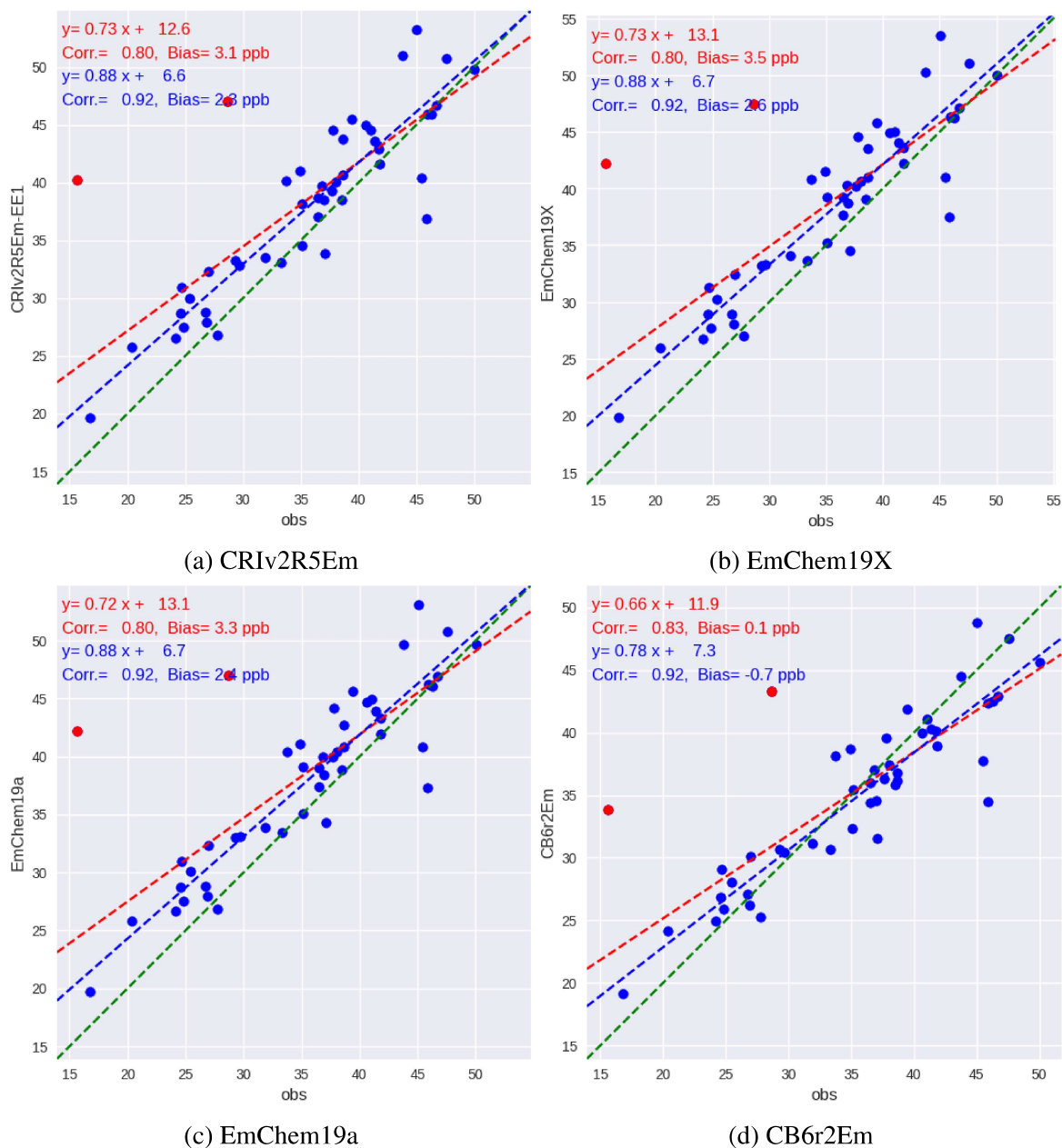


Figure 5.3: Comparison of modelled and observed mean of daily maximum ozone concentrations at GAW sites (alt. ≤ 600m) in 2012. Markers, dashed lines, and statistics (see text) in blue give regression lines for points once outliers are excluded; equivalent in red gives results with all points included. The green dashed line is the 1:1 line. Unit: ppb(v)

6. Discussion and sensitivity tests

The preceding sections have illustrated some of the main similarities and differences between the gas-phase mechanisms at both European and global scale. It would be an enormous job to evaluate the causes of all differences in detail, and any such explanations would vary from location to location, and from season to season, but here we discuss some of the likely factors underlying the differences, especially with respect to comparing the CRI and EmChem schemes (that have some common history and development) and the CB6 scheme which stems from a very different development path. Ch. 6.1–6.4 discuss some reasons for the differences in the mechanisms, including reference to various sensitivity tests made with variations on the chemical mechanisms.

6.1. Inorganic chemistry: the CB6wInorgCRI test

For this work, the inorganic chemistry mechanisms were largely harmonized between CRIv2R5Em and the EmChem19 schemes. For CB6r2Em this was not done, in order to keep the mechanism as similar to the original CB6r2 as possible. In order to investigate the impacts of the differences between the inorganic parts of the mechanisms a global scale model simulation was run with a modified version of CB6r2Em, denoted CB6wInorgCRI, where the inorganic chemistry was replaced by the one used in CRIv2R5Em. The results of this simulation are included in Table 5.3.

For most model species and regions the influence of the differences in the inorganic chemistry is relatively small. The largest relative differences were found for HO_2NO_2 (not shown), which is about 20–30% (25% global areal average) lower when using the modified version of the inorganic chemistry. Fairly large impacts were also seen for the NO_3 radical, which increase by about 10–15% (14% global areal average) for CB6wInorgCRI versus CB6r2Em. Model-simulated OH radical concentrations also increase by ~ 2 –5% (except in the regions with the lowest NO_x/VOC emission ratios). The modified inorganic chemistry caused an increase in annual mean ozone concentrations of about 0.2–1 ppb (1–3%, with average 0.5 ppb, 1.6%) for the global runs compared to the original CB6r2Em. Thus, this is not the most important reason for the large differences in modelled ozone with CB6r2Em compared to the other mechanisms on the global scale, but the impacts of the differences in the inorganic chemistry are not insignificant.

6.2. Monoterpene chemistry: the CRIwMT19X test

We noted in Ch. 4.1 and Ch. 5.1 that EmChem19a produced somewhat more O_3 and OH than CRIv2R5Em, with the differences for OH being very large in northern Europe. This is a region where biogenic emissions dominate over anthropogenic, and where monoterpene (MT) emissions exceed isoprene emissions (Simpson et al. 1999, 2012). An important reason for the differences is related to hydroperoxy (HO_2) and organic peroxy radicals (RO_2), which are of major importance for ozone formation through oxidation of NO to NO_2 . The $HO_2 + NO \rightarrow NO_2 + OH$ reaction is much faster than most of the $RO_2 + NO \rightarrow NO_2 +$ reactions included in the different mechanisms. The simplified monoterpene chemistry in the EmChem19 mechanisms produces much higher concentrations of HO_2 than the more detailed CRIv2R5Em and this contributes to the faster formation of O_3 with the EmChem19 schemes compared to CRIv2R5Em. The greater formation of HO_2 in the EmChem schemes also leads to very large OH formation from the $HO_2 + NO$ reaction.

Indeed, the accumulated amount of NO_2 formed from $HO_2 + NO$ in the lowest model level is about 12% larger with EmChem19X (15% with EmChem19a) than with CRIv2R5Em as a global average; CB6r2Em produce about 8% less NO_2 through this reaction than CRIv2R5Em. For the EmChem19 schemes the differences to CRIv2R5Em are largest for the monoterpene dominated N European region (+60% EmChem19X and +65% EmChem19a) but also large for the tropical rain forest regions, N America and SE USA (with about 18–40% more $HO_2 + NO$ reactions than with CRIv2R5Em). In most regions CB6r2Em leads to (6–16%) fewer $HO_2 + NO$ reactions than CRIv2R5Em; exceptions are the N Europe region and the clean SE Pacific area (both with about 3% more $HO_2 + NO$ reactions).

Another reason for the larger ozone formation with the Emchem19 schemes could be that the CRIv2R5Em forms substantial amounts of organic nitrates in the MT chemistry, which does not occur in the simpler EmChem Schemes. CB6r2Em produces even more organic nitrates as discussed in Sec. 6.4 The larger organic nitrate formation results in lower amounts of NO_x and subsequently ozone in the CRIv2R5Em simulations.

In order to quantify the importance of the MT chemistry further, test simulations were performed with a modified version of the CRIv2R5Em, which we denote CRIwMT19X, where the MT chemistry was replaced by the one used in EmChem19X. As seen in Table 5.3, this modified CRIvMT19X scheme gave results which became much closer to EmChem19X for many compounds (e.g. NO_x , HO_2 , $\sum$ PANs), especially in the areas most affected by biogenic emissions. CRIwMT19X also gives O_3 results for Europe (not shown) in close agreement with EmChem19X over most of Europe (within ± 0.1 ppb(v), except in a few anthropogenic emission hot spots and parts of Italy and the Balkans where the differences were a bit larger), confirming that this monoterpene chemistry is indeed a major cause of the differing O_3 and OH levels in northern Europe.

6.3. Reactivity of biogenic VOC

The reactions of monoterpenes and isoprene in the lowest model level were tracked and this gives an indication of how the reactivity differs between the mechanisms. The EmChem19 schemes are more reactive than CRIv2R5Em in most regions and CB6r2Em has the lowest reactivity. About 31% of the globally emitted isoprene reacts in the lowest model level (with depth of ca. 90 m in these tests) in the EmChem19 simulations and slightly less in the CRIv2R5Em (29%) and CB6r2Em (26%). The OH reaction dominates (22–27%) and only a small fraction reacts with O_3 ($\sim 3\%$) and NO_3 ($< 1\%$) in the lowest model level. About 44% of the emitted monoterpenes reacts in the lowest model level in the EmChem19 simulations (42% with CRIv2r5Em and 38% with CB6r2Em). Most of the MT reacts with O_3 (16–20%) but reactions with NO_3 (11–13%) and OH (10–11%) are also important. The relative importance of the different oxidants vary substantially between different regions — ozone reactions are significant everywhere, but notably suppressed in the regions most influenced by anthropogenic emissions (NE China, Moscow region, NE India); the OH reaction is the most important in the N Italy region (and more important than the O_3 reaction also in the Moscow, NE China and NE India regions; and of clearly less importance in the tropical rainforest regions and Canada); the NO_3 reaction is important in regions with substantial NO_x -emissions but of relatively minor importance in the boreal areas and the Amazon where NO_x -emissions are small.

6.4. Organic nitrate mechanisms

Ch. 6.2 discussed briefly some differences between EmChem19 and CRIv2R5Em organic nitrate formation from monoterpene chemistry. Here we focus on CB6r2Em, which shows very different O_3 formation compared to the other schemes (Fig. 5.1). A major reason for the large differences is the way organic nitrate is formed and evolves in CB6r2Em. Three organic nitrate species are formed, NTR1, NTR2, and INTR. The NTR1 compound, which represents organic nitrates that are predominantly in the gas-phase, undergoes (slow) photolysis that returns NO_x in the form of NO_2 in CB6r2Em. However, NTR1 is also transformed into “particulate organic nitrate” (NTR2) by reaction with OH; no release of NO_2 is included in the reaction. The NTR2 species represents organic nitrates which are partitioned predominantly to the particulate phase (mainly large and multifunctional nitrates; [Hildebrandt Ruiz and Yarwood 2013](#)) and these are treated very differently from all organic nitrates in the CRIv2R5Em and EmChem19 schemes. The only loss process for NTR2 is a transformation into HNO_3 at a constant rate ($1/e$ lifetime 12h), which represents hydrolysis of the organic nitrate in the particulate phase. Photolysis is assumed to be too slow to be important for NTR2 and OH-reactions are also neglected. Finally, the INTR compound represents a separate organic nitrate from isoprene oxidation. INTR contains an alkene bond and reacts rapidly with OH and is partially transformed into NTR2 by this reaction.

Although organic nitrates are formed in the CRIv2R5Em and the EmChem19 schemes as well, these can regenerate NO_x through photolysis and OH reactions, at least to some extent.

For example, for CRIv2R5Em about 25% of the organic nitrate formed in the lowest level reforms NO_2 , and for EmChem19X and EmChem19a the corresponding fractions are about 28% and 20%. The organic nitrates in CB6r2Em, on the other hand, especially NTR2, provide a stronger sink of NO_x , and hence a substantial decrease in ozone formation compared to the other schemes; only about 4% of the NO_x is regenerated from the first level organic nitrate formation.

The relative differences between the CB6r2Em and CRIv2R5Em results (at least for ozone) tend to be smaller in the regions with low isoprene concentrations (e.g. Canada, N Europe, remote Pacific) than elsewhere. The largest differences are found in the tropical rainforest regions where the CB6r2Em simulation gives about 25% lower annual mean ozone and 33% lower OH than CRIv2R5Em. In the regions with high isoprene concentrations (Amazon, WC Africa, SE USA, NE India, NE China) the formation of organic nitrates is very large and in the CB6r2Em scheme this leads to a more substantial loss of NO_x than in the other schemes.

In addition to the fact that less NO_x is regenerated from the organic nitrates with the CB6r2Em mechanism it also forms more organic nitrates than the other mechanisms (35% more than CRIv2R5Em as a global average).

A sensitivity test run was performed with the NTR2 formation turned off (and replacing all NTR2 by NTR1)—this simple test indicates that the impact on ozone concentrations is very large (the global areal mean O_3 in the lowest model level increase by 13% (4 ppb) and is higher than with the other mechanisms; in the different sub-regions the O_3 concentration increase to varying degrees, from 2.1 ppb in NE China to 6.5 ppb in the tropical forest region of C Africa).

This very large impact of the transformation of nitrogen from the gas phase to particulate phase nitrate in the CB6r2Em mechanism indicates that it would be worthwhile to further investigate the coupling of the particulate organic aerosol with the gas-phase chemistry of the EmChem (and CRI) mechanisms. If the CB6r2Em description of the "loss" of nitrogen to the particulate phase occurs at a realistic rate it is likely that the other (effectively pure gas-phase) schemes overestimate the amount of oxidised nitrogen available for photochemical ozone production substantially.

7. CPU time

An important factor when considering the use of the different chemical mechanisms is the CPU usage. This is especially true for the EMEP model which is traditionally used to perform hundreds and even thousands of source-receptor calculations in support of the Air Convention (Simpson 2013). As shown in Table 7.1 the EmChem19a scheme is substantially faster than the other mechanisms, and as we have seen it gives results which are in good agreement with the most complex CRIv2R5Em scheme for most practical applications. The other mechanisms consume more CPU, but all are still manageable within the EMEP MSC-W CTM system for research studies or when further detail is needed. Simpson et al. 2020a presented a similar comparison for global scale $0.5^\circ \times 0.5^\circ$ runs (i.e. $720 \times 360 \times 20$ grid cells), which required 7.3 h for EmChem19a-vbs, 8.0 h for CB6r2Em-vbs, and 10.2 h for CRIv2R5Em-vbs. Thus, as the number of grid cells increases the ‘heavier’ CB6r2Em and CRIv2R5Em become more competitive with EmChem19a, which is a result of the fact that non-chemical calculations, especially advection processes, scale less favourably than chemistry when the number of grid cells increases.

Table 7.1: CPU consumption for EMEP CTM simulations over Europe. (In addition to the gas-phase mechanism, the default ‘vbs’ SOA scheme is also used (c.f. Simpson et al. 2020a), corresponding to typical EMEP usage.)

Mechanism	Time used (hours) [†]	
	in gas-phase chemistry	Total
EmChem19a-vbs	1.10	3.32
EmChem19X-vbs	1.94	4.22
CB6r2Em-vbs	1.66	3.84
CRIv2R5Em-vbs	3.12	5.59

[†] For 16 nodes, 512 processors, on an x86_64 linux supercomputer, with intel mpif90 compiler. The comparison is for an annual simulation on the so-called EMEP0302 grid which is a longitude/latitude grid of $0.3^\circ \times 0.2^\circ$ resolution, 400×260 grid-cells, and with 20 vertical levels.

8. Conclusions

In this report we have documented the development and testing of four chemical mechanisms which are currently implemented in the EMEP and boxChem systems (Ch. 2): EmChem19a, EmChem19X, CB6r2Em and CRIv2R5Em. We have compared these mechanisms with the "Master Chemical Mechanism" (MCMv3.3Em) in a series of box-model tests (Ch. 3), and then in a series of European and global scale simulations (Ch. 4–5). Chapter 6 discusses some of the reasons for the differences in mechanisms. Ch. 7 presents a brief illustration of another important aspect of these mechanisms – the computer time needed to run the EMEP model.

EmChem19a¹ is the current standard scheme for the EMEP MSC-W model. It is a reduced/simplified version of the extended EmChem19X-scheme, which was designed with the GenChem-adapted version of the Master Chemical Mechanism (MCMv3.3Em) as a benchmark scheme, in box model simulations with varying emissions of NO_x, anthropogenic VOC and isoprene, and different temperatures.

Simplified box-model simulations, with limited deposition and no exchange with clean background air, tend to exaggerate the effect of differences due to different chemical mechanisms compared to 3-D chemical transport model simulations (where rapidly changing emissions, dispersion, and deposition processes compete with chemical processes). These simplifications are, however, very useful during mechanism development. In general all four schemes provided similar concentrations, even of radical species, over the first 24 hours, when initial conditions still have a large influence, but differences became more apparent at longer time-scales and at colder temperatures. However, the EmChem schemes showed good agreement with MCM over a wide range of conditions.

The four mechanisms were also tested in chemical transport model runs on the global and European scale with the EMEP CTM. Comparisons with measurements in Europe indicate that the EmChem19a is competitive with the other (more time consuming) mechanisms, at least for ozone and inorganic sulfur and nitrogen components. Some of the CTM-results presented here indicate that the EmChem19 schemes can deviate substantially from CRIv2R5Em in regions dominated by monoterpene emissions and it would be beneficial to develop an improved description of the EmChem19 monoterpene chemistry.

The CB6r2Em scheme gives lower photochemical reactivity than the other schemes, which leads to significantly lower values for accumulated ozone metrics such as AOT40 or W126.

¹EmChem19r, introduced in [Simpson et al. \(2021\)](#) is simply a variation of EmChem19a which tracks residential emissions rather than the wood and fossil fuel tracking used in EmChem19a. We use the term EmChem19a here for both variants.

Major differences between the CB6-based scheme and the other schemes are associated with the formation and properties of organic nitrates and to differences in the inorganic chemistry mechanisms (Ch. 6). The relatively large impact of the loss of nitrogen oxides to organic nitrates in CB6r2Em found in the simulations indicates that it is important to investigate the gas-particle partitioning of the organic nitrates in future studies.

That differences exist between CB6r2Em and the other schemes is not surprising: the EmChem, CRI and MCM schemes all share origins in the same type of chemical mechanism, and have MCM as the reference point for mechanism development. The CB6 schemes are developed in a quite different way, with a larger focus on evaluation against smog-chamber results (e.g. [Yarwood et al. 2010b](#), [Hildebrandt Ruiz and Yarwood 2013](#)). As noted in Ch. 3.1 though, some of the differences in results may also stem from assumptions concerning emission surrogate choices and VOC mapping criteria and methods. The CB-family of schemes is, however, actively developed, and widely used in other CTMs, so the CB6r2Em scheme is a useful addition to the EMEP model system. For example a possible future application of the scheme is to explore halogen chemistry, which is easily available from the original CB6r2h mechanism. In any case, the comparison with surface level ozone measurements cannot discriminate between the different chemical schemes, however, since many other processes and uncertainties affect such comparisons (e.g. anthropogenic and biogenic emissions, transport and dispersion issues). The differences may be seen as an indicator of the uncertainty associated with CTM modelling in general.

For future developments of the EmChem gas-phase mechanisms two of the most important issues are an update of the photolysis treatment and a revision of the monoterpene mechanism. The photolysis rate calculations are currently based upon a system of tabulated values originating in the work of [Kylling et al. \(1995, 1998\)](#) and [Jonson et al. \(2001\)](#). An implementation of the more flexible and dynamic Cloud-J system of [Prather \(2015\)](#) has been started, and will replace the current system in the near future. Implementation of other widely used chemical mechanisms such as MOZART ([Emmons et al. 2010](#), [Knote et al. 2014](#)) would also be useful. Another area for future development is the treatment of semi-volatile organic compounds in a more realistic way, especially regarding organic nitrates in the particulate phase.

Finally, we should note that this report has presented only a brief overview of the many tests which have been conducted in the design of the new EmChem schemes. The focus here has been the gas-phase chemistry, with some consideration of the inorganic particle chemistry. Much work remains to be done to evaluate the impact of these chemical mechanisms on secondary organic aerosols, but that issue is far more complex and unconstrained in terms of both chemistry and emissions than for the gas-phase compounds (e.g. [Hallquist et al. 2009](#), [Jimenez et al. 2009](#), [Bergström et al. 2012](#), [Denier van der Gon et al. 2015](#), [Hodzic et al. 2016](#), [Simpson et al. 2020b](#)).

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9. Acknowledgements

This work was funded by the Swedish Strategic Research project MERGE, the Swedish FORMAS BVOC project, Swedish Research Science Council VR project Photosmog, and EMEP under UN-ECE. We thank Greg Yarwood for providing the CB6r2h code. The computations were partly performed on resources provided by UNINETT Sigma2 - the National Infrastructure for High Performance Computing and Data Storage in Norway (grant NN2890k and NS9005k). IT infrastructure in general was available through the Norwegian Meteorological Institute (MET Norway). The CPU time granted on the supercomputers owned by MET Norway has been of crucial importance, in addition to the CPU time made available by ECMWF to generate meteorology.

Appendices

A. MCMv3.3Em — differences to MCMv3.3.1

The GenChem version of MCM is denoted MCMv3.3Em — the differences to the official MCMv3.3.1 are mainly updates of some reaction rate coefficients to be in agreement with IUPAC recommendations from 2009–2018. A summary of the updates/differences compared to the official MCM version is given below.

- Reaction rates:

- The generic rate coefficient for $\text{RCO}_3 + \text{HO}_2$ reactions (KAPHO2) was updated to the IUPAC recommended rate coefficient (revised in March 2017) for $\text{HO}_2 + \text{CH}_3\text{C}(\text{O})\text{O}_2$: $k = 3.14 \times 10^{-12} \times e^{580/T}$ MCMv3.3.1 uses an older expression, $k = 5.2 \times 10^{-13} \times e^{980/T}$

Note that IUPAC has recently (Dec 2019) updated the recommended rate coefficient again but this update was too late to be included in the EmChem19 schemes and thus, we have kept the 2017 expression also in MCMv3.3Em — this will likely be updated in future versions of EmChem and MCMvEm. The Dec. 2019 recommendation from IUPAC is $k = 1.73 \times 10^{-12} \times e^{730/T}$, which is ca 5–9% slower than the MCMv3.3Em rate coefficient, and about 35–44% faster than the old rate coefficient used in MCMv3.3.1.

- The rate coefficients of three inorganic reactions were updated:
 - * $\text{O}(1\text{D}) + \text{N}_2 \longrightarrow \text{O}(3\text{P}) + \text{N}_2$, IUPAC June 2009: $k = 2.15 \times 10^{-11} \times e^{110/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, which is very similar to the slightly older k used in MCM
 - * $2 \text{NO} + \text{O}_2 \longrightarrow 2 \text{NO}_2$, IUPAC May 2014: $k = 4.25 \times 10^{-39} \times e^{663.5/T} \text{ cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$
 - * $\text{SO}_2 + \text{OH} \longrightarrow \text{HSO}_3$, IUPAC Nov 2017 (MCM use IUPAC 2012)
- The rate coefficients of some biogenic VOC reactions were updated:
 - * $\text{NO}_3 + \text{isoprene}$
 - * $\text{OH} + \text{isoprene}$
 - * $\text{OH} + \text{APINENE}$
 - * $\text{OH} + \text{BPINENE}$
 - * $\text{OH} + \text{LIMONENE}$
 - * $\text{O}_3 + \text{APINENE}$
 - * $\text{O}_3 + \text{BPINENE}$
 - * $\text{O}_3 + \text{LIMONENE}$

- The rate coefficients of three aldehyde + NO₃ reactions were revised:
 - * HCHO + NO₃
 - * GLYOX + NO₃
 - * MGLYOX + NO₃
- Updated rate coefficients and products for the OH oxidation of peroxyacetic acid (CH₃CO₃H), based on IUPAC recommendations Nov. 2017:

$$\text{CH}_3\text{CO}_3\text{H} + \text{OH} \longrightarrow 0.5 \text{ CH}_3\text{CO}_3 + 0.5 \text{ CH}_2\text{O}_2\text{CO}_3\text{H} + \text{H}_2\text{O}, \text{ with } k = 1.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

The peroxy radical product CH₂O₂CO₃H is not included in MCMv3.3.1 but has been added in MCMv3.3Em, assuming that it reacts with NO and NO₃ at “standard” RO₂ + NO and RO₂ + NO₃ rates, in the following simple reactions:

 - CH₂O₂CO₃H + NO → NO₂ + HOCH₂CO₃
 - CH₂O₂CO₃H + NO₃ → NO₂ + HOCH₂CO₃
- Revised pyruvic acid (CH₃COCO₂H) chemistry:
 - OH reaction rate coefficient updated to the IUPAC recommendation from June 2017: $k = 4.9 \times 10^{-14} \times e^{280/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$
 - Changed photolysis products, based on IUPAC recommendation (June 2017):

$$\text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{OH} + h\nu \longrightarrow 0.6 \text{ CH}_3\text{CHO} + 0.05 \text{ CH}_3\text{C}(\text{O})\text{OH} + 0.05 \text{ CO} + 0.35 \text{ CH}_3\text{C}(\text{O})\text{O}_2 + 0.35 \text{ HO}_2$$
- Two bugs were identified in the original version of MCMv3.3.1. These were corrected in MCMv3.3Em, and have now been corrected in MCM v3.3.1 on the MCM website:
 - The products of the M3BU3ECO₃ + HO₂ was corrected (NO₂ was inadvertently and incorrectly included as a reaction product).
 - The rate coefficient for the PPN dissociation reaction (PPN + M → C₂H₅CO₃ + NO₂) contained an error. The term "FPPN" in the final line of the calculation incorrectly appeared as "FCPPN".

B. Additional box model information

Table B.1: Box model VOC-emission split (MCMv3.3Em)

Alkanes		Aldehydes	
C ₂ H ₆	2.47×10^{-2}	HCHO	1.33×10^{-2}
C ₃ H ₈	4.29×10^{-2}	CH ₃ CHO	1.30×10^{-3}
n-C ₄ H ₁₀	1.05×10^{-1}	C ₂ H ₅ CHO	1.03×10^{-3}
i-C ₄ H ₁₀	3.26×10^{-2}	C ₃ H ₇ CHO	5.62×10^{-4}
n-C ₅ H ₁₂	4.93×10^{-2}	2-Methylpropanal	4.56×10^{-4}
i-C ₅ H ₁₂	3.67×10^{-2}	C ₄ H ₉ CHO	4.44×10^{-5}
Neopentane	3.03×10^{-3}		
n-C ₆ H ₁₄	3.04×10^{-2}	Ketones	
i-C ₆ H ₁₄	1.02×10^{-2}	CH ₃ COCH ₃	1.15×10^{-2}
3-Methylpentane	6.50×10^{-3}	2-Butanone	8.99×10^{-3}
2,2-Dimethylbutane	2.14×10^{-3}	3-Methyl-2-butanone	1.63×10^{-6}
2,3-Dimethylbutane	2.82×10^{-3}	3-Pentanone	1.99×10^{-4}
n-C ₇ H ₁₆	1.59×10^{-2}	2-Hexanone	2.64×10^{-4}
2-Methylhexane	5.31×10^{-3}	4-Methyl-2-pentanone	6.10×10^{-3}
3-Methylhexane	5.05×10^{-3}	Cyclohexanone	1.04×10^{-3}
n-C ₈ H ₁₈	2.45×10^{-2}		
n-C ₉ H ₂₀	8.92×10^{-3}	Alcohols and Glycols	
n-C ₁₀ H ₂₂	1.83×10^{-2}	CH ₃ OH	5.63×10^{-3}
n-C ₁₁ H ₂₄	1.47×10^{-2}	C ₂ H ₅ OH	7.44×10^{-2}
n-C ₁₂ H ₂₆	7.12×10^{-3}	n-C ₃ H ₇ OH	6.69×10^{-3}
Cyclohexane	2.00×10^{-2}	i-C ₃ H ₇ OH	7.83×10^{-3}
		n-C ₄ H ₉ OH	5.95×10^{-3}
Alkenes		2-Butanol	2.39×10^{-3}
C ₂ H ₄	3.15×10^{-2}	2-Methyl-1-propanol	1.57×10^{-3}
C ₃ H ₆	1.48×10^{-2}	2-Methyl-2-propanol	6.08×10^{-4}
1-Butene	4.00×10^{-3}	3-Methyl-1-butanol	3.36×10^{-7}
cis-2-Butene	3.91×10^{-3}	3-Methyl-2-butanol	4.05×10^{-5}
trans-2-Butene	3.96×10^{-3}	4-Hydroxy-4-methyl-2-pentanone	1.35×10^{-3}
2-Methylpropene	2.50×10^{-3}	Cyclohexanol	3.33×10^{-4}
1-Pentene	4.51×10^{-3}	1,2-Ethanediol	3.58×10^{-3}
cis-2-Pentene	2.18×10^{-3}	1,2-Propanediol	6.25×10^{-5}
trans-2-Pentene	2.47×10^{-3}		
2-Methyl-1-butene	8.78×10^{-4}	Ethers and Glycol Ethers	
3-Methyl-1-butene	1.11×10^{-3}	CH ₃ OCH ₃	5.70×10^{-4}
2-Methyl-2-butene	1.65×10^{-3}	Ethoxyethane	5.17×10^{-4}
1-Hexene	2.01×10^{-3}	Diisopropylether	2.97×10^{-4}
cis-2-Hexene	1.50×10^{-4}	2-Methoxyethanol	9.34×10^{-8}
trans-2-Hexene	1.50×10^{-4}	1-Methoxy-2-propanol	9.49×10^{-4}
		2-Ethoxyethanol	1.85×10^{-3}
Dialkenes		1-Methoxy-2-propanol	3.33×10^{-3}
1,3-Butadiene	4.23×10^{-3}	1-Butoxy-2-propanol	2.50×10^{-4}
Alkynes		Organic acids	
C ₂ H ₂	1.20×10^{-2}	HCOOH	7.22×10^{-8}
		CH ₃ COOH	1.35×10^{-3}
		C ₂ H ₅ COOH	2.45×10^{-5}
Aromatics			
Benzene	2.02×10^{-2}	Esters	
Toluene	5.82×10^{-2}	CH ₃ OCHO	1.96×10^{-5}
o-Xylene	1.52×10^{-2}	Methylacetate	5.33×10^{-3}
m-Xylene	2.60×10^{-2}	Ethylacetate	9.86×10^{-3}
p-Xylene	2.03×10^{-2}	n-Propylacetate	1.07×10^{-3}
Ethylbenzene	1.42×10^{-2}	i-Propylacetate	3.01×10^{-3}
1,2,3-Trimethylbenzene	3.55×10^{-3}	n-Butylacetate	7.72×10^{-3}
1,2,4-Trimethylbenzene	1.18×10^{-2}	sec-Butylacetate	3.51×10^{-4}
1,3,5-Trimethylbenzene	4.08×10^{-3}		
o-Ethyltoluene	3.24×10^{-3}	Unclassified	
m-Ethyltoluene	5.14×10^{-3}	Dimethylcarbonate	4.06×10^{-6}
p-Ethyltoluene	4.52×10^{-3}		
n-Propylbenzene	2.80×10^{-3}		
i-Propylbenzene	1.50×10^{-3}		
1-Ethyl-3,5-dimethylbenzene	9.26×10^{-3}		
1,3-Diethyl-5-methylbenzene	1.59×10^{-3}		
Ethynylbenzene	3.12×10^{-3}		

Table B.2: Box model VOC-emission split (mass-based) for EmChem19a+EmChem19X, and CRIV2R5Em

Species	EmChem19a, EmChem19X	CRIV2R5Em
Alkanes		
C ₂ H ₆	0.10056	0.0247
C ₃ H ₈	†	0.0429
n-C ₄ H ₁₀	0.39526	0.39849
Alkenes		
C ₂ H ₄	0.04839	0.0315
C ₃ H ₆	0.03162	0.014
trans-2-butene	†	0.03371
Alkynes		
C ₂ H ₂	†	0.012
Aromatics		
Benzene	0.0202	0.0202
Toluene	0.0582	0.0582
o-Xylene	0.12318	0.1263
Aldehydes		
HCHO	0.01797	0.0133
CH ₃ CHO	0.00294	0.00176
C ₂ H ₅ CHO	†	0.00164
Ketones		
2-Butanone	0.02038	0.01659
CH ₃ COCH ₃	†	0.0115
Alcohols		
CH ₃ OH	0.03351	0.01464
C ₂ H ₅ OH	0.09385	0.10356
Unreactive		
Unreactive	0.05395	0.04548

Notes: † indicates species not present in EmChem schemes.

Table B.3: Box model VOC molecular weight (MW) and emission split (fraction, mass-based) for CB6r2Em

CB6-species	MW	Fraction
PAR	12	0.38235
ETHA	30.07	0.0247
PRPA	44.1	0.0429
OLE	24	0.01676
IOLE	48	0.01009
ETH	28.05	0.0315
ETHY	26.04	0.012
BENZ	78.11	0.0202
TOL	84	0.069815
XYL	96	0.089083
FORM	12	0.006
ALD2	24	0.001273
ALDX	24	0.00103
KET	12	0.002553
ACET	58.08	0.0115
MEOH	32.04	0.00563
ETOH	46.07	0.0744
AACD	60.05	0.00135
Other†	N/A	0.19687

Notes: † the “Other” mass-fraction includes hydrogen and oxygen associated with emitted species modelled as PAR, OLE, IOLE, FORM, ALD2, ALDX and KET, as well as the Unreactive fraction of the VOC-emissions.

C. Additional box model results

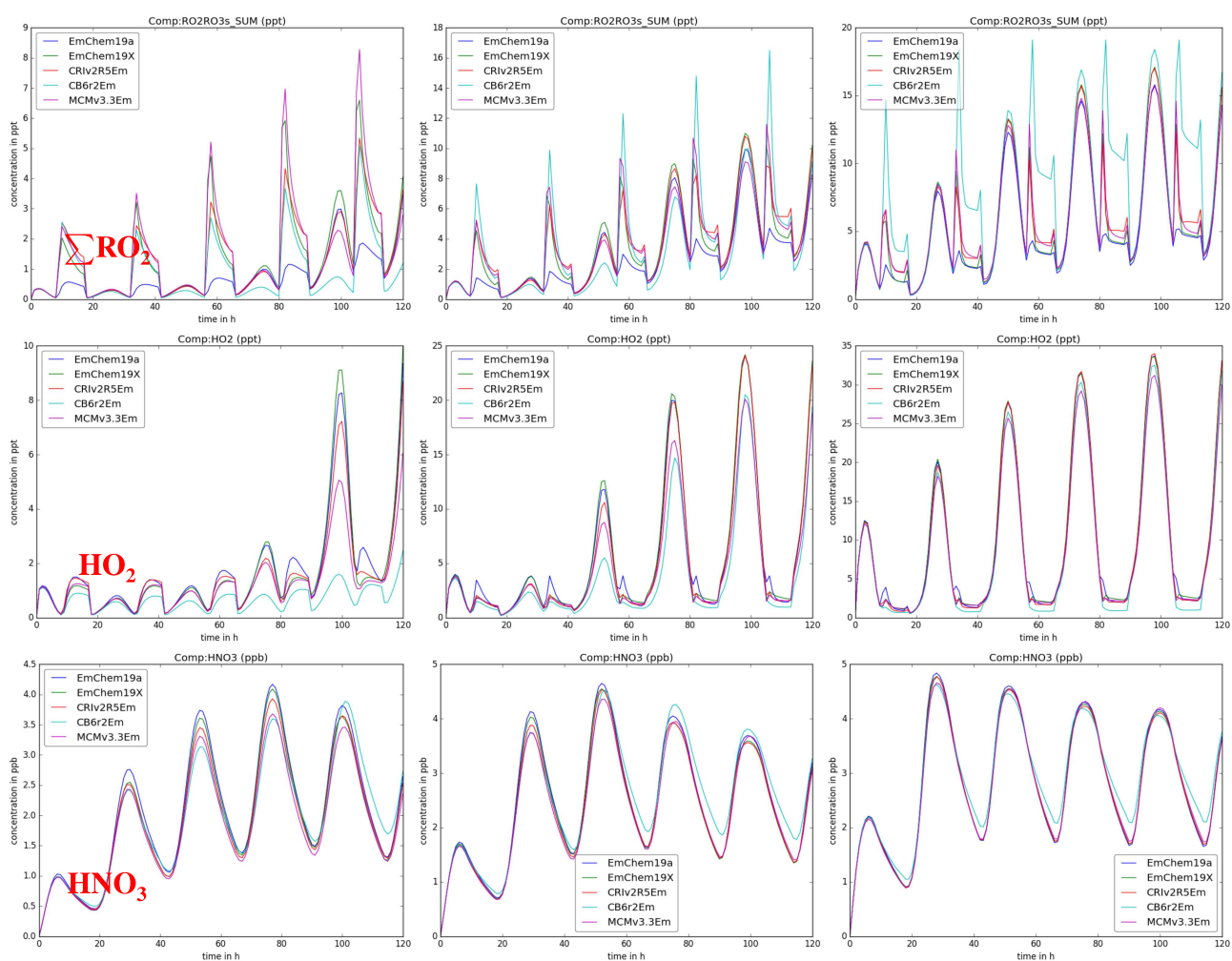


Figure C.1: Model simulated sum of total organic peroxy and acyl peroxy radicals (denoted ΣRO_2 , ppt), HO_2 (ppt), and HNO_3 (ppb). Columns, left to right, give results at $T = 278$, 288 and 299 K. Model set-up: Base-case.

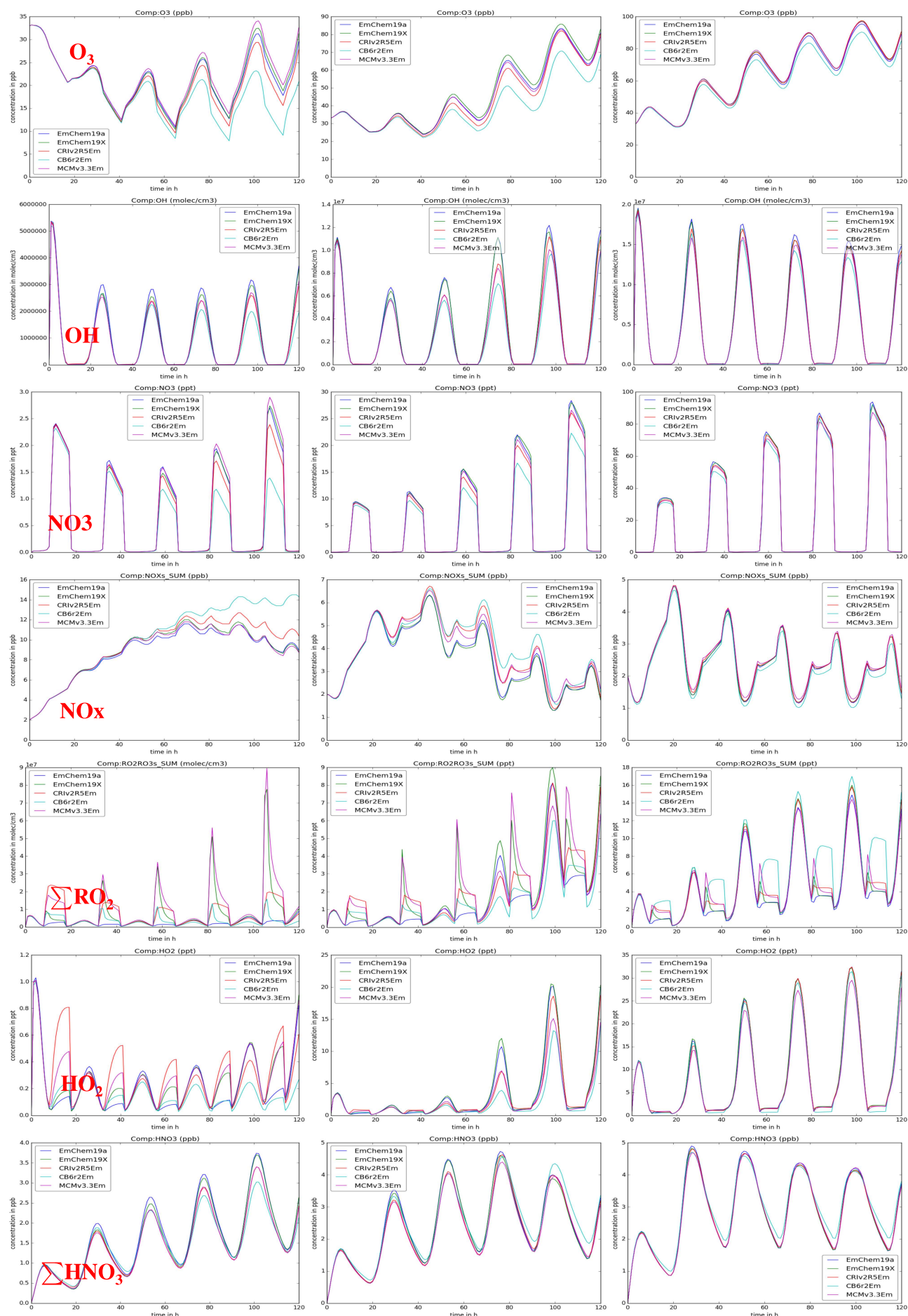


Figure C.2: Model simulated O_3 (ppb), OH (molec/cm³), NO_3 (ppt), NO_x (ppb), ΣRO_2 (molec/cm³ for 278K, otherwise ppt), HO_2 (ppt), and HNO_3 (ppb) at T=278K (left), 288K (middle), and 298K (right). Model set-up: BNOxZBio

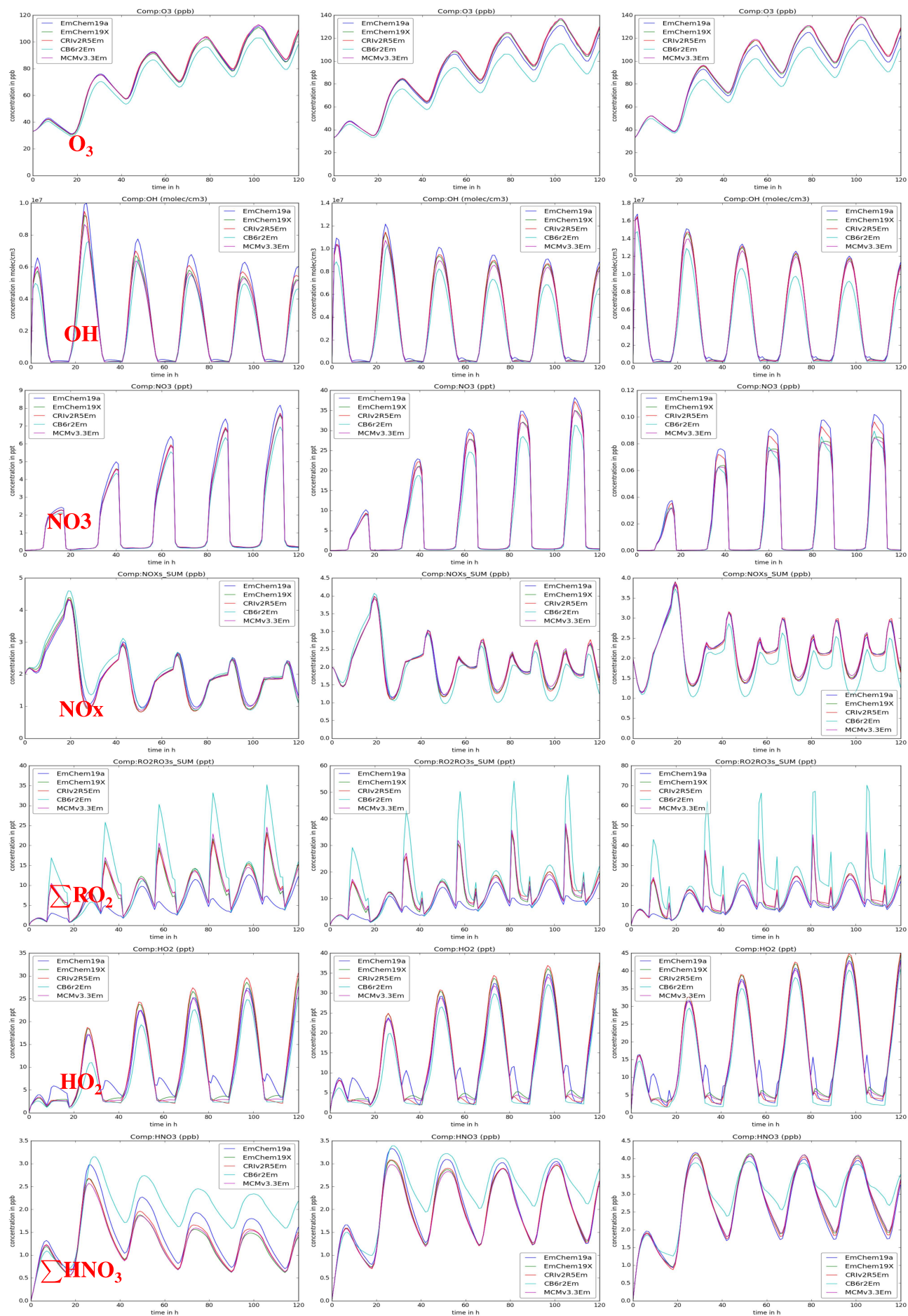


Figure C.3: Model simulated O_3 (ppb), OH (molec/cm³), NO_3 (ppb for T=298, else ppt), NO_x (ppb), ΣRO_2 (ppt), HO_2 (ppt), and HNO_3 (ppb) at T=278K (left), 288K (middle), and 298K (right). Model set-up: BNOxHBio

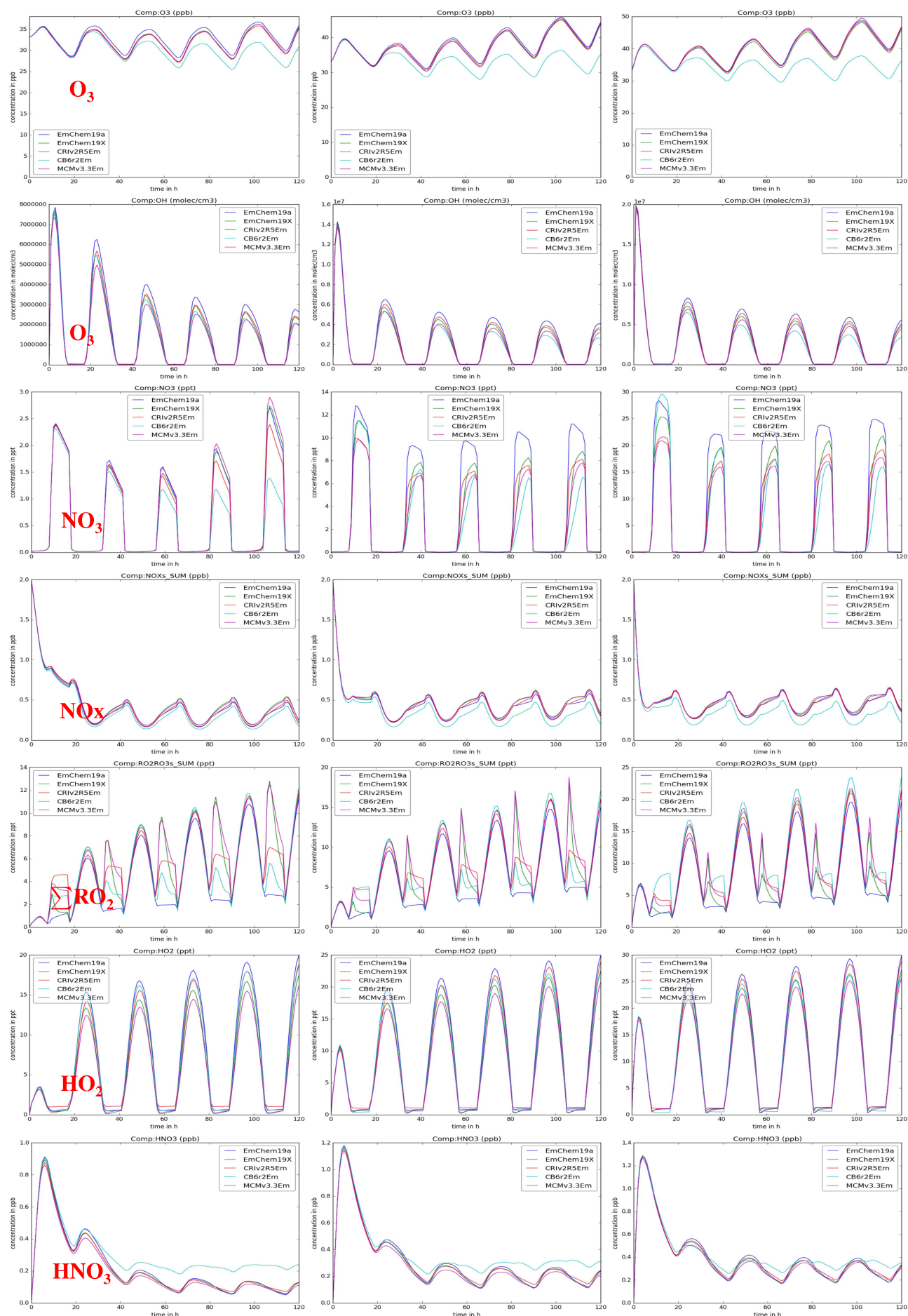


Figure C.4: Model simulated O_3 (ppb), OH (molec/cm³, NO_3 (ppt), NO_x (ppb), ΣRO_2 (ppt), HO_2 (ppt), and HNO_3 (ppb) at T=278K (left), 288K (middle), and 298K (right). Model set-up: LNOxZBio

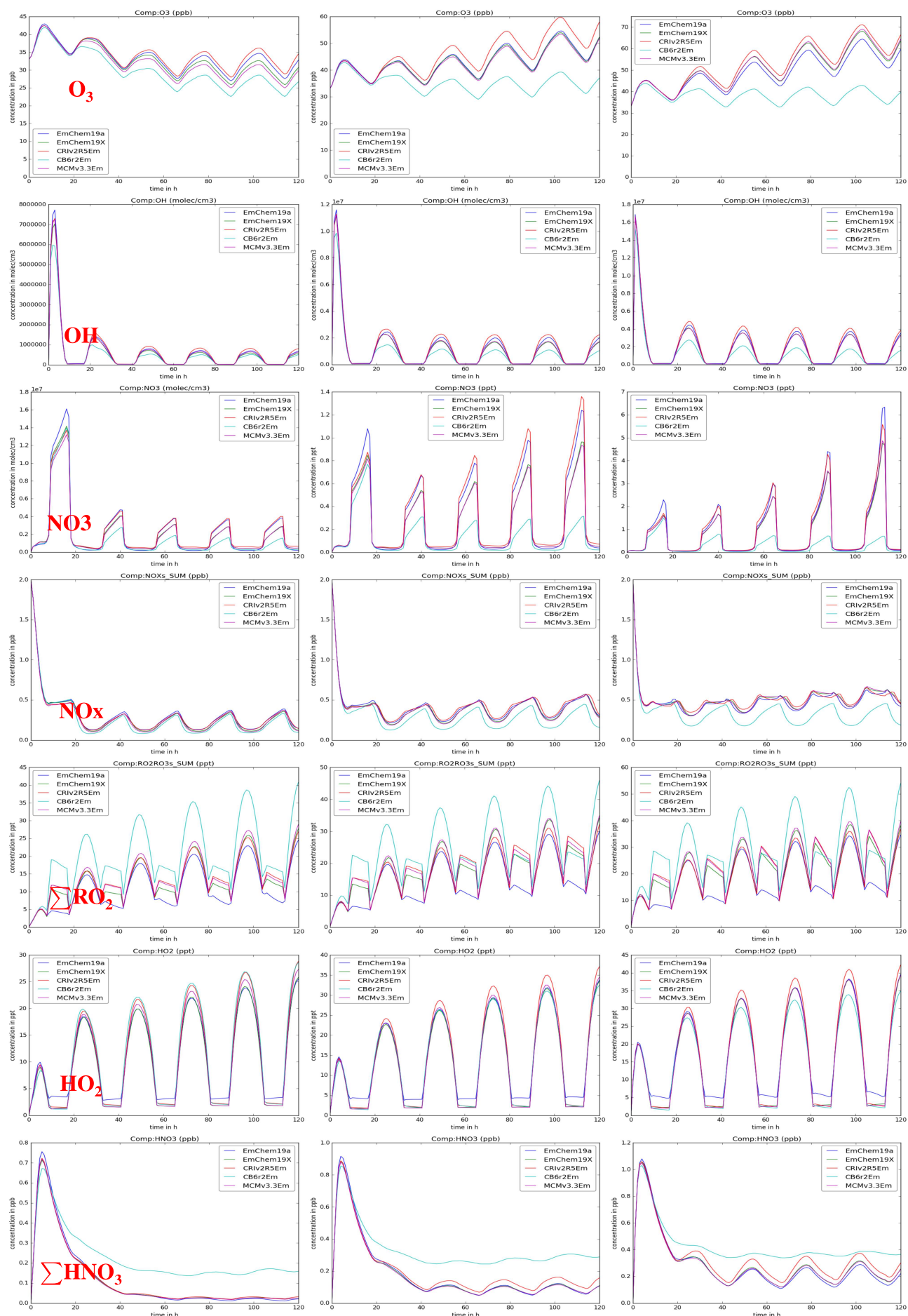


Figure C.5: Model simulated O_3 (ppb), OH (molec/cm³), NO_3 (molec/cm³ for T=278K, otherwise ppt), NO_x (ppb), ΣRO_2 (ppt), HO_2 (ppt), and HNO_3 (ppb) at T=278K (left), 288K (middle), and 298K (right). Model set-up: LNOxHBio

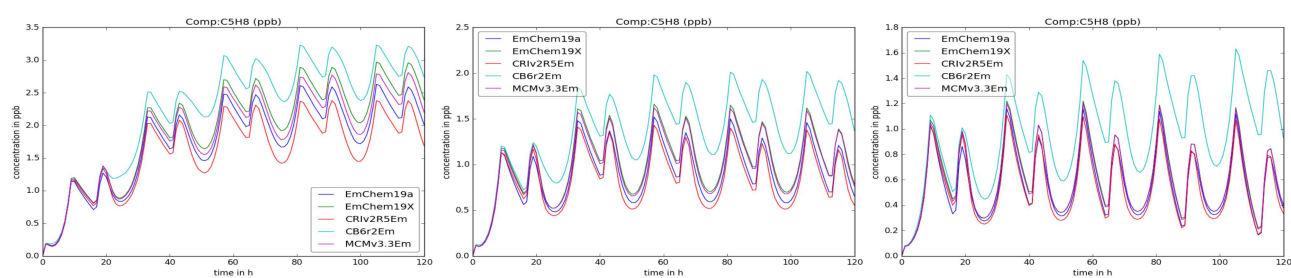


Figure C.6: Model simulated C_5H_8 at $T=278K$ (left), $288K$ (middle), and $298K$ (right). Model set-up: LNOxHBio

D. VOC Emissions mapping

Table D.1: VOC-emission surrogates in EmChem19a and EmChem19X — MCM (emission)
VOC species mapped to EmChem19 species (mass based)

MCM species	VOC	C2H6	NC4H10	C2H4	C3H6	OXYL	APINENE	CH3OH	C2H5OH	HCHO	CH3CHO	MEK
C2H6	ethane	1	0	0	0	0	0	0	0	0	0	0
C3H8	propane	1	0	0	0	0	0	0	0	0	0	0
NC4H10	n-butane	0	1	0	0	0	0	0	0	0	0	0
IC4H10	2-methylpropane	0	1	0	0	0	0	0	0	0	0	0
NC5H12	n-pentane	0	1	0	0	0	0	0	0	0	0	0
IC5H12	2-methyl-butane	0	1	0	0	0	0	0	0	0	0	0
NEOP	2,2-dimethylpropane	1	0	0	0	0	0	0	0	0	0	0
NC6H14	n-hexane	0	1	0	0	0	0	0	0	0	0	0
M2PE	2-methylpentane	0	1	0	0	0	0	0	0	0	0	0
M3PE	3-methylpentane	0	1	0	0	0	0	0	0	0	0	0
M22C4	2,2-dimethylbutane	1	0	0	0	0	0	0	0	0	0	0
M23C4	2,3-dimethylbutane	0	1	0	0	0	0	0	0	0	0	0
NC7H16	n-heptane	0	1	0	0	0	0	0	0	0	0	0
M2HEX	2-methylhexane	0	1	0	0	0	0	0	0	0	0	0
M3HEX	3-methylhexane	0	1	0	0	0	0	0	0	0	0	0
NC8H18	n-octane	0	1	0	0	0	0	0	0	0	0	0
NC9H20	n-nonane	0	1	0	0	0	0	0	0	0	0	0
NC10H22	n-decane	0	1	0	0	0	0	0	0	0	0	0
NC11H24	n-undecane	0	1	0	0	0	0	0	0	0	0	0
NC12H26	n-dodecane	0	1	0	0	0	0	0	0	0	0	0
CHEX	cyclohexane	0	1	0	0	0	0	0	0	0	0	0
C2H4	ethylene	0	0	1	0	0	0	0	0	0	0	0
C3H6	propylene	0	0	0	1	0	0	0	0	0	0	0
BUT1ENE	1-butene	0	0	0	1	0	0	0	0	0	0	0
CBUT2ENE	cis-2-butene	0	0	0	1	0	0	0	0	0	0	0
TBUT2ENE	trans-2-butene	0	0	0	1	0	0	0	0	0	0	0
MEPROPENE	2-methylpropene	0	0	1	0	0	0	0	0	0	0	0
PENT1ENE	1-pentene	0	0	1	0	0	0	0	0	0	0	0
CPENT2ENE	cis-2-pentene	0	0	0	1	0	0	0	0	0	0	0
TPENT2ENE	trans-2-pentene	0	0	0	1	0	0	0	0	0	0	0
ME2BUT1ENE	2-methyl-1-butene	0	0	1	0	0	0	0	0	0	0	0
ME3BUT1ENE	3-methyl-1-butene	0	0	1	0	0	0	0	0	0	0	0
ME2BUT2ENE	2-methyl-2-butene	0	0	1	0	0	0	0	0	0	0	0
HEX1ENE	1-hexene	0	0	1	0	0	0	0	0	0	0	0
CHEX2ENE	cis-2-hexene	0	0	0	1	0	0	0	0	0	0	0
THEX2ENE	trans-2-hexene	0	0	0	1	0	0	0	0	0	0	0
DM23BU2ENE	2,3-dimethyl-1-butene	0	0	0	1	0	0	0	0	0	0	0
C4H6	1,3-butadiene	0	0	1	0	0	0	0	0	0	0	0
APINENE	a-pinene	0	0	0	0	0	1	0	0	0	0	0
BPINENE	b-pinene	0	0	0	0	0	1	0	0	0	0	0
LIMONENE	d-limonene	0	0	0	0	0	1	0	0	0	0	0
C2H2	acetylene	0	0	0	0	0	0	1	0	0	0	0
OXYL	o-xylene	0	0	0	0	1	0	0	0	0	0	0
MXYL	m-xylene	0	0	0	0	1	0	0	0	0	0	0
PXYL	p-xylene	0	0	0	0	1	0	0	0	0	0	0
EBENZ	ethylbenzene	0	0	0	0	1	0	0	0	0	0	0
PBENZ	n-propylbenzene	0	0	0	0	1	0	0	0	0	0	0
IPBENZ	isopropyl benzene	0	0	0	0	1	0	0	0	0	0	0
TM123B	1,2,3-trimethylbenzene	0	0	0	0	1	0	0	0	0	0	0
TM124B	1,2,4-trimethylbenzene	0	0	0	0	1	0	0	0	0	0	0
TM135B	1,3,5-trimethylbenzene	0	0	0	0	1	0	0	0	0	0	0
OETHTOL	o-ethyltoluene	0	0	0	0	1	0	0	0	0	0	0
METHTOL	m-ethyltoluene	0	0	0	0	1	0	0	0	0	0	0
PETHTOL	p-ethyltoluene	0	0	0	0	1	0	0	0	0	0	0
DIME35EB	1-Ethyl-3,5-dimethylbenzene	0	0	0	0	1	0	0	0	0	0	0
DIET35TOL	3,5-diethyltoluene	0	0	0	0	1	0	0	0	0	0	0
CH3OH	methyl alcohol	0	0	0	0	0	0	1	0	0	0	0
C2H5OH	ethyl alcohol	0	0	0	0	0	0	0	1	0	0	0
NPROPOL	n-propyl alcohol	0	0	0	0	0	0	0	1	0	0	0
IPROPOL	isopropyl alcohol	0.5	0	0	0	0	0	0.5	0	0	0	0
NBUTOL	n-butyl alcohol	0	0	0	0	0	0	0	1	0	0	0
BUT2OL	sec-butyl alcohol	0	0	0	0	0	0	0	0	0	0	1
TBUTOL	tert-butyl alcohol	0	0	0	0	0	0	1	0	0	0	0
IBUTOL	isobutyl alcohol	0	0	0	0	0	0	0	1	0	0	0
ME3BUOL	3-methyl-1-butanol	0	0	0	0	0	0	0	0	1	0	0
CYHEXOL	cyclohexanol	0	0	0	0	0	0	0	0	1	0	0
PECOH	3-pentanol	0	0	0	0	0	0	0	0	0	0	1
IPEAOH	2-methyl-1-butanol	0	1	0	0	0	0	0	0	0	0	0
IPECOH	2-methyl-2-butanol	0	0	0	0	0	0	1	0	0	0	0
IPEBOH	3-methyl-2-butanol	0	0	0	0	0	0	0	0	0	0	1

EmChem19 emissions split (continued on next page)

MCM species	VOC	C2H6	NC4H10	C2H4	C3H6	OXYL	APINENE	CH3OH	C2H5OH	HCHO	CH3CHO	MEK
MBO	2-methyl-3-buten-2-ol	0	0	0	1	0	0	0	0	0	0	0
ETHGLY	ethylene glycol	0	0	0	0	0	0	0	0	1	0	0
PROPGLY	propylene glycol	0	0	0	0	0	0	0	1	0	0	0
HCHO	formaldehyde	0	0	0	0	0	0	0	0	1	0	0
CH3CHO	acetaldehyde	0	0	0	0	0	0	0	0	0	1	0
C2H5CHO	propionaldehyde	0	0	0	0	0	0	0	0	0	1	0
C3H7CHO	butyraldehyde	0	0	0	0	0	0	0	0	0	1	0
IPRCHO	isobutyraldehyde	0	0	0	0	0	0	0	0	1	0	0
C4H9CHO	n-pentanal	0	0	0	0	0	0	0	0	0	1	0
CH3COCH3	acetone	0.5	0	0	0	0	0	0.5	0	0	0	0
MEK	methyl ethyl ketone	0	0	0	0	0	0	0	0	0	0	1
MPRK	2-pentanone	0	0	0	0	0	0	0	0	0	1	0
MIPK	methyl isopropyl ketone	0	0	0	0	0	0	0	0	0	0	1
DIEK	3-pentanone	0	0	0	0	0	0	0	0	0	0	1
HEX2ONE	methyl n-butyl ketone	0	0	0	0	0	0	0	0	0	0	1
HEX3ONE	3-hexanone	0	0	0	0	0	0	0	0	0	1	0
MIBK	methyl isobutyl ketone	0	0	0	0	0	0	0	0	0	0	1
MTBK	tert-butyl methyl ketone	0	1	0	0	0	0	0	0	0	0	0
CYHEXONE	cyclohexanone	0.5	0	0	0	0	0	0	0	0	0	0.5
MIBKAOH	4-hydroxy-4-methyl-2-pentanone	0	0	0	0	0	0	0.5	0	0	0	0.5
CH3CO2H	acetic acid	0	0	0	0	0	0	1	0	0	0	0
PROPACID	propionic acid	1	0	0	0	0	0	0	0	0	0	0
CH3OCH3	dimethyl ether	0	0	0	0	0	0	1	0	0	0	0
DIETETHER	ethyl ether	0	1	0	0	0	0	0	0	0	0	0
MTBE	methyl t-butyl ether	0	0	0	0	0	0	1	0	0	0	0
ETBE	ethyl t-butyl ether	0	0	0	0	0	0	1	0	0	0	0
DIIPREETHER	diisopropyl ether	0	0	0	0	0	0	0	0	1	0	0
MO2EOL	2-methoxyethanol	0	1	0	0	0	0	0	0	0	0	0
EOX2EOL	2-ethoxyethanol	0	0	0	0	0	0	0	1	0	0	0
PR2OHMOX	1-methoxy-2-propanol	0	0	0	0	0	0	0	0	0	0	1
BUOX2ETOH	2-butoxyethanol	0	0	0	0	0	0	0	1	0	0	0
BOX2PROL	1-butoxy-2-propanol	0	0	0	0	0	0	0	0	0	0	1
ETHACET	ethyl acetate	1	0	0	0	0	0	0	0	0	0	0
NPROACET	propyl acetate	0	1	0	0	0	0	0	0	0	0	0
IPROACET	isopropyl acetate	0	0	0	0	0	0	1	0	0	0	0
NBUTACET	n-butyl acetate	1	0	0	0	0	0	0	0	0	0	0
SBUTACET	s-butyl acetate	0	1	0	0	0	0	0	0	0	0	0
DMM	dimethoxymethane	1	0	0	0	0	0	0	0	0	0	0
CCL2CH2	1,1-dichloroethene	0	0	0	0	0	0	0	0	1	0	0
TDICLETH	trans-1,2-dichloroethene	0	1	0	0	0	0	0	0	0	0	0
CDICLETH	cis-1,2-dichloroethene	0	1	0	0	0	0	0	0	0	0	0
TRICLETH	trichloroethylene	0	1	0	0	0	0	0	0	0	0	0

Notes:

The following (potentially) emitted VOC species are treated explicitly in the EmChem19a and EmChem19X simulations:

CH4, C5H8, BENZENE, TOLUENE, GLYOX(glyoxal), MGLYOX(methylglyoxal).

The following emitted species (from MCM) are treated as unreactive emissions in the EmChem19a and EmChem19X simulations:

STYRENE, BENZAL(benzaldehyde), HCOOH, CH3OCHO, METHACET(methyl acetate), TBUCET(t-butyl acetate), DMC(dimethyl carbonate),

and all halogenated species except the four included in the Table above.

Table D.2: VOC-emission surrogates in CRIV2R5Em used in the model simulations presented here — MCM emission species mapped to CRIV2R5Em species (mass based); the surrogate choice is based on the R5 reduction of [Watson et al. \(2008\)](#)

MCM species	VOC	C3H8	NC4H10	TBUT2ENE	OXYL	CH3OH	C2H5OH	HCHO	CH3CHO	C2H5CHO	MEK	HCOOH	CH3CO2H
C3H8	propane	1	0	0	0	0	0	0	0	0	0	0	0
NC4H10	n-butane	0	1	0	0	0	0	0	0	0	0	0	0
IC4H10	2-methylpropane	0	1	0	0	0	0	0	0	0	0	0	0
NC5H12	n-pentane	0	1	0	0	0	0	0	0	0	0	0	0
IC5H12	2-methyl-butane	0	1	0	0	0	0	0	0	0	0	0	0
NEOP	2,2-dimethylpropane	0	1	0	0	0	0	0	0	0	0	0	0
NC6H14	n-hexane	0	1	0	0	0	0	0	0	0	0	0	0
M2PE	2-methylpentane	0	1	0	0	0	0	0	0	0	0	0	0
M3PE	3-methylpentane	0	1	0	0	0	0	0	0	0	0	0	0
M22C4	2,2-dimethylbutane	0	1	0	0	0	0	0	0	0	0	0	0
M23C4	2,3-dimethylbutane	0	1	0	0	0	0	0	0	0	0	0	0
NC7H16	n-heptane	0	1	0	0	0	0	0	0	0	0	0	0
M2HEX	2-methylhexane	0	1	0	0	0	0	0	0	0	0	0	0
M3HEX	3-methylhexane	0	1	0	0	0	0	0	0	0	0	0	0
NC8H18	n-octane	0	1	0	0	0	0	0	0	0	0	0	0
NC9H20	n-nonane	0	1	0	0	0	0	0	0	0	0	0	0
NC10H22	n-decane	0	1	0	0	0	0	0	0	0	0	0	0

CRIV2R5Em emissions split (continued on next page)

MCM species	VOC	C3H8	NC4H10	TBUT2ENE	OXYL	CH3OH	C2H5OH	HCHO	CH3CHO	C2H5CHO	MEK	HCOOH	CH3CO2H
NC11H24	n-undecane	0	1	0	0	0	0	0	0	0	0	0	0
NC12H26	n-dodecane	0	1	0	0	0	0	0	0	0	0	0	0
CHEX	cyclohexane	0	1	0	0	0	0	0	0	0	0	0	0
BUT1ENE	1-butene	0	0	1	0	0	0	0	0	0	0	0	0
CBUT2ENE	cis-2-butene	0	0	1	0	0	0	0	0	0	0	0	0
TBUT2ENE	trans-2-butene	0	0	1	0	0	0	0	0	0	0	0	0
MEPROPENE	2-methylpropene	0	0	1	0	0	0	0	0	0	0	0	0
PENT1ENE	1-pentene	0	0	1	0	0	0	0	0	0	0	0	0
CPENT2ENE	cis-2-pentene	0	0	1	0	0	0	0	0	0	0	0	0
TPENT2ENE	trans-2-pentene	0	0	1	0	0	0	0	0	0	0	0	0
ME2BUT1ENE	2-methyl-1-butene	0	0	1	0	0	0	0	0	0	0	0	0
ME3BUT1ENE	3-methyl-1-butene	0	0	1	0	0	0	0	0	0	0	0	0
ME2BUT2ENE	2-methyl-2-butene	0	0	1	0	0	0	0	0	0	0	0	0
HEX1ENE	1-hexene	0	0	1	0	0	0	0	0	0	0	0	0
CHEX2ENE	cis-2-hexene	0	0	1	0	0	0	0	0	0	0	0	0
THEX2ENE	trans-2-hexene	0	0	1	0	0	0	0	0	0	0	0	0
DM23BU2ENE	2,3-dimethyl-1-butene	0	0	1	0	0	0	0	0	0	0	0	0
C4H6	1,3-butadiene	0	0	1	0	0	0	0	0	0	0	0	0
OXYL	o-xylene	0	0	0	1	0	0	0	0	0	0	0	0
MXYL	m-xylene	0	0	0	1	0	0	0	0	0	0	0	0
PXYL	p-xylene	0	0	0	1	0	0	0	0	0	0	0	0
EBENZ	ethylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
PBENZ	n-propylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
IPBENZ	isopropyl benzene	0	0	0	1	0	0	0	0	0	0	0	0
TM123B	1,2,3-trimethylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
TM124B	1,2,4-trimethylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
TM135B	1,3,5-trimethylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
OETHTOL	o-ethyltoluene	0	0	0	1	0	0	0	0	0	0	0	0
METHTOL	m-ethyltoluene	0	0	0	1	0	0	0	0	0	0	0	0
PETHTOL	p-ethyltoluene	0	0	0	1	0	0	0	0	0	0	0	0
DIME35EB	1-Ethyl-3,5-dimethylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
DIET35TOL	3,5-diethyltoluene	0	0	0	1	0	0	0	0	0	0	0	0
STYRENE	ethenylbenzene	0	0	0	1	0	0	0	0	0	0	0	0
BENZAL	benzaldehyde	0	0	0	1	0	0	0	0	0	0	0	0
PHENOL	phenol	0	0	0	1	0	0	0	0	0	0	0	0
CRESOL	2-methylphenol	0	0	0	1	0	0	0	0	0	0	0	0
CATECHOL	1,2-benzenediol	0	0	0	1	0	0	0	0	0	0	0	0
PHCOME	acetophenone	0	0	0	1	0	0	0	0	0	0	0	0
CH3OH	methyl alcohol	0	0	0	0	1	0	0	0	0	0	0	0
C2H5OH	ethyl alcohol	0	0	0	0	0	1	0	0	0	0	0	0
NPROPOL	n-propyl alcohol	0	0	0	0	0	1	0	0	0	0	0	0
IPROPOL	isopropyl alcohol	0	0	0	0	1	0	0	0	0	0	0	0
NBUTOL	n-butyl alcohol	0	0	0	0	0	1	0	0	0	0	0	0
BUT2OL	sec-butyl alcohol	0	0	0	0	0	1	0	0	0	0	0	0
TBUTOL	tert-butyl alcohol	0	0	0	0	1	0	0	0	0	0	0	0
IBUTOL	isobutyl alcohol	0	0	0	0	0	1	0	0	0	0	0	0
ME3BUOL	3-methyl-1-butanol	0	0	0	0	0	1	0	0	0	0	0	0
CYHEXOL	cyclohexanol	0	0	0	0	0	1	0	0	0	0	0	0
PECOH	3-pentanol	0	0	0	0	0	1	0	0	0	0	0	0
IPEAOH	2-methyl-1-butanol	0	0	0	0	0	1	0	0	0	0	0	0
IPECOH	2-methyl-2-butanol	0	0	0	0	1	0	0	0	0	0	0	0
IPEBOH	3-methyl-2-butanol	0	0	0	0	0	1	0	0	0	0	0	0
MIBKAOH	4-hydroxy-4-methyl-2-pentanone	0	0	0	0	0	1	0	0	0	0	0	0
MBO	2-methyl-3-buten-2-ol	0	0	0	0	0	1	0	0	0	0	0	0
ETHGLY	ethylene glycol	0	0	0	0	0	1	0	0	0	0	0	0
PROGLY	propylene glycol	0	0	0	0	0	1	0	0	0	0	0	0
HCHO	formaldehyde	0	0	0	0	0	0	1	0	0	0	0	0
CH3CHO	acetaldehyde	0	0	0	0	0	0	0	1	0	0	0	0
C2H5CHO	propionaldehyde	0	0	0	0	0	0	0	0	1	0	0	0
C3H7CHO	butyraldehyde	0	0	0	0	0	0	0	0	1	0	0	0
IPRCHO	isobutyraldehyde	0	0	0	0	0	0	0	1	0	0	0	0
C4H9CHO	n-pentanal	0	0	0	0	0	0	0	0	1	0	0	0
ACR	acrolein	0	0	0	0	0	0	0	1	0	0	0	0
MACR	methacrolein	0	0	0	0	0	0	0	0	1	0	0	0
C4ALDB	2-butenal	0	0	0	0	0	0	0	0	1	0	0	0
MEK	methyl ethyl ketone	0	0	0	0	0	0	0	0	0	1	0	0
MPRK	2-pentanone	0	0	0	0	0	0	0	0	0	1	0	0
MIPK	methyl isopropyl ketone	0	0	0	0	0	0	0	0	0	1	0	0
DIEK	3-pentanone	0	0	0	0	0	0	0	0	0	1	0	0
HEX2ONE	methyl n-butyl ketone	0	0	0	0	0	0	0	0	0	1	0	0
HEX3ONE	3-hexanone	0	0	0	0	0	0	0	0	0	1	0	0
MIBK	methyl isobutyl ketone	0	0	0	0	0	0	0	0	0	1	0	0
MTBK	tert-butyl methyl ketone	0	0	0	0	0	0	0	0	0	1	0	0
CYHEXONE	cyclohexanone	0	0	0	0	0	0	0	0	0	1	0	0
MVK	methyl vinyl ketone	0	0	0	0	0	0	0	0	0	1	0	0
MVMK	3-methyl-3-buten-2-one	0	0	0	0	0	0	0	0	0	1	0	0
GLYOX	ethanedial	0	0	0	0	0	0	0	1	0	0	0	0
MGLYOX	2-oxo-propanal	0	0	0	0	0	0	0	0	1	0	0	0
EGLYOX	2-oxo-butanal	0	0	0	0	0	0	0	0	1	0	0	0

CRIV2R5Em emissions split (continued on next page)

MCM species	VOC	C3H8	NC4H10	TBUT2ENE	OXYL	CH3OH	C2H5OH	HCHO	CH3CHO	C2H5CHO	MEK	HCOOH	CH3CO2H
BIACET	2,3-butanedione	0	0	0	0	0	0	0	0	0	1	0	0
HCOOH	formic acid	0	0	0	0	0	0	0	0	0	0	1	0
CH3CO2H	acetic acid	0	0	0	0	0	0	0	0	0	0	0	1
PROPACID	propionic acid	0	0	0	0	0	0	0	0	0	0	0	1
CH3OCH3	dimethyl ether	0	0	0	0	1	0	0	0	0	0	0	0
DIETETHER	ethyl ether	0	0	0	0	0	1	0	0	0	0	0	0
MTBE	methyl t-butyl ether	0	0	0	0	1	0	0	0	0	0	0	0
ETBE	ethyl t-butyl ether	0	0	0	0	1	0	0	0	0	0	0	0
DIIPREETHER	diisopropyl ether	0	0	0	0	0	1	0	0	0	0	0	0
MO2EOL	2-methoxyethanol	0	0	0	0	0	1	0	0	0	0	0	0
EOX2EOL	2-ethoxyethanol	0	0	0	0	0	1	0	0	0	0	0	0
PR2OHMOX	1-methoxy-2-propanol	0	0	0	0	0	1	0	0	0	0	0	0
BUOX2ETOH	2-butoxyethanol	0	0	0	0	0	1	0	0	0	0	0	0
BOX2PROL	1-butoxy-2-propanol	0	0	0	0	0	1	0	0	0	0	0	0
CH3OCHO	methyl formate	0	0	0	0	0	0	0	0	0	0	1	0
METHACET	methyl acetate	0	0	0	0	0	0	0	0	0	0	1	0
ETHACET	ethyl acetate	0	0	0	0	0	0	0	0	0	0	0	1
NPROACET	propyl acetate	0	0	0	0	0	0	0	0	0	0	0	1
IPOACET	isopropyl acetate	0	0	0	0	0	0	0	0	0	0	0	1
NBUTACET	n-butyl acetate	0	0	0	0	0	0	0	0	0	0	0	1
SBUTACET	s-butyl acetate	0	0	0	0	0	0	0	0	0	0	0	1
TBUACET	t-butyl acetate	0	0	0	0	0	0	0	0	0	0	0	1
DMM	dimethoxymethane	1	0	0	0	0	0	0	0	0	0	0	0
DMC	dimethyl carbonate	0	0	0	0	0	0	0	0	0	0	1	0
CCL2CH2	1,1-dichloroethene	0	0	0	0	0	0	1	0	0	0	0	0
TDICLETH	trans-1,2-dichloroethene	1	0	0	0	0	0	0	0	0	0	0	0
CDICLETH	cis-1,2-dichloroethene	0	1	0	0	0	0	0	0	0	0	0	0
TRICLETH	trichloroethylene	1	0	0	0	0	0	0	0	0	0	0	0

Notes:

The following (potentially) emitted VOC species are treated explicitly in the CRIV2R5Em simulations presented here:

CH4, C2H6, C2H4, C3H6, C2H2, C5H8(isoprene), BENZENE, TOLUENE, CH3COCH3;

APINENE and BPINENE can be treated as individual emitted species or lumped together and using APINENE as surrogate for all monoterpene emissions.

All halogenated species except the four included in the Table above are treated as unreactive emissions in the CRIV2R5Em simulations.

Note that other emission surrogate choices are possible — e.g. including NPROPOL, IPROPOL, GLYOX, MGLYOX, MACR and MVK emissions, or choosing the surrogate species based on photochemical ozone creation potential (POCP), for example using C2H4 and C3H6 as surrogates for some of the larger alkenes or TOLUENE for some aromatics with lower POCP than o-xylene; species with very low POCP (e.g. benzaldehyde and styrene) may be treated as unreactive.

Table D.3: VOC-emission surrogates in CB6r2Em — MCM (emission) VOC species mapped to CB6 species (mole based)

MCM species	VOC	PAR	ETH	OLE	IOLE	FORM	ALD2	TERP	TOL	XYL	ALDX	KET
NC4H10	n-butane	4	0	0	0	0	0	0	0	0	0	0
IC4H10	2-methylpropane	4	0	0	0	0	0	0	0	0	0	0
NC5H12	n-pentane	5	0	0	0	0	0	0	0	0	0	0
IC5H12	2-methyl-butane	5	0	0	0	0	0	0	0	0	0	0
NEOP	2,2-dimethylpropane	4	0	0	0	0	0	0	0	0	0	0
NC6H14	n-hexane	6	0	0	0	0	0	0	0	0	0	0
M2PE	2-methylpentane	6	0	0	0	0	0	0	0	0	0	0
M3PE	3-methylpentane	6	0	0	0	0	0	0	0	0	0	0
M22C4	2,2-dimethylbutane	5	0	0	0	0	0	0	0	0	0	0
M23C4	2,3-dimethylbutane	6	0	0	0	0	0	0	0	0	0	0
NC7H16	n-heptane	7	0	0	0	0	0	0	0	0	0	0
M2HEX	2-methylhexane	7	0	0	0	0	0	0	0	0	0	0
M3HEX	3-methylhexane	7	0	0	0	0	0	0	0	0	0	0
NC8H18	n-octane	7	0	0	0	0	0	0	0	0	0	0
NC9H20	n-nonane	7	0	0	0	0	0	0	0	0	0	0
NC10H22	n-decane	7	0	0	0	0	0	0	0	0	0	0
NC11H24	n-undecane	8	0	0	0	0	0	0	0	0	0	0
NC12H26	n-dodecane	8	0	0	0	0	0	0	0	0	0	0
CHEX	cyclohexane	6	0	0	0	0	0	0	0	0	0	0
C2H4	ethylene	0	1	0	0	0	0	0	0	0	0	0
C3H6	propylene	1	0	1	0	0	0	0	0	0	0	0

CB6 emissions split (continued on next page)

MCM species	VOC	PAR	ETH	OLE	IOLE	FORM	ALD2	TERP	TOL	XYL	ALDX	KET
BUT1ENE	1-butene	2	0	1	0	0	0	0	0	0	0	0
CBUT2ENE	cis-2-butene	0	0	0	1	0	0	0	0	0	0	0
MEPROPENE	2-methylpropene	3	0	0	0	1	0	0	0	0	0	0
PENT1ENE	1-pentene	3	0	1	0	0	0	0	0	0	0	0
CPENT2ENE	cis-2-pentene	1	0	0	1	0	0	0	0	0	0	0
ME2BUT1ENE	2-methyl-1-butene	4	0	0	0	1	0	0	0	0	0	0
ME3BUT1ENE	3-methyl-1-butene	3	0	1	0	0	0	0	0	0	0	0
ME2BUT2ENE	2-methyl-2-butene	3	0	0	0	0	1	0	0	0	0	0
HEX1ENE	1-hexene	4	0	1	0	0	0	0	0	0	0	0
CHEX2ENE	cis-2-hexene	2	0	0	1	0	0	0	0	0	0	0
C4H6	1,3-butadiene	0	0	2	0	0	0	0	0	0	0	0
APINENE	a-pinene	0	0	0	0	0	0	1	0	0	0	0
BPINENE	b-pinene	0	0	0	0	0	0	1	0	0	0	0
LIMONENE	d-limonene	0	0	0	0	0	0	1	0	0	0	0
TOLUENE	toluene	0	0	0	0	0	0	0	1	0	0	0
OXYL	o-xylene	0	0	0	0	0	0	0	0	1	0	0
MXYL	m-xylene	0	0	0	0	0	0	0	0	1	0	0
PXYL	p-xylene	0	0	0	0	0	0	0	0	1	0	0
EBENZ	ethylbenzene	1	0	0	0	0	0	0	1	0	0	0
PBENZ	n-propylbenzene	2	0	0	0	0	0	0	1	0	0	0
IPBENZ	isopropyl benzene	2	0	0	0	0	0	0	1	0	0	0
TM123B	1,2,3-trimethylbenzene	1	0	0	0	0	0	0	0	1	0	0
TM124B	1,2,4-trimethylbenzene	1	0	0	0	0	0	0	0	1	0	0
TM135B	1,3,5-trimethylbenzene	1	0	0	0	0	0	0	0	1	0	0
OETHTOL	o-ethyltoluene	1	0	0	0	0	0	0	0	1	0	0
METHTOL	m-ethyltoluene	1	0	0	0	0	0	0	0	1	0	0
PETHTOL	p-ethyltoluene	1	0	0	0	0	0	0	0	1	0	0
DIME35EB	1-Ethyl-3,5-dimethylbenzene	2	0	0	0	0	0	0	0	1	0	0
STYRENE	styrene	0	0	0.5	0	0	0	0	1	0	0	0
NPROPOL	n-propyl alcohol	3	0	0	0	0	0	0	0	0	0	0
IPROPOL	isopropyl alcohol	3	0	0	0	0	0	0	0	0	0	0
NBUTOL	n-butyl alcohol	4	0	0	0	0	0	0	0	0	0	0
BUT2OL	sec-butyl alcohol	4	0	0	0	0	0	0	0	0	0	0
IBUTOL	isobutyl alcohol	4	0	0	0	0	0	0	0	0	0	0
ME3BUOL	3-methyl-1-butanol	5	0	0	0	0	0	0	0	0	0	0
CYHEXOL	cyclohexanol	6	0	0	0	0	0	0	0	0	0	0
ETHGLY	ethylene glycol	2	0	0	0	0	0	0	0	0	0	0
PROPGLY	propylene glycol	3	0	0	0	0	0	0	0	0	0	0
HCHO	formaldehyde	0	0	0	0	1	0	0	0	0	0	0
CH3CHO	acetaldehyde	0	0	0	0	0	1	0	0	0	0	0
C2H5CHO	propionaldehyde	1	0	0	0	0	0	0	0	0	1	0
C3H7CHO	butyraldehyde	2	0	0	0	0	0	0	0	0	1	0
IPRCHO	isobutyraldehyde	2	0	0	0	0	0	0	0	0	1	0
C4H9CHO	n-pentanal	3	0	0	0	0	0	0	0	0	1	0
ACR	acrolein	0	0	0.5	0	0	0	0	0	0	1	0
MACR	methacrolein	1	0	0.5	0	0	0	0	0	0	1	0
MEK	methyl ethyl ketone	3	0	0	0	0	0	0	0	0	0	1
MPRK	2-pentanone	4	0	0	0	0	0	0	0	0	0	1
DIEK	3-pentanone	4	0	0	0	0	0	0	0	0	0	1
MIBK	methyl isobutyl ketone	5	0	0	0	0	0	0	0	0	0	1
CYHEXONE	cyclohexanone	5	0	0	0	0	0	0	0	0	0	1
MIBKAOH	4-hydroxy-4-methyl-2-pentanone	5	0	0	0	0	0	0	0	0	0	1
PROPACID	propionic acid	2	0	0	0	0	0	0	0	0	0	0
CH3OCH3	dimethyl ether	2	0	0	0	0	0	0	0	0	0	0
DIETETHER	ethyl ether	4	0	0	0	0	0	0	0	0	0	0
MTBE	methyl t-butyl ether	4	0	0	0	0	0	0	0	0	0	0
DIIPREETHER	diisopropyl ether	6	0	0	0	0	0	0	0	0	0	0
MO2EOL	2-methoxyethanol	3	0	0	0	0	0	0	0	0	0	0

CB6 emissions split (continued on next page)

MCM species	VOC	PAR	ETH	OLE	IOLE	FORM	ALD2	TERP	TOL	XYL	ALDX	KET
EOX2EOL	2-ethoxyethanol	4	0	0	0	0	0	0	0	0	0	0
PR2OHMOX	1-methoxy-2-propanol	2	0	0	0	0	0	0	0	0	1	0
BUOX2ETOH	2-butoxyethanol	6	0	0	0	0	0	0	0	0	0	0
BOX2PROL	1-butoxy-2-propanol	7	0	0	0	0	0	0	0	0	0	0
CH3OCHO	methyl formate	1	0	0	0	0	0	0	0	0	0	0
METHACET	methyl acetate	2	0	0	0	0	0	0	0	0	0	0
ETHACET	ethyl acetate	3	0	0	0	0	0	0	0	0	0	0
NPROACET	propyl acetate	4	0	0	0	0	0	0	0	0	0	0
IPROACET	isopropyl acetate	4	0	0	0	0	0	0	0	0	0	0
NBUTACET	n-butyl acetate	5	0	0	0	0	0	0	0	0	0	0
DMM	dimethoxymethane	3	0	0	0	0	0	0	0	0	0	0
TRICLETH	trichloroethylene	0	1	0	0	0	0	0	0	0	0	0
CCL2CH2	1,1-dichloroethene	2	0	0	0	0	0	0	0	0	0	0

Notes:

The following (potentially) emitted species are treated explicitly in the CB6r2Em simulations:

CH₄, ETHA(ethane), PRPA(propane), ETHY(acetylene), C₅H₈, BENZ(benzene), MEOH(methanol), ETOH(ethanol), ACET(acetone), GLY(glyoxal), MGly(methylglyoxal), FACD(formic acid), AACD(acetic acid).

The following emitted species (from MCM) are treated as unreactive in the CB6r2Em simulations:

BENZAL(benzaldehyde), CH₃CL, CH₂CL₂, CHCL₃, CH₃CCL₃, TCE(tetrachloroethene), CDICLETH(cis-1,2-dichloroethene), CH₂CLCH₂CL, CHCL₂CH₃, CH₃CH₂CL, CHCL₂CHCL₂, CH₃BR.

E. Ozone Evaluation, European simulations

Table E.1: EECCA scale modelled mean ozone concentrations compared to measurements at selected regional (and global) background sites within the EMEP monitoring network during 2011. The comparisons are based on the hours with available measurements (data coverage, dc, in % of the days of the year with valid measurements). Concentrations in ppb(v). Correlation coefficients (R) given in parenthesis after the annual mean of the daily mean concentrations for the different model schemes.

Station	°N	°E	Alt	dc(%)	Obs	EmChem19a	EmChem19X	CRIV2R5Em	CB6r2Em	EmChem16	EmChem09
AT02	47.77	16.77	117	100	30.10	31.91 (0.850)	31.86 (0.850)	31.56 (0.849)	29.86 (0.850)	31.49 (0.838)	30.72 (0.839)
BE32	50.63	6.00	295	98	26.03	28.50 (0.867)	28.51 (0.868)	28.29 (0.869)	27.04 (0.858)	28.39 (0.850)	27.77 (0.855)
CH02	46.81	6.94	489	100	25.83	33.37 (0.816)	33.33 (0.817)	32.97 (0.825)	31.37 (0.819)	33.22 (0.776)	32.00 (0.810)
CY02	35.04	33.06	532	99	48.84	39.61 (0.806)	39.66 (0.808)	39.32 (0.806)	37.51 (0.776)	38.55 (0.753)	38.18 (0.759)
CZ03	49.57	15.08	535	96	31.13	33.35 (0.801)	33.30 (0.802)	32.99 (0.807)	31.50 (0.806)	33.14 (0.791)	32.14 (0.796)
DE02	52.80	10.76	74	100	27.13	29.29 (0.870)	29.28 (0.869)	28.96 (0.871)	27.81 (0.875)	29.47 (0.867)	28.37 (0.869)
DK31	56.28	8.43	10	99	27.49	32.95 (0.692)	32.95 (0.694)	32.62 (0.702)	31.65 (0.706)	33.06 (0.700)	32.25 (0.706)
EE09	59.50	25.90	32	99	28.53	31.12 (0.730)	31.03 (0.731)	30.48 (0.740)	29.38 (0.751)	30.97 (0.752)	30.07 (0.750)
ES10	42.32	3.32	23	100	39.79	40.36 (0.817)	40.41 (0.822)	40.19 (0.821)	38.14 (0.767)	39.88 (0.786)	39.17 (0.787)
FI09	59.78	21.38	7	97	33.04	35.67 (0.769)	35.57 (0.767)	35.02 (0.755)	33.82 (0.723)	35.52 (0.756)	34.56 (0.729)
FR15	46.65	-0.75	133	100	30.28	32.00 (0.809)	32.03 (0.809)	31.86 (0.809)	30.72 (0.791)	31.74 (0.795)	31.30 (0.797)
IE31	53.33	-9.90	5	100	36.46	36.89 (0.790)	36.90 (0.791)	36.74 (0.791)	36.21 (0.793)	36.72 (0.786)	36.41 (0.794)
IT04	45.80	8.63	209	98	17.18	34.10 (0.817)	34.20 (0.816)	33.96 (0.814)	31.48 (0.825)	34.37 (0.821)	32.92 (0.821)
LV16	57.14	25.91	188	86	29.53	29.29 (0.724)	29.22 (0.725)	28.77 (0.739)	27.59 (0.772)	29.01 (0.755)	28.31 (0.759)
GB36	51.57	-1.32	137	99	27.50	28.01 (0.844)	28.04 (0.847)	27.86 (0.849)	27.01 (0.833)	28.02 (0.823)	27.52 (0.841)
NL09	53.33	6.28	1	97	24.99	30.45 (0.870)	30.46 (0.870)	30.20 (0.871)	29.15 (0.866)	30.71 (0.864)	29.84 (0.863)
NO01	58.38	8.25	190	77	25.83	34.04 (0.785)	34.03 (0.783)	33.60 (0.790)	32.46 (0.802)	33.97 (0.795)	33.01 (0.798)
PL02	51.82	21.98	180	100	26.75	30.16 (0.846)	30.09 (0.845)	29.75 (0.847)	28.42 (0.860)	29.98 (0.858)	29.11 (0.855)
SE11	56.02	13.15	175	99	29.28	29.74 (0.763)	29.72 (0.763)	29.37 (0.759)	28.29 (0.741)	29.82 (0.762)	28.89 (0.743)
SK06	49.05	22.27	345	100	29.92	34.17 (0.773)	34.06 (0.768)	33.75 (0.770)	32.12 (0.820)	33.91 (0.815)	33.04 (0.801)

Table E.2: EECCA scale modelled mean of daily maximum ozone concentrations compared to measurements at selected regional (and global) background sites within the EMEP monitoring network during 2011. The comparisons are based on the hours with available measurements (data coverage, dc, in % of the days of the year with valid measurements). Concentrations in ppb(v). Correlation coefficients (R) given in parenthesis after the annual mean of the daily mean concentrations for the different model schemes.

Station	°N	°E	Alt	dc(%)	Obs	EmChem19a	EmChem19X	CRIV2R5Em	CB6r2Em	EmChem16	EmChem09
AT02	47.77	16.77	117	100	43.23	41.29 (0.851)	41.22 (0.852)	40.82 (0.852)	38.57 (0.850)	40.50 (0.832)	39.70 (0.841)
BE32	50.63	6.00	295	98	37.96	36.10 (0.883)	36.14 (0.884)	35.90 (0.883)	34.27 (0.862)	35.79 (0.858)	35.28 (0.863)
CH02	46.81	6.94	489	100	41.37	42.94 (0.822)	42.87 (0.823)	42.48 (0.830)	40.38 (0.819)	42.55 (0.768)	41.25 (0.811)
CY02	35.04	33.06	532	99	54.50	47.00 (0.840)	47.01 (0.843)	46.48 (0.839)	44.35 (0.813)	45.76 (0.778)	45.13 (0.785)
CZ03	49.57	15.08	535	96	41.59	40.57 (0.820)	40.51 (0.821)	40.14 (0.823)	38.28 (0.816)	40.12 (0.809)	39.04 (0.810)
DE02	52.80	10.76	74	100	38.96	36.50 (0.885)	36.50 (0.886)	36.11 (0.886)	34.57 (0.878)	36.58 (0.878)	35.26 (0.875)
DK31	56.28	8.43	10	99	33.94	37.91 (0.703)	37.92 (0.707)	37.57 (0.713)	36.48 (0.690)	37.97 (0.701)	37.11 (0.702)
EE09	59.50	25.90	32	99	38.02	35.96 (0.752)	35.87 (0.750)	35.27 (0.742)	33.97 (0.712)	35.66 (0.752)	34.72 (0.721)
ES10	42.32	3.32	23	100	47.65	45.57 (0.840)	45.64 (0.845)	45.38 (0.843)	42.92 (0.790)	44.84 (0.806)	44.17 (0.815)
FI09	59.78	21.38	7	97	39.40	40.04 (0.774)	39.96 (0.770)	39.41 (0.746)	38.09 (0.678)	39.75 (0.739)	38.84 (0.689)
FR15	46.65	-0.75	133	100	41.02	39.08 (0.834)	39.12 (0.832)	38.91 (0.830)	37.36 (0.826)	38.58 (0.820)	38.16 (0.817)
IE31	53.33	-9.90	5	100	41.23	39.93 (0.780)	39.95 (0.780)	39.78 (0.782)	39.18 (0.786)	39.73 (0.785)	39.41 (0.792)
IT04	45.80	8.63	209	98	35.61	48.95 (0.793)	49.10 (0.795)	48.80 (0.793)	45.33 (0.796)	49.32 (0.792)	47.32 (0.790)
LV16	57.14	25.91	188	86	39.79	34.59 (0.791)	34.52 (0.789)	34.04 (0.787)	32.56 (0.780)	34.12 (0.794)	33.41 (0.790)
GB36	51.57	-1.32	137	99	37.06	35.08 (0.848)	35.11 (0.851)	34.91 (0.851)	33.82 (0.828)	35.06 (0.817)	34.54 (0.835)
NL09	53.33	6.28	1	97	35.38	36.73 (0.823)	36.77 (0.825)	36.48 (0.823)	35.17 (0.797)	36.98 (0.819)	36.02 (0.804)
NO01	58.38	8.25	190	77	36.74	38.57 (0.777)	38.57 (0.778)	38.06 (0.776)	36.75 (0.758)	38.42 (0.790)	37.37 (0.770)
PL02	51.82	21.98	180	100	39.52	37.51 (0.864)	37.44 (0.863)	37.02 (0.862)	35.29 (0.863)	37.09 (0.865)	36.18 (0.863)
SE11	56.02	13.15	175	99	37.91	35.82 (0.763)	35.82 (0.765)	35.42 (0.759)	34.13 (0.721)	35.83 (0.755)	34.84 (0.727)
SK06	49.05	22.27	345	100	42.36	40.69 (0.841)	40.58 (0.839)	40.22 (0.840)	38.19 (0.849)	40.16 (0.850)	39.34 (0.842)

Table E.3: EECCA scale modelled AOT40 concentrations of ozone compared to measurements at selected regional (and global) background sites within the EMEP monitoring network during 2011. The comparisons are based on the hours with available measurements (data coverage, dc, in % of the days of the year with valid measurements). Concentrations in ppb hours. Correlation coefficients (R) given in parenthesis after the annual mean of the daily mean concentrations for the different model schemes.

Station	°N	°E	Alt	dc(%)	Obs	EmChem19a	EmChem19X	CRIV2R5Em	CB6r2Em	EmChem16	EmChem09
AT02	47.77	16.77	117	99	17.86	13.13 (-26%)	13.23 (-26%)	12.52 (-30%)	7.17 (-60%)	9.69 (-46%)	9.37 (-48%)
BE32	50.63	6.00	295	98	9.81	4.91 (-50%)	5.01 (-49%)	4.81 (-51%)	2.77 (-72%)	4.12 (-58%)	3.81 (-61%)
CH02	46.81	6.94	489	99	17.00	15.21 (-11%)	15.16 (-11%)	14.56 (-14%)	9.74 (-43%)	12.73 (-25%)	11.23 (-34%)
CY02	35.04	33.06	532	96	31.77	18.70 (-41%)	18.89 (-41%)	17.61 (-45%)	12.17 (-62%)	13.67 (-57%)	12.56 (-60%)
CZ03	49.57	15.08	535	96	12.32	10.16 (-18%)	10.17 (-17%)	9.52 (-23%)	5.58 (-55%)	8.12 (-34%)	6.75 (-45%)
DE02	52.80	10.76	74	99	12.71	6.10 (-52%)	6.15 (-52%)	5.66 (-55%)	3.44 (-73%)	5.77 (-55%)	4.33 (-66%)
DK31	56.28	8.43	10	95	2.02	4.25 (110%)	4.30 (113%)	3.89 (93%)	2.57 (27%)	4.37 (116%)	3.32 (64%)
EE09	59.50	25.90	32	98	4.92	1.96 (-60%)	1.88 (-62%)	1.45 (-71%)	0.68 (-86%)	1.64 (-67%)	1.00 (-80%)
ES10	42.32	3.32	23	98	18.56	15.49 (-17%)	15.81 (-15%)	15.47 (-17%)	9.65 (-48%)	12.28 (-34%)	11.80 (-36%)
FI09	59.78	21.38	7	95	3.88	5.67 (46%)	5.51 (42%)	4.49 (16%)	2.31 (-40%)	4.60 (19%)	3.11 (-20%)
FR15	46.65	-0.75	133	99	10.83	6.54 (-40%)	6.68 (-38%)	6.49 (-40%)	3.86 (-64%)	5.14 (-53%)	5.10 (-53%)
IE31	53.33	-9.90	5	99	3.97	3.83 (-4%)	3.85 (-3%)	3.67 (-8%)	3.01 (-24%)	3.75 (-6%)	3.33 (-16%)
IT04	45.80	8.63	209	91	9.72	35.42 (264%)	36.22 (273%)	35.43 (265%)	26.37 (171%)	33.39 (244%)	30.31 (212%)
GB36	51.57	-1.32	137	98	4.70	3.04 (-35%)	3.12 (-34%)	2.95 (-37%)	1.85 (-61%)	2.92 (-38%)	2.48 (-47%)
NL09	53.33	6.28	1	97	4.97	3.42 (-31%)	3.49 (-30%)	3.16 (-36%)	1.9 (-62%)	3.57 (-28%)	2.63 (-47%)
NO01	58.38	8.25	190	96	4.21	2.62 (-38%)	2.64 (-37%)	2.24 (-47%)	1.38 (-67%)	2.63 (-38%)	1.75 (-58%)
PL02	51.82	21.98	180	98	10.41	7.79 (-25%)	7.77 (-25%)	7.17 (-31%)	4.06 (-61%)	6.13 (-41%)	5.31 (-49%)
SE11	56.02	13.15	175	96	5.80	3.28 (-43%)	3.32 (-43%)	2.96 (-49%)	1.6 (-72%)	3.19 (-45%)	2.23 (-62%)
SK06	49.05	22.27	345	100	9.88	9.14 (-7%)	9.13 (-8%)	8.59 (-13%)	4.8 (-51%)	6.97 (-29%)	6.43 (-35%)

F. Ozone Evaluation, Global simulations

Table F.1: Global scale EMEP MSC-W chemical transport model mean of daily maximum ozone concentrations compared to measurements at GAW sites (with alt. $\leq 600\text{m}$) during 2012. The comparisons are based on the hours with available measurements (data coverage, dc, in % of the days of the year with valid measurements). Concentrations in ppb(v). Correlation coefficients (R) given in parenthesis after the annual means of the daily maximum concentrations for the different model schemes.

Station	$^{\circ}\text{N}$	$^{\circ}\text{E}$	Alt	Obs	dc(%)	EmChem19a	EmChem19X	CRIv2R5Em	CB6r2Em	EmChem16	EmChem09
<i>Antarctica</i>											
Arrival Heights	-77.8	166.67	184	27.78	99	26.88 (0.822)	26.99 (0.823)	26.82 (0.825)	25.23 (0.816)	25.44 (0.811)	28.55 (0.857)
Halley	-75.62	-26.18	38	24.18	62	26.69 (0.499)	26.78 (0.501)	26.57 (0.508)	24.93 (0.491)	25.32 (0.475)	28.15 (0.572)
Neumayer	-70.67	-8.27	49	26.86	100	27.94 (0.855)	28.06 (0.856)	27.89 (0.859)	26.23 (0.849)	26.38 (0.845)	29.66 (0.889)
Syowa Station	-69	39.58	16	26.73	100	28.83 (0.863)	28.96 (0.864)	28.79 (0.867)	27.09 (0.859)	27.23 (0.852)	30.60 (0.894)
Marambio	-64.24	-56.62	198	20.38	74	25.80 (0.834)	25.92 (0.834)	25.73 (0.837)	24.14 (0.831)	24.39 (0.828)	27.44 (0.861)
<i>S. hemisphere</i>											
Ushuaia, Argentina	-54.83	-68.3	18	24.83	99	27.57 (0.899)	27.70 (0.900)	27.52 (0.903)	25.86 (0.903)	25.92 (0.890)	29.38 (0.921)
Pilar Obs., Argentina	-31.67	-63.88	338	38.66	18	42.72 (0.472)	43.48 (0.469)	43.80 (0.493)	36.18 (0.493)	39.97 (0.477)	47.59 (0.406)
Cape Point, South Africa	-34.35	18.48	230	26.98	96	32.31 (0.764)	32.44 (0.765)	32.35 (0.756)	30.13 (0.794)	30.56 (0.749)	34.32 (0.811)
Lauder, New Zealand	-45.03	169.67	370	24.60	95	28.76 (0.658)	28.91 (0.661)	28.70 (0.667)	26.83 (0.667)	27.03 (0.641)	30.64 (0.658)
Baring Head, New Zealand	-41.41	174.87	85	25.42	96	30.09 (0.819)	30.23 (0.821)	30.01 (0.826)	28.04 (0.832)	28.35 (0.804)	32.04 (0.831)
Cape Grim, Tasmania	-40.68	144.68	94	29.31	100	33.05 (0.834)	33.24 (0.835)	33.25 (0.830)	30.68 (0.852)	31.42 (0.818)	34.95 (0.856)
Cape Matatula, Samoa	-14.24	-170.57	42	16.77	97	19.71 (0.786)	19.81 (0.787)	19.67 (0.792)	19.12 (0.795)	17.59 (0.781)	20.50 (0.783)
<i>Asia</i>											
Danum Valley, Borneo	4.97	117.83	426	15.63	87	42.20 (0.528)	42.17 (0.534)	40.21 (0.555)	33.85 (0.554)	39.33 (0.526)	42.69 (0.479)
Minamitorishima, Japan	24.28	153.98	8	33.73	99	40.41 (0.917)	40.79 (0.917)	40.16 (0.917)	38.18 (0.916)	38.53 (0.915)	40.83 (0.922)
Yonagunijima, Japan	24.47	123.02	30	45.04	100	53.06 (0.805)	53.51 (0.807)	53.19 (0.807)	48.77 (0.815)	52.17 (0.809)	53.93 (0.816)
Ryori, Japan East Coast	39.03	141.82	260	46.31	100	46.04 (0.813)	46.25 (0.815)	45.89 (0.813)	42.55 (0.787)	45.03 (0.803)	47.14 (0.791)
<i>N. America</i>											
Trinidad Head, N Calif. coast	41.05	-124.15	120	35.13	100	39.15 (0.678)	39.27 (0.681)	38.15 (0.712)	35.45 (0.782)	37.42 (0.713)	39.92 (0.718)
Saturna, Canada west coast	48.78	-123.13	178	37.66	100	40.00 (0.761)	40.22 (0.760)	39.25 (0.760)	36.33 (0.765)	40.03 (0.752)	40.05 (0.743)
Egbert, Canada	44.23	-79.78	253	43.77	100	49.64 (0.877)	50.23 (0.876)	50.99 (0.872)	44.51 (0.880)	49.18 (0.873)	51.91 (0.869)
Kejimikujik, Canada	44.43	-65.2	127	37.76	99	44.17 (0.561)	44.55 (0.551)	44.51 (0.534)	39.55 (0.615)	42.93 (0.581)	46.00 (0.534)
Algoma, Canada	47.03	-84.38	411	40.63	99	44.66 (0.708)	44.93 (0.709)	44.99 (0.707)	39.97 (0.699)	43.60 (0.707)	46.46 (0.711)
Exp. Lakes Area, Canada	49.67	-93.72	369	38.63	100	40.85 (0.744)	41.00 (0.743)	40.69 (0.738)	36.78 (0.770)	39.32 (0.745)	42.31 (0.744)
Chapais, Canada	49.82	-74.98	381	36.96	100	38.44 (0.796)	38.69 (0.792)	38.49 (0.782)	34.58 (0.832)	36.91 (0.811)	40.07 (0.788)
Bratts Lake, Canada	50.20	-104.71	595	39.42	97	45.59 (0.741)	45.80 (0.744)	45.52 (0.743)	41.85 (0.720)	44.29 (0.723)	47.22 (0.721)
<i>N. Atlantic islands</i>											
Ragged Point, N Barbados	13.17	-59.43	45	24.65	86	30.97 (0.807)	31.30 (0.806)	30.96 (0.807)	29.04 (0.816)	28.25 (0.815)	30.75 (0.814)
Cape Verde Obs., Cape Verde	16.86	-24.87	10	34.90	100	41.07 (0.897)	41.48 (0.895)	40.98 (0.897)	38.72 (0.900)	38.70 (0.900)	41.58 (0.894)
Tudor Hill, Bermuda	32.27	-64.87	30	28.66	98	46.99 (0.738)	47.43 (0.735)	47.02 (0.729)	43.32 (0.769)	45.00 (0.763)	48.01 (0.742)
<i>Europe</i>											
Mace Head, Ireland west coast	53.33	-9.9	8	41.78	100	43.31 (0.731)	43.59 (0.733)	42.89 (0.735)	40.09 (0.715)	42.05 (0.729)	44.80 (0.729)
Giordan Lighthouse, Malta	36.07	14.22	160	47.55	99	50.75 (0.657)	51.08 (0.672)	50.76 (0.696)	47.50 (0.636)	49.48 (0.589)	50.70 (0.485)
Zingst, Germany (Baltic coast)	54.43	12.73	1	38.06	100	40.41 (0.788)	40.61 (0.790)	40.02 (0.793)	37.41 (0.772)	39.84 (0.767)	41.12 (0.738)
Westerland, Germany (N. Sea)	54.93	8.32	12	41.82	100	41.94 (0.765)	42.20 (0.770)	41.57 (0.772)	38.95 (0.739)	41.25 (0.738)	43.06 (0.724)
Iskrba, Slovenia	45.57	14.87	520	46.71	100	46.96 (0.854)	47.10 (0.853)	46.71 (0.855)	42.94 (0.838)	46.27 (0.844)	46.74 (0.818)
Kovk, Slovenia	46.12	15.1	600	45.93	98	46.23 (0.873)	46.36 (0.873)	45.90 (0.879)	42.34 (0.851)	45.55 (0.855)	45.80 (0.836)
Payenne, Switzerland	46.82	6.95	490	41.04	100	44.93 (0.734)	45.03 (0.739)	44.50 (0.756)	41.12 (0.726)	44.32 (0.669)	44.68 (0.702)
K-puszta, Hungary	46.97	19.55	125	50.02	83	49.70 (0.895)	49.95 (0.897)	49.77 (0.895)	45.62 (0.892)	48.80 (0.882)	49.64 (0.880)
Kosice, Czech Rep.	49.58	15.08	534	41.38	99	43.89 (0.837)	44.02 (0.838)	43.56 (0.838)	40.32 (0.830)	43.30 (0.818)	43.63 (0.800)
Waldhof, Germany	52.8	10.77	74	38.51	100	38.88 (0.857)	39.09 (0.859)	38.53 (0.862)	35.84 (0.852)	38.48 (0.837)	39.33 (0.827)
Neuglobsow, Germany	53.17	13.03	65	36.50	100	39.06 (0.826)	39.25 (0.826)	38.66 (0.821)	36.00 (0.830)	38.58 (0.814)	39.35 (0.819)
Kollumerwaard, Netherlands	53.33	6.28	0	36.81	99	39.99 (0.786)	40.26 (0.791)	39.68 (0.795)	37.00 (0.765)	39.53 (0.769)	41.03 (0.738)
Rucava, Latvia	56.16	21.17	18	45.46	95	40.87 (0.780)	41.01 (0.776)	40.42 (0.766)	37.75 (0.799)	40.14 (0.789)	41.37 (0.759)
Zoseni, Latvia	57.14	25.91	182	45.87	100	37.33 (0.818)	37.47 (0.817)	36.83 (0.813)	34.45 (0.833)	36.54 (0.822)	37.97 (0.814)
Vindeln, Sweden	64.25	19.77	271	35.08	98	35.09 (0.864)	35.21 (0.865)	34.56 (0.863)	32.35 (0.855)	34.14 (0.859)	36.31 (0.857)
Pallas-Sammaltunturi, Finland	67.97	24.12	560	37.06	98	34.33 (0.788)	34.48 (0.786)	33.84 (0.793)	31.58 (0.803)	33.29 (0.795)	35.72 (0.790)
<i>Arctic</i>											
Barrow, N Alaska	71.32	-156.6	11	29.69	100	33.13 (-0.045)	33.33 (-0.039)	32.79 (-0.031)	30.46 (-0.053)	32.09 (-0.063)	34.77 (-0.024)
Zeppelin mountain, Svalbard	78.91	-11.89	474	36.50	98	37.43 (0.757)	37.64 (0.753)	37.01 (0.778)	34.44 (0.788)	36.30 (0.774)	39.16 (0.769)
Villum, N Greenland	81.6	-16.67	20	31.88	99	33.91 (0.102)	34.12 (0.098)	33.55 (0.128)	31.17 (0.142)	32.87 (0.107)	35.48 (0.138)
Alert, N Nunavut, Canada	82.45	-62.52	210	33.33	100	33.41 (-0.003)	33.62 (-0.013)	33.05 (0.039)	30.66 (0.113)	32.34 (0.048)	34.99 (0.029)

G. EmChem19a mechanism

Table G.1: Gas-phase Chemistry of EmChem19a

N	Rate coefficient	Reaction
1	$5.681 \times 10^{-34} \times (T/300)^{-2.6}$	$\text{OP} + \langle \text{O}_2 \rangle + \langle \text{M} \rangle \longrightarrow \text{O}_3$
2	$2.15 \times 10^{-11} e^{110/T}$	$\text{OD} + \langle \text{N}_2 \rangle \longrightarrow \text{OP}$
3	$3.2 \times 10^{-11} e^{67/T}$	$\text{OD} + \langle \text{O}_2 \rangle \longrightarrow \text{OP}$
4	2.14×10^{-10}	$\text{OD} + \langle \text{H}_2\text{O} \rangle \longrightarrow 2 \text{OH}$
5	$4.8 \times 10^{-11} e^{250/T}$	$\text{OH} + \text{HO}_2 \longrightarrow \langle \text{H}_2\text{O} \rangle + \langle \text{O}_2 \rangle$
6	$2.9 \times 10^{-12} e^{-160/T}$	$\text{OH} + \text{H}_2\text{O}_2 \longrightarrow \text{HO}_2 + \langle \text{H}_2\text{O} \rangle$
7	$7.7 \times 10^{-12} e^{-2100/T}$	$\text{OH} + \text{H}_2 \longrightarrow \text{HO}_2 + \langle \text{H}_2\text{O} \rangle$
8	$\text{FH}_2\text{O} \times 2.2 \times 10^{-13} e^{600/T}$	$\text{HO}_2 + \text{HO}_2 \longrightarrow \text{H}_2\text{O}_2$
9	$\text{FH}_2\text{O} \times 1.9 \times 10^{-33} e^{980/T}$	$\text{HO}_2 + \text{HO}_2 + \langle \text{M} \rangle \longrightarrow \text{H}_2\text{O}_2$
10	KMT01	$\text{OP} + \text{NO} + \text{M} \longrightarrow \text{NO}_2$
11	$1.4 \times 10^{-12} e^{-1310/T}$	$\text{O}_3 + \text{NO} \longrightarrow \text{NO}_2 + \langle \text{O}_2 \rangle$
12	$1.4 \times 10^{-13} e^{-2470/T}$	$\text{O}_3 + \text{NO}_2 \longrightarrow \text{NO}_3 + \langle \text{O}_2 \rangle$
13	$1.7 \times 10^{-12} e^{-940/T}$	$\text{O}_3 + \text{OH} \longrightarrow \text{HO}_2 + \langle \text{O}_2 \rangle$
14	$2.03 \times 10^{-16} \times (T/300)^{4.57} e^{693/T}$	$\text{O}_3 + \text{HO}_2 \longrightarrow \text{OH} + 2 \langle \text{O}_2 \rangle$
15	$1.8 \times 10^{-11} e^{110/T}$	$\text{NO} + \text{NO}_3 \longrightarrow 2 \text{NO}_2$
16	$3.45 \times 10^{-12} e^{270/T}$	$\text{NO} + \text{HO}_2 \longrightarrow \text{NO}_2 + \text{OH}$
17	$4.5 \times 10^{-14} e^{-1260/T}$	$\text{NO}_2 + \text{NO}_3 \longrightarrow \text{NO} + \text{NO}_2$
18	KMT03	$\text{NO}_2 + \text{NO}_3 \longrightarrow \text{N}_2\text{O}_5$
19	KMT04	$\text{N}_2\text{O}_5 \longrightarrow \text{NO}_2 + \text{NO}_3$
20	KMT08	$\text{NO}_2 + \text{OH} + \text{M} \longrightarrow \text{HNO}_3$
21	KMT3-OH-HNO3	$\text{OH} + \text{HNO}_3 \longrightarrow \text{NO}_3 + \langle \text{H}_2\text{O} \rangle$
22	KMT07	$\text{OH} + \text{NO} \longrightarrow \text{HONO}$
23	$2.5 \times 10^{-12} e^{260/T}$	$\text{OH} + \text{HONO} \longrightarrow \text{NO}_2$
24	2.0×10^{-11}	$\text{OH} + \text{NO}_3 \longrightarrow \text{HO}_2 + \text{NO}_2$
25	4.0×10^{-12}	$\text{HO}_2 + \text{NO}_3 \longrightarrow \text{OH} + \text{NO}_2$
26	KMT09	$\text{HO}_2 + \text{NO}_2 \longrightarrow \text{HO}_2\text{NO}_2$
27	KMT10	$\text{HO}_2\text{NO}_2 \longrightarrow \text{HO}_2 + \text{NO}_2$
28	$3.2 \times 10^{-13} e^{690/T}$	$\text{OH} + \text{HO}_2\text{NO}_2 \longrightarrow \text{NO}_2$
29	$1.85 \times 10^{-12} e^{-1690/T}$	$\text{CH}_4 + \text{OH} \longrightarrow \text{CH}_3\text{O}_2$
30	KMT05	$\text{CO} + \text{OH} \longrightarrow \text{HO}_2$
31	1.2×10^{-12}	$\text{CH}_3\text{O}_2 + \text{NO}_3 \longrightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$
32	$2.3 \times 10^{-12} e^{360/T}$	$\text{CH}_3\text{O}_2 + \text{NO} \longrightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$
33	$1.48 \times 10^{-12} e^{-520/T}$	$\text{CH}_3\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{HCHO} + \text{HO}_2$
34	$2.06 \times 10^{-13} e^{365/T} - 1.48 \times 10^{-12} e^{-520/T}$	$\text{CH}_3\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.5 \text{HCHO} + 0.5 \text{CH}_3\text{OH}$
35	$3.8 \times 10^{-13} e^{780/T}$	$\text{CH}_3\text{O}_2 + \text{HO}_2 \longrightarrow 0.9 \text{CH}_3\text{OOH} + 0.1 \text{HCHO}$
36	$2.85 \times 10^{-12} e^{-345/T}$	$\text{CH}_3\text{OH} + \text{OH} \longrightarrow \text{HO}_2 + \text{HCHO}$
37	$5.3 \times 10^{-12} e^{190/T}$	$\text{CH}_3\text{OOH} + \text{OH} \longrightarrow 0.4 \text{HCHO} + 0.4 \text{OH} + 0.6 \text{CH}_3\text{O}_2 + 0.6 \langle \text{H}_2\text{O} \rangle$
38	$5.4 \times 10^{-12} e^{135/T}$	$\text{HCHO} + \text{OH} \longrightarrow \text{HO}_2 + \text{CO}$
39	$2.0 \times 10^{-12} e^{-2440/T}$	$\text{HCHO} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$
40	$6.9 \times 10^{-12} e^{-1000/T}$	$\text{C}_2\text{H}_6 + \text{OH} \longrightarrow \text{C}_2\text{H}_5\text{O}_2 + \langle \text{H}_2\text{O} \rangle$
41	$2.55 \times 10^{-12} e^{380/T}$	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \longrightarrow \text{HO}_2 + \text{CH}_3\text{CHO} + \text{NO}_2$
42	KRO2NO3	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \longrightarrow \text{HO}_2 + \text{CH}_3\text{CHO} + \text{NO}_2$
43	$6.4 \times 10^{-13} e^{710/T}$	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \longrightarrow \text{C}_2\text{H}_5\text{OOH}$
44	1.17×10^{-11}	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \longrightarrow 0.69 \text{CH}_3\text{CHO} + 0.69 \text{OH} + 0.31 \text{C}_2\text{H}_5\text{O}_2$
45	$4.7 \times 10^{-12} e^{345/T}$	$\text{CH}_3\text{CHO} + \text{OH} \longrightarrow 0.95 \text{CH}_3\text{CO}_3 + 0.05 \text{CH}_3\text{O}_2 + 0.05 \text{CO}$
46	KNO3AL	$\text{CH}_3\text{CHO} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{CH}_3\text{CO}_3$
47	KAPNO	$\text{CH}_3\text{CO}_3 + \text{NO} \longrightarrow \text{NO}_2 + \text{CH}_3\text{O}_2 + \langle \text{CO}_2 \rangle$
48	4.0×10^{-12}	$\text{CH}_3\text{CO}_3 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{CH}_3\text{O}_2$
49	KFPAN	$\text{CH}_3\text{CO}_3 + \text{NO}_2 + \text{M} \longrightarrow \text{PAN}$
50	KBPAN	$\text{PAN} + \text{M} \longrightarrow \text{CH}_3\text{CO}_3 + \text{NO}_2$

EmChem19a (continued on next page)

	Rate coefficient	Reaction
51	KAPHO2	$\text{CH}_3\text{CO}_3 + \text{HO}_2 \longrightarrow 0.454 \text{CH}_3\text{O}_2 + 0.454 \text{OH} + 0.384 \text{CH}_3\text{CO}_3\text{H} + 0.162 \text{O}_3 + 0.162 <\text{CH}_3\text{COOH}>$
52	1.0×10^{-11}	$\text{CH}_3\text{CO}_3 + [\text{RO}_2\text{POOL}] \longrightarrow 0.7 \text{CH}_3\text{O}_2 + 0.3 <\text{CH}_3\text{COOH}>$
53	1.1×10^{-11}	$\text{CH}_3\text{CO}_3\text{H} + \text{OH} \longrightarrow \text{CH}_3\text{CO}_3$
54	3.22×10^{-12}	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \longrightarrow 0.05 \text{ETRO}_2 + 0.95 \text{CH}_3\text{CHO} + 0.95 \text{HO}_2$
55	$9.8 \times 10^{-12} \text{e}^{-425/T}$	$\text{NC}_4\text{H}_{10} + \text{OH} \longrightarrow \text{C}_4\text{H}_9\text{O}_2$
56	$\text{KHO}_2\text{RO}_2 \times 0.625$	$\text{C}_4\text{H}_9\text{O}_2 + \text{HO}_2 \longrightarrow \text{BURO}_2\text{H}$
57	2.4×10^{-11}	$\text{BURO}_2\text{H} + \text{OH} \longrightarrow 0.847 \text{OH} + 0.847 \text{MEK} + 0.153 \text{C}_4\text{H}_9\text{O}_2$
58	KRO2NO	$\text{C}_4\text{H}_9\text{O}_2 + \text{NO} \longrightarrow 0.917 \text{NO}_2 + 0.083 \text{SC}_4\text{H}_9\text{NO}_3 + 0.654 \text{HO}_2 + 0.654 \text{MEK} + 0.264 \text{CH}_3\text{CHO} + 0.264 \text{C}_2\text{H}_5\text{O}_2$
59	KRO2NO3	$\text{C}_4\text{H}_9\text{O}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + 0.716 \text{MEK} + 0.716 \text{HO}_2 + 0.284 \text{CH}_3\text{CHO} + 0.284 \text{C}_2\text{H}_5\text{O}_2$
60	8.6×10^{-13}	$\text{SC}_4\text{H}_9\text{NO}_3 + \text{OH} \longrightarrow \text{MEK} + \text{NO}_2$
61	1.1×10^{-12}	$\text{MEK} + \text{OH} \longrightarrow \text{MEKO}_2$
62	KRO2NO	$\text{MEKO}_2 + \text{NO} \longrightarrow \text{NO}_2 + \text{CH}_3\text{CO}_3 + \text{CH}_3\text{CHO}$
63	KRO2NO3	$\text{MEKO}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{CH}_3\text{CO}_3 + \text{CH}_3\text{CHO}$
64	$\text{KHO}_2\text{RO}_2 \times 0.625$	$\text{MEKO}_2 + \text{HO}_2 \longrightarrow \text{MEKO}_2\text{H}$
65	1.04×10^{-12}	$\text{MEKO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.2135 \text{BIACET} + 0.75 \text{CH}_3\text{CO}_3 + 0.6405 \text{CH}_3\text{CHO} + 0.0365 \text{MGLYOX} + 0.073 \text{C}_2\text{H}_6 + 0.1095 \text{HCHO}$
66	2.1×10^{-11}	$\text{MEKO}_2\text{H} + \text{OH} \longrightarrow 0.826 \text{OH} + 0.7054 \text{BIACET} + 0.1206 \text{MGLYOX} + 0.0603 \text{C}_2\text{H}_6 + 0.174 \text{MEKO}_2$
67	2.3×10^{-13}	$\text{BIACET} + \text{OH} \longrightarrow \text{CH}_3\text{CO}_3 + \text{HCHO} + \text{CO}$
68	KMT15	$\text{C}_2\text{H}_4 + \text{OH} + \text{M} \longrightarrow \text{ETRO}_2$
69	KRO2NO	$\text{ETRO}_2 + \text{NO} \longrightarrow \text{NO}_2 + 2 \text{HCHO} + \text{HO}_2$
70	$1.53 \times 10^{-13} \text{e}^{1300/T}$	$\text{ETRO}_2 + \text{HO}_2 \longrightarrow \text{ETRO}_2\text{H}$
71	1.7475×10^{-11}	$\text{ETRO}_2\text{H} + \text{OH} \longrightarrow 0.79 \text{CH}_3\text{CHO} + 0.79 \text{OH} + 0.21 \text{ETRO}_2$
72	$6.82 \times 10^{-15} \text{e}^{-2500/T}$	$\text{C}_2\text{H}_4 + \text{O}_3 \longrightarrow 1.1575 \text{HCHO} + 0.17 \text{OH} + 0.35 \text{CO} + 0.27 \text{HO}_2 + 0.18 \text{H}_2 + 0.2625 <\text{HCOOH}> + 0.1575 \text{H}_2\text{O}_2$
73	KMT16	$\text{C}_3\text{H}_6 + \text{OH} + \text{M} \longrightarrow \text{PRRO}_2$
74	$5.77 \times 10^{-15} \text{e}^{-1880/T}$	$\text{C}_3\text{H}_6 + \text{O}_3 \longrightarrow 0.489 \text{CH}_3\text{CHO} + 0.68 \text{HCHO} + 0.169 \text{H}_2\text{O}_2 + 0.3646 \text{OH} + 0.483 \text{CO} + 0.0684 \text{H}_2 + 0.038 \text{HO}_2 + 0.3 \text{CH}_3\text{O}_2 + 0.05 \text{CH}_3\text{OH} + 0.04 \text{CH}_4 + 0.1 <\text{HCOOH}> + 0.181 <\text{CH}_3\text{CO}_2\text{H}>$
75	KRO2NO	$\text{PRRO}_2 + \text{NO} \longrightarrow \text{NO}_2 + \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$
76	KRO2NO3	$\text{PRRO}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$
77	$\text{KHO}_2\text{RO}_2 \times 0.52$	$\text{PRRO}_2 + \text{HO}_2 \longrightarrow \text{ACETOL}$
78	$4.60 \times 10^{-13} \text{e}^{-1155/T}$	$\text{C}_3\text{H}_6 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{C}_2\text{H}_5\text{O}_2 + \text{HCHO}$
79	$2.3 \times 10^{-12} \text{e}^{-190/T}$	$\text{BENZENE} + \text{OH} \longrightarrow 0.53 <\text{PHENOL}> + 0.648 <\text{HO}_2> + 0.259 \text{OXYO}_2 + 0.118 <\text{BZEPOXMUC}>$
80	$1.8 \times 10^{-12} \text{e}^{340/T}$	$\text{TOLUENE} + \text{OH} \longrightarrow 0.18 <\text{CRESOL}> + 0.564 \text{OXYO}_2 + 0.28 <\text{HO}_2> + 0.1 <\text{TLEPOXMUC}> + 0.07 <\text{C}_6\text{H}_5\text{SCH}_2\text{O}_2>$
81	1.36×10^{-11}	$\text{OXYL} + \text{OH} \longrightarrow 0.55 \text{OXYO}_2 + 0.24 <\text{OXYEPOXMUC}> + 0.4 <\text{HO}_2> + 0.16 <\text{OXYLOL}> + 0.05 <\text{OXYLO}_2>$
82	KRO2NO	$\text{OXYO}_2 + \text{NO} \longrightarrow \text{NO}_2 + \text{MGLYOX} + \text{C}_5\text{DICARB} + \text{HO}_2$
83	KRO2NO3	$\text{OXYO}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{MGLYOX} + \text{C}_5\text{DICARB} + \text{HO}_2$
84	$\text{KHO}_2\text{RO}_2 \times 0.859$	$\text{OXYO}_2 + \text{HO}_2 \longrightarrow \text{OXYO}_2\text{H}$
85	7.62×10^{-11}	$\text{OXYO}_2\text{H} + \text{OH} \longrightarrow \text{OXYO}_2$
86	6.2×10^{-11}	$\text{C}_5\text{DICARB} + \text{OH} \longrightarrow \text{C}_5\text{DICARBO}_2$
87	KRO2NO	$\text{C}_5\text{DICARBO}_2 + \text{NO} \longrightarrow \text{NO}_2 + \text{HO}_2 + \text{MGLYOX} + \text{GLYOX}$
88	KRO2NO3	$\text{C}_5\text{DICARBO}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{HO}_2 + \text{MGLYOX} + \text{GLYOX}$
89	$\text{KHO}_2\text{RO}_2 \times 0.706$	$\text{C}_5\text{DICARBO}_2 + \text{HO}_2 \longrightarrow \text{C}_5\text{DICAROOH}$
90	$1.9 \times 10^{-12} \text{e}^{190/T}$	$\text{C}_5\text{DICAROOH} + \text{OH} \longrightarrow \text{C}_5\text{DICARBO}_2$
91	$3.1 \times 10^{-12} \text{e}^{340/T}$	$\text{GLYOX} + \text{OH} \longrightarrow 0.416 \text{HO}_2 + 1.416 \text{CO} + 0.584 \text{OH}$
92	$1.9 \times 10^{-12} \text{e}^{575/T}$	$\text{MGLYOX} + \text{OH} \longrightarrow \text{CH}_3\text{CO}_3 + \text{CO}$
93	$2.7 \times 10^{-11} \text{e}^{390/T}$	$\text{C}_5\text{H}_8 + \text{OH} \longrightarrow \text{ISRO}_2$
94	$1.05 \times 10^{-14} \text{e}^{-2000/T}$	$\text{C}_5\text{H}_8 + \text{O}_3 \longrightarrow 0.25 \text{HO}_2 + 0.25 \text{OH} + 0.08 \text{CH}_3\text{O}_2 + 0.14 \text{CO} + 0.09 \text{H}_2\text{O}_2 + 0.28 <\text{HCOOH}> + 0.1 \text{CH}_3\text{CO}_3 + 0.1 \text{MACRO}_2 + 0.65 \text{MACR} + 0.58 \text{HCHO}$
95	$2.95 \times 10^{-12} \text{e}^{-450/T}$	$\text{C}_5\text{H}_8 + \text{NO}_3 \longrightarrow \text{ISON} + \text{HO}_2$
96	KRO2NO	$\text{ISRO}_2 + \text{NO} \longrightarrow 0.9 \text{NO}_2 + 0.9 \text{MACR} + 0.9 \text{HCHO} + 0.9 \text{HO}_2 + 0.1 \text{ISON}$
97	$\text{KHO}_2\text{RO}_2 \times 0.706$	$\text{ISRO}_2 + \text{HO}_2 \longrightarrow \text{ISRO}_2\text{H}$
98	4.0×10^{-12}	$\text{ISRO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{MACR} + \text{HCHO} + \text{HO}_2$
99	8.94×10^{-11}	$\text{ISRO}_2\text{H} + \text{OH} \longrightarrow 0.9 \text{IEPOX} + \text{OH} + 0.1 \text{MACR}$
100	9.13×10^{-12}	$\text{IEPOX} + \text{OH} \longrightarrow \text{MACRO}_2$
101	3.34×10^{-11}	$\text{ISON} + \text{OH} \longrightarrow 0.78 \text{ACETOL} + 0.78 \text{NALD} + 0.78 \text{HO}_2 + 0.22 \text{NO}_2 + 0.22 \text{MACR} + 0.22 \text{HCHO}$
102	9.2×10^{-17}	$\text{ISON} + \text{O}_3 \longrightarrow 0.67 \text{NALD} + 0.67 \text{OH} + 0.33 \text{MACR} + 0.33 \text{HCHO} + 0.33 \text{NO}_2$
103	$1.3 \times 10^{-12} \text{e}^{610/T}$	$\text{MACR} + \text{OH} \longrightarrow \text{MACRO}_2$
104	$4.0 \times 10^{-12} \text{e}^{380/T}$	$\text{MACR} + \text{OH} \longrightarrow \text{MACRO}_2$
105	$4.26 \times 10^{-16} \text{e}^{-1520/T}$	$\text{MACR} + \text{O}_3 \longrightarrow 0.9 \text{MGLYOX} + 0.45 <\text{HCOOH}> + 0.32 \text{HO}_2 + 0.22 \text{CO} + 0.19 \text{OH} + 0.1 \text{CH}_3\text{CO}_3$
106	$7.0 \times 10^{-16} \text{e}^{-2100/T}$	$\text{MACR} + \text{O}_3 \longrightarrow 0.9 \text{MGLYOX} + 0.45 <\text{HCOOH}> + 0.32 \text{HO}_2 + 0.22 \text{CO} + 0.19 \text{OH} + 0.1 \text{CH}_3\text{CO}_3$
107	KRO2NO	$\text{MACRO}_2 + \text{NO} \longrightarrow \text{NO}_2 + 0.25 \text{CH}_3\text{CO}_3 + 0.25 \text{ACETOL} + 0.25 \text{CO} + 0.5 \text{MGLYOX} + 0.75 \text{HCHO} + 0.75 \text{HO}_2$
108	$\text{KHO}_2\text{RO}_2 \times 0.625$	$\text{MACRO}_2 + \text{HO}_2 \longrightarrow \text{MACROOH}$
109	2.9×10^{-11}	$\text{MPAN} + \text{OH} \longrightarrow \text{ACETOL} + \text{NO}_2$
110	3.0×10^{-11}	$\text{MACROOH} + \text{OH} \longrightarrow \text{ACETOL} + \text{CO} + \text{OH}$
111	$1.6 \times 10^{-12} \text{e}^{305/T}$	$\text{ACETOL} + \text{OH} \longrightarrow \text{MGLYOX} + \text{HO}_2$
112	1.55×10^{-12}	$\text{NALD} + \text{OH} \longrightarrow \text{HCHO} + \text{CO} + \text{NO}_2$
113	$\text{KFPAN} \times 0.107$	$\text{MACRO}_2 + \text{NO}_2 \longrightarrow \text{MPAN}$
114	KBPAN	$\text{MPAN} \longrightarrow \text{MACRO}_2 + \text{NO}_2$
115	$1.88 \times 10^9 \text{e}^{-7261/T} \times 0.052$	$\text{ISRO}_2 \longrightarrow \text{HPALD} + \text{HO}_2$
116	$1.45 \times 10^{12} \text{e}^{-10688/T}$	$\text{ISRO}_2 \longrightarrow \text{MACR} + \text{HCHO} + \text{OH}$
117	7.61×10^{-11}	$\text{HPALD} + \text{OH} \longrightarrow \text{MGLYOX} + \text{CO} + \text{HCHO} + \text{OH}$
118	$1.34 \times 10^{-11} \text{e}^{410/T}$	$\text{APINENE} + \text{OH} \longrightarrow \text{TERPO}_2$
119	$8.22 \times 10^{-16} \text{e}^{-640/T}$	$\text{APINENE} + \text{O}_3 \longrightarrow 0.7 \text{OH} + 2 \text{MACR} + \text{HO}_2$

EmChem19a (continued on next page)

	Rate coefficient	Reaction
120	$1.2 \times 10^{-12} e^{490/T}$	APINENE + NO ₃ → TERPO ₂ + NO ₂
121	KRO ₂ NO	TERPO ₂ + NO → HO ₂ + 2 MACR + NO ₂ + 0.19 C ₂ H ₆
122	KRO ₂ NO ₃	TERPO ₂ + NO ₃ → HO ₂ + 2 MACR + NO ₂ + 0.19 C ₂ H ₆
123	$7.5 \times 10^{-13} e^{700/T}$	TERPO ₂ + HO ₂ → TERPOOH
124	$3.8 \times 10^{-12} e^{200/T}$	TERPOOH + OH → TERPO ₂
125	RCPHOT(IDO ₃ -O ₁ D)	O ₃ → OD
126	RCPHOT(IDO ₃ -O ₃ P)	O ₃ → OP
127	RCPHOT(IDH ₂ O ₂)	H ₂ O ₂ → 2 OH
128	RCPHOT(IDNO ₂)	NO ₂ → OP + NO
129	RCPHOT(IDNO ₃)	NO ₃ → 0.127 NO + 0.873 NO ₂ + 0.873 OP
130	RCPHOT(IDHONO)	HONO → OH + NO
131	RCPHOT(IDHNO ₃)	HNO ₃ → NO ₂ + OH
132	RCPHOT(IDHO ₂ NO ₂)	HO ₂ NO ₂ → 0.333 OH + 0.333 NO ₃ + 0.667 NO ₂ + 0.667 HO ₂
133	RCPHOT(IDHCHO-H)	HCHO → CO + 2 HO ₂
134	RCPHOT(IDHCHO-H ₂)	HCHO → CO + H ₂
135	RCPHOT(IDCH ₃ CHO)	CH ₃ CHO → CH ₃ O ₂ + HO ₂ + CO
136	RCPHOT(IDCH ₃ CHO)	NALD → HCHO + CO + NO ₂ + HO ₂
137	RCPHOT(IDMEK)	MEK → CH ₃ CO ₃ + C ₂ H ₅ O ₂
138	RCPHOT(IDMEK)	ACETOL → CH ₃ CO ₃ + HCHO + HO ₂
139	RCPHOT(IDCHOCHO)	GLYOX → 1.9 CO + 0.1 HCHO + 0.5 HO ₂
140	RCPHOT(IDR ₂ COCHO)	MGLYOX → CH ₃ CO ₃ + CO + HO ₂
141	RCPHOT(IDCH ₃ COY)	BIACET → 2 CH ₃ CO ₃
142	RCPHOT(IDHCHO-H ₂) × 0.0474	MACR → CH ₃ CO ₃ + HCHO + CO + HO ₂
143	RCPHOT(IDNO ₂) × 0.2	C ₅ DICARB → C ₅ DICARBO ₂ + HO ₂
144	RCPHOT(IDHCHO-H ₂) × 12	HPALD → PACALD + HO ₂ + OH
145	RCPHOT(IDHCHO-H ₂) × 24	PACALD → CO + HO ₂ + MGLYOX + OH
146	RCPHOT(IDHCHO-H) × 0.9	C ₅ DICAROOH → OH + HO ₂ + MGLYOX + GLYOX
147	RCPHOT(IDCH ₃ O ₂ H)	CH ₃ OOH → HCHO + OH + HO ₂
148	RCPHOT(IDCH ₃ O ₂ H)	C ₂ H ₅ OOH → HO ₂ + CH ₃ CHO + OH
149	RCPHOT(IDCH ₃ O ₂ H)	BURO ₂ H → OH + 0.716 HO ₂ + 0.716 MEK + 0.284 CH ₃ CHO + 0.284 C ₂ H ₅ O ₂
150	RCPHOT(IDCH ₃ O ₂ H)	ETRO ₂ H → HO ₂ + OH + 1.56 HCHO + 0.22 CH ₃ CHO
151	RCPHOT(IDCH ₃ O ₂ H)	CH ₃ CO ₃ H → CH ₃ O ₂ + OH
152	RCPHOT(IDCH ₃ O ₂ H)	MEKO ₂ H → CH ₃ CHO + CH ₃ CO ₃ + OH
153	RCPHOT(IDMEK)	MEKO ₂ H → CH ₃ CHO + CH ₃ CO ₃ + OH
154	RCPHOT(IDCH ₃ O ₂ H)	MACROOH → OH + HO ₂ + 0.5 ACETOL + 0.5 CO + 0.5 MGLYOX + 0.5 HCHO
155	RCPHOT(IDCH ₃ O ₂ H)	OXYO ₂ H → OH + MGLYOX + C ₅ DICARB + HO ₂
156	RCPHOT(IDCH ₃ O ₂ H)	ISRO ₂ H → OH + MACR + HCHO + HO ₂
157	RCPHOT(IDMEK) × 0.78	SC ₄ H ₉ NO ₃ → NO ₂ + 0.652 MEK + 0.652 HO ₂ + 0.348 CH ₃ CHO + 0.348 C ₂ H ₅ O ₂
158	RCPHOT(IDMEK) × 0.78	ISON → NO ₂ + MACR + HCHO + HO ₂

Notes:

"T" is temperature, "M" is third body, RCPHOT are photolysis rates.

Reaction coefficients are in units of s⁻¹ for unimolecular reactions, cm³ molecule⁻¹ s⁻¹ for bimolecular reactions, and cm⁶ molecule⁻² s⁻² for termolecular reactions.

$$\text{FH}_2\text{O} = 1.0 + 1.41 \times 10^{-21} e^{2200/T} \times [\text{H}_2\text{O}]$$

$$\text{KAPHO}_2 = 3.14 \times 10^{-12} e^{580/T}$$

$$\text{KAPNO} = 7.5 \times 10^{-12} e^{290/T}$$

$$\text{KHO}_2\text{RO}_2 = 2.91 \times 10^{-13} e^{1300/T}$$

$$\text{KMT05} = 1.44 \times 10^{-13} + [\text{M}] \times 3.43 \times 10^{-33}$$

$$\text{KNO}_3\text{AL} = 1.4 \times 10^{-12} e^{-1860/T}$$

$$\text{KRO}_2\text{NO} = 2.7 \times 10^{-12} e^{360/T}$$

$$\text{KRO}_2\text{NO}_3 = 2.3 \times 10^{-12}$$

Some complex 3-body rate-expressions are given in Tables [G.3](#) and [G.4](#)

Table G.2: Gas-phase species in EmChem19a (note that most of the organic species represent a number of different compounds and in some cases their reactions have been adjusted (rates and/or products) to take this into account)

Model species	description
non-advected (short-lived) species	
OD	O(¹ D)
OP	O(³ P)
OH	OH
HO2	HO ₂
CH3O2	CH ₃ O ₂ , RO ₂
C2H5O2	C ₂ H ₅ O ₂ , RO ₂
C4H9O2	C ₄ H ₉ O ₂ , RO ₂
ISRO2	HOC ₅ H ₈ O ₂ , RO ₂
ETRO2	HOCH ₂ CH ₂ O ₂ , RO ₂
PRRO2	CH ₃ CHO ₂ CH ₂ OH, RO ₂
OXYO2	C ₈ H ₁₁ O ₅ , RO ₂
MEKO2	CH ₃ COCHO ₂ CH ₃ and CH ₃ COCH ₂ CH ₂ O ₂ , RO ₂
C5DICARBO2	CH ₃ COCH(O ₂)CH(OH)CHO, RO ₂
MACRO2	C ₄ H ₇ O ₄ , RO ₂
TERPO2	C ₁₀ H ₁₇ O ₃ , RO ₂
advected species	
CH3CO3	CH ₃ COO ₂ , RO ₂
O3	O ₃
NO	NO, NO _x , OXN
NO2	NO ₂ , NO _x , OXN
NO3	NO ₃ , OXN
N2O5	N ₂ O ₅ , OXN
H2	H ₂
H2O2	H ₂ O ₂
HONO	HONO, OXN
HNO3	HNO ₃ , OXN
HO2NO2	HO ₂ NO ₂ , OXN
CO	CO
CH4	CH ₄
C2H6	C ₂ H ₆
NC4H10	n-C ₄ H ₁₀
C2H4	C ₂ H ₄
C3H6	C ₃ H ₆
BENZENE	C ₆ H ₆
TOLUENE	C ₆ H ₅ CH ₃
OXYL	o-C ₆ H ₄ (CH ₃)CH ₃
C5H8	CH ₂ =C(CH ₃)CH=CH ₂ , isoprene
APINENE	C ₁₀ H ₁₆ (α-pinene), monoterpene
CH3OH	CH ₃ OH
C2H5OH	C ₂ H ₅ OH
HCHO	HCHO, carbonyl
CH3CHO	CH ₃ CHO, carbonyl
MACR	CH ₂ =C(CH ₃)CHO (also representing MVK, CH ₂ =CHCOCH ₃), carbonyl
MEK	CH ₃ C(O)C ₂ H ₅ , carbonyl
ACETOL	CH ₃ C(O)CH ₂ OH, carbonyl
GLYOX	HCOHCO, glyoxal, carbonyl
MGLYOX	CH ₃ C(O)CHO, methyl glyoxal, carbonyl
<i>EmChem19a species (continued on next page)</i>	

Model species	description
BIACET	$\text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3$, 2,3-butanedione, carbonyl
C5DICARB	$\text{CH}_3\text{C}(\text{O})\text{CH}=\text{CHCHO}$, 4-oxopent-2-enal, carbonyl
CH3OOH	CH_3OOH , ROOH
C2H5OOH	$\text{C}_2\text{H}_5\text{OOH}$, ROOH
BURO2H	sec- $\text{C}_4\text{H}_9\text{OOH}$, ROOH
ETRO2H	$\text{HOCH}_2\text{CH}_2\text{OOH}$, ROOH
MEKO2H	$\text{CH}_3\text{C}(\text{O})\text{CH}(\text{CH}_3)\text{OOH}$, carbonyl, ROOH
ISRO2H	$\text{C}_5\text{H}_8(\text{OH})(\text{OOH})$, hydroperoxides from isoprene (several isomers), ROOH
C5DICAROOH	$\text{CH}_3\text{COCH}(\text{OOH})\text{CH}(\text{OH})\text{CHO}$, ROOH, carbonyl
HPALD	$\text{HCOCH}=\text{C}(\text{CH}_3)\text{CH}_2\text{OOH}$ and $\text{HCOC}(\text{CH}_3)=\text{CHCH}_2\text{OOH}$, ROOH, carbonyl
MACROOH	$\text{O}=\text{CHC}(\text{CH}_3)(\text{OOH})\text{CH}_2\text{OH}$ (also represents other species), ROOH, carbonyl
OXYO2H	$\text{C}_8\text{H}_{12}\text{O}_5$ (multifunctional), ROOH
CH3CO3H	$\text{CH}_3\text{C}(\text{O})\text{OOH}$, peroxyacid
PACALD	$\text{HCOCH}=\text{C}(\text{CH}_3)\text{C}(\text{O})\text{OOH}$ and $\text{HCOC}(\text{CH}_3)=\text{CHC}(\text{O})\text{OOH}$, peroxyacid, carbonyl
IEPOX	$\text{C}_5\text{H}_{10}\text{O}_3$ (epoxide with two OH groups)
SC4H9NO3	sec- $\text{C}_4\text{H}_9\text{NO}_3$, OXN, organic nitrate
NALD	$\text{O}_2\text{NOCH}_2\text{CHO}$ (represents second- and subsequent-generation nitrates from isoprene degradation), OXN, organic nitrate, carbonyl
ISON	$\text{C}_5\text{H}_8(\text{OH})(\text{NO}_3)$ (lumped species, repr first-gen nitrates from isoprene degradation), OXN, organic nitrate
PAN	$\text{CH}_3\text{C}(\text{O})\text{OONO}_2$, OXN, PANs
MPAN	$\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(=\text{O})\text{OONO}_2$, OXN, PANs
TERPOOH	$\text{C}_{10}\text{H}_{16}(\text{OH})(\text{OOH})$, ROOH
SO2	SO_2
NH3	NH_3

Notes:

RO_2 : organic peroxy radicals, carbonyl: aldehydes and/or ketones, ROOH: organic hydroperoxides,

OXN: species containing oxidised nitrogen, PANs: peroxyacyl nitrates, organic nitrate: species containing R-ONO2 (excl. PANs)

Table G.3: Rate coefficients for 3-body reactions using the Troe expression. The reaction rate coefficients are calculated as: $k = \frac{k_0 k_\infty}{k_0 + k_\infty} F$, with the broadening factor F calculated using the approximate expression: $\log_{10} F \cong \frac{\log_{10} F_c}{1 + [\log_{10}(k_0/k_\infty)/N]^2}$ where $N = [0.75 - 1.27 \log_{10} F_c]$ The first column (Rate coeff.) refers to the notation in Table G.1.

Rate coeff.	$k_0/[M]$	k_∞	F_c
KMT01	$1.0 \times 10^{-31} (300/T)^{1.6}$	$5.0 \times 10^{-11} (300/T)^{0.3}$	0.85
KMT02	$1.3 \times 10^{-31} (300/T)^{1.5}$	$2.3 \times 10^{-11} (300/T)^{-0.24}$	0.6
KMT03	$3.6 \times 10^{-30} (300/T)^{4.1}$	$1.9 \times 10^{-12} (300/T)^{-0.2}$	0.35
KMT04	$1.3 \times 10^{-3} (300/T)^{3.5} e^{(-11000/T)}$	$9.7 \times 10^{14} (300/T)^{-0.1} e^{(-11080/T)}$	0.35
KMT07	$7.4 \times 10^{-31} (300/T)^{2.4}$	$3.3 \times 10^{-11} (300/T)^{0.3}$	0.81
KMT07CRI	$7.4 \times 10^{-31} (300/T)^{2.4}$	$3.3 \times 10^{-11} (300/T)^{0.3}$	$e^{(-T/1420)}$
KMT08	$3.2 \times 10^{-30} (300/T)^{4.5}$	3.0×10^{-11}	0.41
KMT09	$1.4 \times 10^{-31} (300/T)^{3.1}$	4.0×10^{-12}	0.4
KMT10	$4.1 \times 10^{-5} \exp(-10650/T)$	$6.0 \times 10^{15} \exp(-11170/T)$	0.4
KMT12box	$2.8 \times 10^{-31} (300/T)^{2.6}$	2.0×10^{-12}	$e^{(-T/1420)}$
KMT15	$8.6 \times 10^{-29} (300/T)^{3.1}$	$9.0 \times 10^{-12} (300/T)^{0.85}$	0.48
KMT16	$8.0 \times 10^{-27} (300/T)^{3.5}$	$9.0 \times 10^{-9}/T$	0.5
KMT17	$5.0 \times 10^{-30} (300/T)^{1.5}$	1.0×10^{-12}	$0.17 e^{(-51/T)} + e^{(-T/204)}$
KFPAN	$3.28 \times 10^{-28} (300/T)^{6.87}$	$1.125 \times 10^{-11} (300/T)^{1.105}$	0.3
KBPAN	$1.1 \times 10^{-5} (300/T)^{-10100}$	$1.9 \times 10^{17} \exp(-14100/T)$	0.3
KBPPN	$1.7 \times 10^{-3} \exp(-11280/T)$	$8.3 \times 10^{16} \exp(-13940/T)$	0.36

Table G.4: Other rate coefficients

No.	Rate coeff.
KMT3-OH-HNO3	$= K_1 + (K_3[M])/(1.0 + (K_3[M])/K_4)$, where $K_1 = 2.4 \times 10^{-14} \exp(460/T)$, $K_3 = 6.5 \times 10^{-34} \exp(1335/T)$, $K_4 = 2.7 \times 10^{-17} \exp(2199/T)$

H. EmChem19X mechanism

Table H.1: Gas-phase Chemistry of EmChem19X

N	Rate coefficient	Reaction
1	$5.681 \times 10^{-34} \times (T/300)^{-2.6}$	$\text{OP} + \langle \text{O}_2 \rangle + \langle \text{M} \rangle \rightarrow \text{O}_3$
2	$2.15 \times 10^{-11} e^{110/T}$	$\text{OD} + \langle \text{N}_2 \rangle \rightarrow \text{OP}$
3	$3.2 \times 10^{-11} e^{67/T}$	$\text{OD} + \langle \text{O}_2 \rangle \rightarrow \text{OP}$
4	2.14×10^{-10}	$\text{OD} + \langle \text{H}_2\text{O} \rangle \rightarrow 2 \text{OH}$
5	$4.8 \times 10^{-11} e^{250/T}$	$\text{OH} + \text{HO}_2 \rightarrow \langle \text{H}_2\text{O} \rangle + \langle \text{O}_2 \rangle$
6	$2.9 \times 10^{-12} e^{-160/T}$	$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \langle \text{H}_2\text{O} \rangle$
7	$7.7 \times 10^{-12} e^{-2100/T}$	$\text{OH} + \text{H}_2 \rightarrow \text{HO}_2 + \langle \text{H}_2\text{O} \rangle$
8	$\text{FH}_2\text{O} \times 2.2 \times 10^{-13} e^{600/T}$	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2$
9	$\text{FH}_2\text{O} \times 1.9 \times 10^{-33} e^{980/T}$	$\text{HO}_2 + \text{HO}_2 + \langle \text{M} \rangle \rightarrow \text{H}_2\text{O}_2$
10	KMT01	$\text{OP} + \text{NO} + \text{M} \rightarrow \text{NO}_2$
11	$1.4 \times 10^{-12} e^{-1310/T}$	$\text{O}_3 + \text{NO} \rightarrow \text{NO}_2 + \langle \text{O}_2 \rangle$
12	$1.4 \times 10^{-13} e^{-2470/T}$	$\text{O}_3 + \text{NO}_2 \rightarrow \text{NO}_3 + \langle \text{O}_2 \rangle$
13	$1.7 \times 10^{-12} e^{-940/T}$	$\text{O}_3 + \text{OH} \rightarrow \text{HO}_2 + \langle \text{O}_2 \rangle$
14	$2.03 \times 10^{-16} \times (T/300)^{4.57} e^{693/T}$	$\text{O}_3 + \text{HO}_2 \rightarrow \text{OH} + 2 \langle \text{O}_2 \rangle$
15	$1.8 \times 10^{-11} e^{110/T}$	$\text{NO} + \text{NO}_3 \rightarrow 2 \text{NO}_2$
16	$3.45 \times 10^{-12} e^{270/T}$	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$
17	$4.5 \times 10^{-14} e^{-1260/T}$	$\text{NO}_2 + \text{NO}_3 \rightarrow \text{NO} + \text{NO}_2$
18	KMT03	$\text{NO}_2 + \text{NO}_3 \rightarrow \text{N}_2\text{O}_5$
19	KMT04	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$
20	KMT08	$\text{NO}_2 + \text{OH} + \text{M} \rightarrow \text{HNO}_3$
21	KMT3-OH-HNO3	$\text{OH} + \text{HNO}_3 \rightarrow \text{NO}_3 + \langle \text{H}_2\text{O} \rangle$
22	KMT07	$\text{OH} + \text{NO} \rightarrow \text{HONO}$
23	$2.5 \times 10^{-12} e^{260/T}$	$\text{OH} + \text{HONO} \rightarrow \text{NO}_2$
24	2.0×10^{-11}	$\text{OH} + \text{NO}_3 \rightarrow \text{HO}_2 + \text{NO}_2$
25	4.0×10^{-12}	$\text{HO}_2 + \text{NO}_3 \rightarrow \text{OH} + \text{NO}_2$
26	KMT09	$\text{HO}_2 + \text{NO}_2 \rightarrow \text{HO}_2\text{NO}_2$
27	KMT10	$\text{HO}_2\text{NO}_2 \rightarrow \text{HO}_2 + \text{NO}_2$
28	$3.2 \times 10^{-13} e^{690/T}$	$\text{OH} + \text{HO}_2\text{NO}_2 \rightarrow \text{NO}_2$
29	$1.85 \times 10^{-12} e^{-1690/T}$	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2$
30	KMT05	$\text{CO} + \text{OH} \rightarrow \text{HO}_2$
31	1.2×10^{-12}	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$
32	$2.3 \times 10^{-12} e^{360/T}$	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$
33	$1.48 \times 10^{-12} e^{-520/T}$	$\text{CH}_3\text{O}_2 + [\text{RO}_2\text{POOL}] \rightarrow \text{HCHO} + \text{HO}_2$
34	$2.06 \times 10^{-13} e^{365/T}$	$\text{CH}_3\text{O}_2 + [\text{RO}_2\text{POOL}] \rightarrow 0.5 \text{HCHO} + 0.5 \text{CH}_3\text{OH}$
	$1.48 \times 10^{-12} e^{-520/T}$	
35	$3.8 \times 10^{-13} e^{780/T}$	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow 0.9 \text{CH}_3\text{OOH} + 0.1 \text{HCHO}$

EmChem19X (continued on next page)

	Rate coefficient	Reaction
36	$2.85 \times 10^{-12} e^{-345/T}$	$\text{CH}_3\text{OH} + \text{OH} \longrightarrow \text{HO}_2 + \text{HCHO}$
37	$5.3 \times 10^{-12} e^{190/T}$	$\text{CH}_3\text{OOH} + \text{OH} \longrightarrow 0.4 \text{HCHO} + 0.4 \text{OH} + 0.6 \text{CH}_3\text{O}_2 + 0.6 \text{<H}_2\text{O>}$
38	$5.4 \times 10^{-12} e^{135/T}$	$\text{HCHO} + \text{OH} \longrightarrow \text{HO}_2 + \text{CO}$
39	$2.0 \times 10^{-12} e^{-2440/T}$	$\text{HCHO} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$
40	$6.9 \times 10^{-12} e^{-1000/T}$	$\text{C}_2\text{H}_6 + \text{OH} \longrightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{<H}_2\text{O>}$
41	$2.55 \times 10^{-12} e^{380/T}$	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \longrightarrow \text{HO}_2 + \text{CH}_3\text{CHO} + \text{NO}_2$
42	KRO2NO3	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \longrightarrow \text{HO}_2 + \text{CH}_3\text{CHO} + \text{NO}_2$
43	$6.4 \times 10^{-13} e^{710/T}$	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \longrightarrow \text{C}_2\text{H}_5\text{OOH}$
44	3.10×10^{-13}	$\text{C}_2\text{H}_5\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.8 \text{CH}_3\text{CHO} + 0.6 \text{HO}_2 + 0.2 \text{C}_2\text{H}_5\text{OH}$
45	1.17×10^{-11}	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \longrightarrow 0.69 \text{CH}_3\text{CHO} + 0.69 \text{OH} + 0.31 \text{C}_2\text{H}_5\text{O}_2$
46	$4.7 \times 10^{-12} e^{345/T}$	$\text{CH}_3\text{CHO} + \text{OH} \longrightarrow 0.95 \text{CH}_3\text{CO}_3 + 0.05 \text{HCOCH}_2\text{O}_2$
47	KNO3AL	$\text{CH}_3\text{CHO} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{CH}_3\text{CO}_3$
48	KAPNO	$\text{CH}_3\text{CO}_3 + \text{NO} \longrightarrow \text{NO}_2 + \text{CH}_3\text{O}_2 + \text{<CO}_2\text{>}$
49	4.0×10^{-12}	$\text{CH}_3\text{CO}_3 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{CH}_3\text{O}_2$
50	KFPAN	$\text{CH}_3\text{CO}_3 + \text{NO}_2 + \text{M} \longrightarrow \text{PAN}$
51	KBPAN	$\text{PAN} + \text{M} \longrightarrow \text{CH}_3\text{CO}_3 + \text{NO}_2$
52	KAPHO2	$\text{CH}_3\text{CO}_3 + \text{HO}_2 \longrightarrow 0.454 \text{CH}_3\text{O}_2 + 0.454 \text{OH} + 0.384 \text{CH}_3\text{CO}_3\text{H} + 0.162 \text{O}_3 + 0.162 \text{<CH}_3\text{COOH>}$
53	1.0×10^{-11}	$\text{CH}_3\text{CO}_3 + [\text{RO}_2\text{POOL}] \longrightarrow 0.7 \text{CH}_3\text{O}_2 + 0.3 \text{<CH}_3\text{COOH>}$
54	1.1×10^{-11}	$\text{CH}_3\text{CO}_3\text{H} + \text{OH} \longrightarrow 0.5 \text{CH}_3\text{CO}_3 + 0.5 \text{CH}_2\text{O}_2\text{CO}_3\text{H}$
55	KRO2NO	$\text{CH}_2\text{O}_2\text{CO}_3\text{H} + \text{NO} \longrightarrow \text{NO}_2 + \text{HOCH}_2\text{CO}_3$
56	KRO2NO3	$\text{CH}_2\text{O}_2\text{CO}_3\text{H} + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{HOCH}_2\text{CO}_3$
57	KHO2RO2×0.387	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \longrightarrow \text{HCOCH}_2\text{OOH}$
58	KRO2NO	$\text{HCOCH}_2\text{O}_2 + \text{NO} \longrightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$
59	KRO2NO3	$\text{HCOCH}_2\text{O}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$
60	2.0×10^{-12}	$\text{HCOCH}_2\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.2 \text{GLYOX} + 0.2 \text{HOCH}_2\text{CHO} + 0.6 \text{HCHO} + 0.6 \text{HO}_2 + 0.6 \text{CO}$
61	3.3×10^{-11}	$\text{HCOCH}_2\text{OOH} + \text{OH} \longrightarrow 0.89 \text{GLYOX} + 0.89 \text{OH} + 0.11 \text{HCOCH}_2\text{O}_2$
62	3.22×10^{-12}	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \longrightarrow 0.05 \text{ETRO}_2 + 0.95 \text{CH}_3\text{CHO} + 0.95 \text{HO}_2$
63	$9.8 \times 10^{-12} e^{-425/T}$	$\text{NC}_4\text{H}_{10} + \text{OH} \longrightarrow \text{C}_4\text{H}_9\text{O}_2$
64	KHO2RO2×0.625	$\text{C}_4\text{H}_9\text{O}_2 + \text{HO}_2 \longrightarrow \text{BURO}_2\text{H}$
65	2.4×10^{-11}	$\text{BURO}_2\text{H} + \text{OH} \longrightarrow 0.847 \text{OH} + 0.847 \text{MEK} + 0.153 \text{C}_4\text{H}_9\text{O}_2$
66	KRO2NO	$\text{C}_4\text{H}_9\text{O}_2 + \text{NO} \longrightarrow 0.917 \text{NO}_2 + 0.083 \text{SC}_4\text{H}_9\text{NO}_3 + 0.654 \text{HO}_2 + 0.654 \text{MEK} + 0.264 \text{CH}_3\text{CHO} + 0.264 \text{C}_2\text{H}_5\text{O}_2$
67	KRO2NO3	$\text{C}_4\text{H}_9\text{O}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + 0.716 \text{MEK} + 0.716 \text{HO}_2 + 0.284 \text{CH}_3\text{CHO} + 0.284 \text{C}_2\text{H}_5\text{O}_2$
68	8.6×10^{-13}	$\text{SC}_4\text{H}_9\text{NO}_3 + \text{OH} \longrightarrow \text{MEK} + \text{NO}_2$
69	1.1×10^{-12}	$\text{MEK} + \text{OH} \longrightarrow \text{MEKO}_2$
70	KRO2NO	$\text{MEKO}_2 + \text{NO} \longrightarrow \text{NO}_2 + 0.854 \text{CH}_3\text{CO}_3 + 0.854 \text{CH}_3\text{CHO} + 0.146 \text{C}_2\text{H}_5\text{CO}_3 + 0.146 \text{HCHO}$
71	KRO2NO3	$\text{MEKO}_2 + \text{NO}_3 \longrightarrow \text{NO}_2 + 0.854 \text{CH}_3\text{CO}_3 + 0.854 \text{CH}_3\text{CHO} + 0.146 \text{C}_2\text{H}_5\text{CO}_3 + 0.146 \text{HCHO}$
72	KHO2RO2×0.625	$\text{MEKO}_2 + \text{HO}_2 \longrightarrow \text{MEKO}_2\text{H}$
73	1.04×10^{-12}	$\text{MEKO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.2135 \text{BIACET} + 0.6405 \text{CH}_3\text{CO}_3 + 0.6405 \text{CH}_3\text{CHO} + 0.0365 \text{EGLYOX} + 0.1095 \text{C}_2\text{H}_5\text{CO}_3 + 0.1095 \text{HCHO}$
74	2.1×10^{-11}	$\text{MEKO}_2\text{H} + \text{OH} \longrightarrow 0.826 \text{OH} + 0.7054 \text{BIACET} + 0.1206 \text{EGLYOX} + 0.174 \text{MEKO}_2$
75	2.3×10^{-13}	$\text{BIACET} + \text{OH} \longrightarrow \text{CH}_3\text{CO}_3 + \text{HCHO} + \text{CO}$
76	KAPHO2	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \longrightarrow 0.75 \text{C}_2\text{H}_5\text{O}_2 + 0.75 \text{OH} + 0.25 \text{O}_3 + 0.25 \text{<PROPACID>}$
77	$6.7 \times 10^{-12} e^{340/T}$	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO} \longrightarrow \text{NO}_2 + \text{C}_2\text{H}_5\text{O}_2$
78	KFPAN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \longrightarrow \text{PPN}$
79	4.0×10^{-12}	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_3 \longrightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$
80	1.0×10^{-11}	$\text{C}_2\text{H}_5\text{CO}_3 + [\text{RO}_2\text{POOL}] \longrightarrow 0.7 \text{C}_2\text{H}_5\text{O}_2 + 0.3 \text{<PROPACID>}$
81	1.27×10^{-12}	$\text{PPN} + \text{OH} \longrightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{NO}_2$
82	KBPPN	$\text{PPN} \longrightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$
83	$5.6 \times 10^{-12} e^{-1860/T}$	$\text{EGLYOX} + \text{NO}_3 \longrightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{CO} + \text{HNO}_3$
84	1.39×10^{-11}	$\text{EGLYOX} + \text{OH} \longrightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{CO}$

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	Rate coefficient	Reaction
85	KMT15	$C_2H_4 + OH + M \longrightarrow ETRO_2$
86	KRO2NO	$ETRO_2 + NO \longrightarrow NO_2 + HOCH_2CH_2O$
87	KRO2NO3	$ETRO_2 + NO_3 \longrightarrow NO_2 + HOCH_2CH_2O$
88	$1.53 \times 10^{-13} e^{1300/T}$	$ETRO_2 + HO_2 \longrightarrow ETRO_2H$
89	1.9×10^{-12}	$ETRO_2 + [RO_2POOL] \longrightarrow 0.4 HOCH_2CHO + 0.6 HOCH_2CH_2O$
90	$9.5 \times 10^{13} e^{-5988/T}$	$HOCH_2CH_2O \longrightarrow HO_2 + 2 HCHO$
91	KROPRIM	$HOCH_2CH_2O + <O_2> \longrightarrow HO_2 + HOCH_2CHO$
92	1.7475×10^{-11}	$ETRO_2H + OH \longrightarrow 0.79 HOCH_2CHO + 0.79 OH + 0.21 ETRO_2$
93	1.0×10^{-11}	$HOCH_2CHO + OH \longrightarrow 0.2 GLYOX + 0.2 HO_2 + 0.8 HOCH_2CO_3$
94	KNO3AL	$HOCH_2CHO + NO_3 \longrightarrow HOCH_2CO_3 + HNO_3$
95	KAPHO2	$HOCH_2CO_3 + HO_2 \longrightarrow 0.75 HO_2 + 0.75 HCHO + 0.75 OH + 0.25 O_3 + 0.25 HOCH_2CO_2H$
96	KAPNO	$HOCH_2CO_3 + NO \longrightarrow NO_2 + HO_2 + HCHO$
97	KFPAN	$HOCH_2CO_3 + NO_2 \longrightarrow PHAN$
98	4.0×10^{-12}	$HOCH_2CO_3 + NO_3 \longrightarrow NO_2 + HO_2 + HCHO$
99	1.0×10^{-11}	$HOCH_2CO_3 + [RO_2POOL] \longrightarrow 0.7 HCHO + 0.7 HO_2 + 0.3 HOCH_2CO_2H$
100	2.73×10^{-12}	$HOCH_2CO_2H + OH \longrightarrow HCHO + HO_2$
101	1.12×10^{-12}	$PHAN + OH \longrightarrow HCHO + CO + NO_2$
102	KBPAN	$PHAN \longrightarrow HOCH_2CO_3 + NO_2$
103	$6.82 \times 10^{-15} e^{-2500/T}$	$C_2H_4 + O_3 \longrightarrow 1.1575 HCHO + 0.17 OH + 0.35 CO + 0.27 HO_2 + 0.18 H_2 + 0.2625 <HCOOH> + 0.1575 H_2O_2$
104	KMT16	$C_3H_6 + OH + M \longrightarrow PRRO_2$
105	$5.77 \times 10^{-15} e^{-1880/T}$	$C_3H_6 + O_3 \longrightarrow 0.489 CH_3CHO + 0.68 HCHO + 0.169 H_2O_2 + 0.3646 OH + 0.183 CO + 0.0684 H_2 + 0.038 HO_2 + 0.3 HCOCH_2O_2 + 0.05 CH_3OH + 0.04 CH_4 + 0.1 <HCOOH> + 0.181 <CH_3CO_2H>$
106	KRO2NO	$PRRO_2 + NO \longrightarrow NO_2 + CH_3CHO + HCHO + HO_2$
107	KRO2NO3	$PRRO_2 + NO_3 \longrightarrow NO_2 + CH_3CHO + HCHO + HO_2$
108	KHO2RO2 $\times 0.52$	$PRRO_2 + HO_2 \longrightarrow ACETOL$
109	8.8×10^{-13}	$PRRO_2 + [RO_2POOL] \longrightarrow 0.4 ACETOL + 0.6 CH_3CHO + 0.6 HCHO + 0.6 HO_2$
110	$4.6 \times 10^{-13} e^{-1155/T}$	$C_3H_6 + NO_3 \longrightarrow NRN9O_2$
111	KHO2RO2 $\times 0.52$	$NRN9O_2 + HO_2 \longrightarrow NOA$
112	KRO2NO	$NRN9O_2 + NO \longrightarrow 1.13 NO_2 + 0.87 NOA + 0.87 HO_2 + 0.13 CH_3CHO + 0.13 HCHO$
113	KRO2NO3	$NRN9O_2 + NO_3 \longrightarrow 1.13 NO_2 + 0.87 NOA + 0.87 HO_2 + 0.13 CH_3CHO + 0.13 HCHO$
114	6.7×10^{-13}	$NOA + OH \longrightarrow MGLYOX + NO_2$
115	KHO2RO2 $\times 0.625$	$IBUTOLBO_2 + HO_2 \longrightarrow C_2H_5OH + C_2H_5OOH$
116	KRO2NO	$IBUTOLBO_2 + NO \longrightarrow NO_2 + HCHO + HO_2 + C_2H_6 + CH_3OH$
117	KRO2NO3	$IBUTOLBO_2 + NO_3 \longrightarrow NO_2 + HCHO + HO_2 + C_2H_6 + CH_3OH$
118	$2.3 \times 10^{-12} e^{-190/T}$	$BENZENE + OH \longrightarrow 0.39 OXYLOL + 0.654 HO_2 + 0.346 OXYBIPERO_2$
119	$1.8 \times 10^{-12} e^{340/T}$	$TOLUENE + OH \longrightarrow 0.16 OXYLOL + 0.29 HO_2 + 0.71 OXYBIPERO_2$
120	1.36×10^{-11}	$OXYL + OH \longrightarrow 0.84 OXYBIPERO_2 + 0.16 HO_2 + 0.16 OXYLOL$
121	KRO2NO	$OXYBIPERO_2 + NO \longrightarrow 0.138 NOXYOLOOH + 0.862 NO_2 + 0.862 HO_2 + 0.3017 BIACET + 0.58185 BZFUONE + 0.28015 C_5DICARB + 0.28015 MGLYOX + 0.28015 EGLYOX$
122	KRO2NO3	$OXYBIPERO_2 + NO_3 \longrightarrow NO_2 + HO_2 + 0.35 BIACET + 0.325 C_5DICARB + 0.325 MGLYOX + 0.675 BZFUONE + 0.325 EGLYOX$
123	KHO2RO2 $\times 0.859$	$OXYBIPERO_2 + HO_2 \longrightarrow OXYBPEROOH$
124	7.62×10^{-11}	$OXYBPEROOH + OH \longrightarrow OXYBIPERO_2$
125	6.1×10^{-11}	$OXYLOL + OH \longrightarrow 0.17 OXYIO + 0.83 HO_2 + 0.83 OXYCATECH$
126	2.1×10^{-11}	$OXYLOL + NO_3 \longrightarrow 0.61 NOXYOLO_2 + 0.39 OXYIO + 0.39 HNO_3$
127	2.05×10^{-10}	$OXYCATECH + OH \longrightarrow OXCATEC1O$
128	2.01×10^{-10}	$OXYCATECH + NO_3 \longrightarrow HNO_3 + OXCATEC1O$
129	2.08×10^{-12}	$OXCATEC1O + NO_2 \longrightarrow OXNCATECH$
130	2.86×10^{-13}	$OXCATEC1O + O_3 \longrightarrow OXCATEC1O_2$
131	6.83×10^{-12}	$OXNCATECH + OH \longrightarrow OXNCATECO_2$
132	5.03×10^{-12}	$OXNCATECH + NO_3 \longrightarrow OXNNCATCO_2$

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	Rate coefficient	Reaction
133	$\text{KHO2RO2} \times 0.859$	$\text{OXNCATECO2} + \text{HO2} \rightarrow \text{OXNCATCOOH}$
134	KRO2NO	$\text{OXNCATECO2} + \text{NO} \rightarrow \text{NO2} + \text{CH3COCO2H} + \text{HO2} + \text{NC4MDCO2H}$
135	KRO2NO3	$\text{OXNCATECO2} + \text{NO3} \rightarrow \text{NO2} + \text{CH3COCO2H} + \text{HO2} + \text{NC4MDCO2H}$
136	8.0×10^{-13}	$\text{OXNCATECO2} + [\text{RO2POOL}] \rightarrow \text{CH3COCO2H} + \text{HO2} + \text{NC4MDCO2H}$
137	$1.9 \times 10^{-12} e^{190/T}$	$\text{NC4MDCO2H} + \text{OH} \rightarrow \text{NO2} + \text{<MMALANHY>}$
138	$1.9 \times 10^{-12} e^{190/T}$	$\text{OXNCATCOOH} + \text{OH} \rightarrow \text{OXNCATECO2}$
139	$\text{KHO2RO2} \times 0.859$	$\text{OXNNCATCO2} + \text{HO2} \rightarrow \text{OXNNCATOOH}$
140	KRO2NO	$\text{OXNNCATCO2} + \text{NO} \rightarrow 2 \text{NO2} + \text{CH3COCO2H} + \text{NC4MDCO2H}$
141	KRO2NO3	$\text{OXNNCATCO2} + \text{NO3} \rightarrow 2 \text{NO2} + \text{CH3COCO2H} + \text{NC4MDCO2H}$
142	8.0×10^{-13}	$\text{OXNNCATCO2} + [\text{RO2POOL}] \rightarrow \text{CH3COCO2H} + \text{NO2} + \text{NC4MDCO2H}$
143	$1.9 \times 10^{-12} e^{190/T}$	$\text{OXNNCATOOH} + \text{OH} \rightarrow \text{OXNNCATCO2}$
144	$\text{KHO2RO2} \times 0.859$	$\text{OXCATEC1O2} + \text{HO2} \rightarrow \text{OXCATEC1OOH}$
145	KRO2NO	$\text{OXCATEC1O2} + \text{NO} \rightarrow \text{NO2} + \text{OXCATEC1O}$
146	KRO2NO3	$\text{OXCATEC1O2} + \text{NO3} \rightarrow \text{NO2} + \text{OXCATEC1O}$
147	8.8×10^{-13}	$\text{OXCATEC1O2} + [\text{RO2POOL}] \rightarrow \text{OXCATEC1O}$
148	2.05×10^{-10}	$\text{OXCATEC1OOH} + \text{OH} \rightarrow \text{OXCATEC1O2}$
149	2.08×10^{-12}	$\text{OXY1O} + \text{NO2} \rightarrow \text{OXY1OHNO2}$
150	2.86×10^{-13}	$\text{OXY1O} + \text{O3} \rightarrow \text{DM123O2}$
151	1.53×10^{-12}	$\text{OXY1OHNO2} + \text{OH} \rightarrow \text{NOXYOL1O}$
152	3.13×10^{-13}	$\text{OXY1OHNO2} + \text{NO3} \rightarrow \text{HNO3} + \text{NOXYOL1O}$
153	2.08×10^{-12}	$\text{NOXYOL1O} + \text{NO2} \rightarrow \text{<DNOXYOL>}$
154	2.86×10^{-13}	$\text{NOXYOL1O} + \text{O3} \rightarrow \text{NOXYOL1O2}$
155	$\text{KHO2RO2} \times 0.859$	$\text{NOXYOL1O2} + \text{HO2} \rightarrow \text{NOXYOL1OOH}$
156	KRO2NO	$\text{NOXYOL1O2} + \text{NO} \rightarrow \text{NO2} + \text{NOXYOL1O}$
157	KRO2NO3	$\text{NOXYOL1O2} + \text{NO3} \rightarrow \text{NO2} + \text{NOXYOL1O}$
158	1.53×10^{-12}	$\text{NOXYOL1OOH} + \text{OH} \rightarrow \text{NOXYOL1O2}$
159	$\text{KHO2RO2} \times 0.859$	$\text{DM123O2} + \text{HO2} \rightarrow \text{DM123OOH}$
160	KRO2NO	$\text{DM123O2} + \text{NO} \rightarrow \text{NO2} + \text{OXY1O}$
161	KRO2NO3	$\text{DM123O2} + \text{NO3} \rightarrow \text{NO2} + \text{OXY1O}$
162	4.65×10^{-11}	$\text{DM123OOH} + \text{OH} \rightarrow \text{DM123O2}$
163	$\text{KHO2RO2} \times 0.859$	$\text{NOXYOLO2} + \text{HO2} \rightarrow \text{NOXYOLOOH}$
164	KRO2NO	$\text{NOXYOLO2} + \text{NO} \rightarrow 2 \text{NO2} + \text{GLYOX} + \text{CH3COCO2H} + \text{C3H6}$
165	KRO2NO3	$\text{NOXYOLO2} + \text{NO3} \rightarrow 2 \text{NO2} + \text{GLYOX} + \text{CH3COCO2H} + \text{C3H6}$
166	8.0×10^{-13}	$\text{NOXYOLO2} + [\text{RO2POOL}] \rightarrow \text{NO2} + \text{GLYOX} + \text{CH3COCO2H} + \text{C3H6}$
167	1.43×10^{-10}	$\text{NOXYOLOOH} + \text{OH} \rightarrow \text{NOXYOLO2}$
168	3.0×10^{-13}	$\text{BZFUONE} + \text{NO3} \rightarrow \text{NO2} + \text{IBUTOLBO2}$
169	4.45×10^{-11}	$\text{BZFUONE} + \text{OH} \rightarrow \text{IBUTOLBO2}$
170	6.2×10^{-11}	$\text{C5DICARB} + \text{OH} \rightarrow \text{C5DICARBO2}$
171	KRO2NO	$\text{C5DICARBO2} + \text{NO} \rightarrow \text{NO2} + \text{HO2} + \text{MGLYOX} + \text{GLYOX}$
172	KRO2NO3	$\text{C5DICARBO2} + \text{NO3} \rightarrow \text{NO2} + \text{HO2} + \text{MGLYOX} + \text{GLYOX}$
173	$\text{KHO2RO2} \times 0.706$	$\text{C5DICARBO2} + \text{HO2} \rightarrow \text{C5DICAROOH}$
174	$1.9 \times 10^{-12} e^{190/T}$	$\text{C5DICAROOH} + \text{OH} \rightarrow \text{C5DICARBO2}$
175	$3.1 \times 10^{-12} e^{340/T}$	$\text{GLYOX} + \text{OH} \rightarrow 0.416 \text{HO2} + 1.417 \text{CO} + 0.584 \text{OH}$
176	$1.9 \times 10^{-12} e^{575/T}$	$\text{MGLYOX} + \text{OH} \rightarrow \text{CH3CO3} + \text{CO}$
177	$2.7 \times 10^{-11} e^{390/T}$	$\text{C5H8} + \text{OH} \rightarrow \text{ISRO2}$
178	$1.05 \times 10^{-14} e^{-2000/T}$	$\text{C5H8} + \text{O3} \rightarrow 0.363 \text{MACR} + 0.312 \text{MVK} + 0.364 \text{CO} + 0.1725 \text{HO2} + 0.25 \text{OH} + 0.175 \text{<HCOOH>} + 0.7775 \text{HCHO} + 0.28 \text{H2O2} + 0.0475 \text{C3H6} + 0.1535 \text{CH3CO3} + 0.105 \text{MACO2H}$
179	$2.95 \times 10^{-12} e^{-450/T}$	$\text{C5H8} + \text{NO3} \rightarrow \text{NISOP02}$
180	KRO2NO	$\text{ISRO2} + \text{NO} \rightarrow 0.9 \text{NO2} + 0.6 \text{MVK} + 0.3 \text{MACR} + 0.9 \text{HCHO} + 0.9 \text{HO2} + 0.1 \text{ISON}$
181	KRO2NO3	$\text{ISRO2} + \text{NO3} \rightarrow \text{NO2} + 0.667 \text{MVK} + 0.333 \text{MACR} + \text{HCHO} + \text{HO2}$
182	$\text{KHO2RO2} \times 0.706$	$\text{ISRO2} + \text{HO2} \rightarrow \text{ISRO2H}$
183	1.45×10^{-12}	$\text{ISRO2} + [\text{RO2POOL}] \rightarrow 0.6665 \text{MVK} + \text{HCHO} + \text{HO2} + 0.3335 \text{MACR}$
184	$1.88 \times 10^9 e^{-7261/T} \times 0.052$	$\text{ISRO2} \rightarrow \text{HPALD} + \text{HO2}$
185	$1.45 \times 10^{12} e^{-10688/T}$	$\text{ISRO2} \rightarrow \text{MACR} + \text{HCHO} + \text{OH}$
186	6.0×10^{-11}	$\text{ISRO2H} + \text{OH} \rightarrow 0.93 \text{IEPOX} + 0.07 \text{ISRO2} + 0.93 \text{OH}$

EmChem19X (continued on next page)

	Rate coefficient	Reaction
187	1.16×10^{-11}	IEPOX + OH $\longrightarrow$ 0.74 HMVKO2 + 0.15 MACRO2 + 0.89 CH3OH + 0.11 BIACETOH + 0.11 CH4
188	3.25×10^{-11}	ISON + OH $\longrightarrow$ 0.6 ACETOL + 0.6 NALD + 0.6 HO2 + 0.4 NO2 + 0.2 MACR + 0.2 MVK + 0.4 HCHO
189	$8.0 \times 10^{-12} e^{380/T}$	MACR + OH $\longrightarrow$ 0.45 MACO3 + 0.55 MACRO2
190	$1.36 \times 10^{-15} e^{-2112/T}$	MACR + O3 $\longrightarrow$ 0.9016 MGLYOX + 0.1408 HO2 + 0.6528 CO + 0.2392 OH + 0.2035 <HCOOH> + 0.1437 H2O2 + 0.2421 HCHO + 0.0984 CH3CO3
191	3.4×10^{-15}	MACR + NO3 $\longrightarrow$ MACO3 + HNO3
192	KRO2NO	MACRO2 + NO $\longrightarrow$ NO2 + HO2 + 0.85 ACETOL + 0.85 CO + 0.15 MGLYOX + 0.15 HCHO
193	KRO2NO3	MACRO2 + NO3 $\longrightarrow$ NO2 + HO2 + 0.85 ACETOL + 0.85 CO + 0.15 MGLYOX + 0.15 HCHO
194	KHO2RO2 $\times 0.625$	MACRO2 + HO2 $\longrightarrow$ MACROOH
195	K14ISOM1	MACRO2 $\longrightarrow$ ACETOL + CO + OH
196	KFPAN	MACO3 + NO2 $\longrightarrow$ MPAN
197	$1.6 \times 10^{16} e^{-13500/T}$	MPAN $\longrightarrow$ MACO3 + NO2
198	KAPHO2	MACO3 + HO2 $\longrightarrow$ 0.44 OH + 0.44 HCHO + 0.56 O3 + 0.56 MACO2H + 0.154 CH3CO3 + 0.286 CH3O2 + 0.286 CO
199	1.0×10^{-11}	MACO3 + [RO2POOL] $\longrightarrow$ 0.3 MACO2H + 0.7 HCHO + 0.455 CH3O2 + 0.455 CO + 0.245 CH3CO3
200	$8.7 \times 10^{-12} e^{290/T}$	MACO3 + NO $\longrightarrow$ NO2 + HCHO + 0.35 CH3CO3 + 0.65 CH3O2 + 0.65 CO
201	4.0×10^{-12}	MACO3 + NO3 $\longrightarrow$ NO2 + HCHO + 0.35 CH3CO3 + 0.65 CH3O2 + 0.65 CO
202	2.9×10^{-11}	MPAN + OH $\longrightarrow$ ACETOL + NO3 + CO
203	8.2×10^{-18}	MPAN + O3 $\longrightarrow$ HCHO + CH3CO3 + NO3
204	3.77×10^{-11}	MACROOH + OH $\longrightarrow$ ACETOL + CO + OH
205	$1.6 \times 10^{-12} e^{305/T}$	ACETOL + OH $\longrightarrow$ MGLYOX + HO2
206	1.55×10^{-12}	NALD + OH $\longrightarrow$ HCHO + CO + NO2
207	$2.6 \times 10^{-12} e^{610/T}$	MVK + OH $\longrightarrow$ HMVKO2
208	$8.5 \times 10^{-16} e^{-1520/T}$	MVK + O3 $\longrightarrow$ 0.545 MGLYOX + 0.645 HCHO + 0.56 CO + 0.36 OH + 0.28 HO2 + 0.075 <HCOOH> + 0.09 H2O2 + 0.1 CH3CHO + 0.28 CH3CO3 + 0.075 CH3COCO2H
209	KRO2NO	HMVKO2 + NO $\longrightarrow$ 0.0352 MVKNO3 + 0.9648 NO2 + 0.67536 CH3CO3 + 0.67536 HOCH2CHO + 0.28944 MGLYOX + 0.28944 HCHO + 0.28944 HO2
210	KRO2NO3	HMVKO2 + NO3 $\longrightarrow$ NO2 + 0.7 CH3CO3 + 0.7 HOCH2CHO + 0.3 MGLYOX + 0.3 HCHO + 0.3 HO2
211	KHO2RO2 $\times 0.625$	HMVKO2 + HO2 $\longrightarrow$ MVKO2H
212	1.22×10^{-12}	HMVKO2 + [RO2POOL] $\longrightarrow$ 0.28 BIACETOH + 0.42 CH3CO3 + 0.42 HOCH2CHO + 0.12 CO2H3CHO + 0.18 MGLYOX + 0.18 HO2 + 0.18 HCHO
213	4.5×10^{-11}	MVKO2H + OH $\longrightarrow$ 0.7 BIACETOH + OH + 0.3 CO2H3CHO
214	2.96×10^{-12}	BIACETOH + OH $\longrightarrow$ CO23C3CHO + HO2
215	1.23×10^{-11}	CO23C3CHO + OH $\longrightarrow$ CH3CO3 + 2 CO
216	KNO3AL $\times 4$	CO23C3CHO + NO3 $\longrightarrow$ CH3CO3 + 2 CO + HNO3
217	2.45×10^{-11}	CO2H3CHO + OH $\longrightarrow$ CO2H3CO3
218	KNO3AL $\times 4$	CO2H3CHO + NO3 $\longrightarrow$ HNO3 + CO2H3CO3
219	KAPHO2	CO2H3CO3 + HO2 $\longrightarrow$ 0.56 CO2H3CO3H + 0.44 MGLYOX + 0.44 HO2 + 0.44 OH
220	KAPNO	CO2H3CO3 + NO $\longrightarrow$ MGLYOX + HO2 + NO2
221	4.0×10^{-12}	CO2H3CO3 + NO3 $\longrightarrow$ MGLYOX + HO2 + NO2
222	1.0×10^{-11}	CO2H3CO3 + [RO2POOL] $\longrightarrow$ MGLYOX + HO2
223	KFPAN	CO2H3CO3 + NO2 $\longrightarrow$ C4PAN6
224	3.74×10^{-12}	C4PAN6 + OH $\longrightarrow$ MGLYOX + CO + NO2
225	KBPAN	C4PAN6 $\longrightarrow$ CO2H3CO3 + NO2
226	7.34×10^{-12}	CO2H3CO3H + OH $\longrightarrow$ CO2H3CO3
227	1.33×10^{-12}	MVKNO3 + OH $\longrightarrow$ 0.67 CO2N3CHO + 0.67 HO2 + 0.33 BIACETOH + 0.33 NO2
228	KHO2RO2 $\times 0.706$	NISOP2 + HO2 $\longrightarrow$ ISON2
229	KRO2NO	NISOP2 + NO $\longrightarrow$ NO2 + ISON2 + HO2
230	KRO2NO3	NISOP2 + NO3 $\longrightarrow$ NO2 + ISON2 + HO2

EmChem19X (continued on next page)

	Rate coefficient	Reaction
231	1.3×10^{-12}	$\text{NISOP} \text{O}_2 + [\text{RO}_2\text{POOL}] \rightarrow 0.2 \text{ ISON} + 0.8 \text{ ISON}_2 + 0.6 \text{ HO}_2$
232	4.16×10^{-11}	$\text{ISON}_2 + \text{OH} \rightarrow \text{NC}_4\text{CO}_3$
233	2.4×10^{-17}	$\text{ISON}_2 + \text{O}_3 \rightarrow 0.555 \text{ NOA} + 0.555 \text{ GLYOX} + 0.89 \text{ OH} + 0.445 \text{ HO}_2 + 0.89 \text{ CO} + 0.0756 \text{ H}_2\text{O}_2 + 0.445 \text{ MGLYOX} + 0.445 \text{ NO}_2$
234	$\text{KNO}_3\text{AL} \times 4.25$	$\text{ISON}_2 + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{NC}_4\text{CO}_3$
235	KAPHO2	$\text{NC}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{NOA} + \text{CO} + \text{HO}_2 + \text{OH}$
236	KAPNO	$\text{NC}_4\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{NOA} + \text{CO} + \text{HO}_2$
237	4.0×10^{-12}	$\text{NC}_4\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NOA} + \text{CO} + \text{HO}_2$
238	KFPAN	$\text{NC}_4\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_5\text{PAN}_{18}$
239	1.0×10^{-11}	$\text{NC}_4\text{CO}_3 + [\text{RO}_2\text{POOL}] \rightarrow \text{NOA} + \text{HO}_2 + \text{CO}$
240	KBPAN	$\text{C}_5\text{PAN}_{18} \rightarrow \text{NC}_4\text{CO}_3 + \text{NO}_2$
241	2.16×10^{-11}	$\text{C}_5\text{PAN}_{18} + \text{OH} \rightarrow \text{NOA} + 2 \text{ CO} + \text{NO}_2$
242	7.61×10^{-11}	$\text{HPALD} + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{HCHO} + \text{OH}$
243	1.51×10^{-11}	$\text{MACO}_2\text{H} + \text{OH} \rightarrow 0.35 \text{ CH}_3\text{CO}_3 + \text{HCHO} + 0.65 \text{ CO} + 0.65 \text{ CH}_3\text{O}_2$
244	$1.34 \times 10^{-11} e^{410/T}$	$\text{APINENE} + \text{OH} \rightarrow \text{TERPO}_2$
245	$8.22 \times 10^{-16} e^{-640/T}$	$\text{APINENE} + \text{O}_3 \rightarrow 0.7 \text{ OH} + \text{MVK} + \text{MACR} + \text{HO}_2$
246	$1.2 \times 10^{-12} e^{490/T}$	$\text{APINENE} + \text{NO}_3 \rightarrow \text{TERPO}_2 + \text{NO}_2$
247	KRO2NO	$\text{TERPO}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{MVK} + \text{MACR} + \text{NO}_2 + 0.19 \text{ C}_2\text{H}_6$
248	KRO2NO3	$\text{TERPO}_2 + \text{NO}_3 \rightarrow \text{HO}_2 + \text{MVK} + \text{MACR} + \text{NO}_2 + 0.19 \text{ C}_2\text{H}_6$
249	$7.5 \times 10^{-13} e^{700/T}$	$\text{TERPO}_2 + \text{HO}_2 \rightarrow \text{TERPOOH}$
250	$3.8 \times 10^{-12} e^{200/T}$	$\text{TERPOOH} + \text{OH} \rightarrow \text{TERPO}_2$
251	RCPHOT(IDO3-O1D)	$\text{O}_3 \rightarrow \text{OD}$
252	RCPHOT(IDO3-O3P)	$\text{O}_3 \rightarrow \text{OP}$
253	RCPHOT(IDH2O2)	$\text{H}_2\text{O}_2 \rightarrow 2 \text{ OH}$
254	RCPHOT(IDNO2)	$\text{NO}_2 \rightarrow \text{OP} + \text{NO}$
255	RCPHOT(IDNO3)	$\text{NO}_3 \rightarrow 0.127 \text{ NO} + 0.873 \text{ NO}_2 + 0.873 \text{ OP}$
256	RCPHOT(IDHONO)	$\text{HONO} \rightarrow \text{OH} + \text{NO}$
257	RCPHOT(IDHNO3)	$\text{HNO}_3 \rightarrow \text{NO}_2 + \text{OH}$
258	RCPHOT(IDHO2NO2)	$\text{HO}_2\text{NO}_2 \rightarrow 0.333 \text{ OH} + 0.333 \text{ NO}_3 + 0.667 \text{ NO}_2 + 0.667 \text{ HO}_2$
259	RCPHOT(IDHCHO-H)	$\text{HCHO} \rightarrow \text{CO} + 2 \text{ HO}_2$
260	RCPHOT(IDHCHO-H2)	$\text{HCHO} \rightarrow \text{CO} + \text{H}_2$
261	$\text{RCPHOT}(\text{IDHCHO-H}) \times 0.6$	$\text{HOCH}_2\text{CHO} \rightarrow 2 \text{ HO}_2 + \text{HCHO} + \text{CO}$
262	$\text{RCPHOT}(\text{IDHCHO-H}) \times 0.6$	$\text{CO}_2\text{H}_3\text{CHO} \rightarrow 2 \text{ HO}_2 + \text{MGLYOX} + \text{CO}$
263	$\text{RCPHOT}(\text{IDHCHO-H}_2) \times 0.078$	$\text{MVK} \rightarrow 0.5 \text{ C}_3\text{H}_6 + \text{CO} + 0.5 \text{ CH}_3\text{CO}_3 + 0.5 \text{ HCHO} + 0.5 \text{ HO}_2$
264	$\text{RCPHOT}(\text{IDHCHO-H}_2) \times 0.04767$	$\text{MACR} \rightarrow 0.5 \text{ MACO}_3 + \text{HO}_2 + 0.825 \text{ CO} + 0.5 \text{ HCHO} + 0.325 \text{ CH}_3\text{O}_2 + 0.175 \text{ CH}_3\text{CO}_3$
265	$\text{RCPHOT}(\text{IDHCHO-H}_2) \times 12$	$\text{HPALD} \rightarrow 0.32 \text{ CH}_3\text{CO}_3 + 0.32 \text{ HOCH}_2\text{CHO} + 1.68 \text{ CO} + \text{OH} + 0.68 \text{ ACETOL} + 0.68 \text{ HO}_2$
266	RCPHOT(IDCH3CHO)	$\text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{O}_2 + \text{HO}_2 + \text{CO}$
267	RCPHOT(IDCH3CHO)	$\text{NALD} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{HO}_2$
268	RCPHOT(IDMEK)	$\text{MEK} \rightarrow \text{CH}_3\text{CO}_3 + \text{C}_2\text{H}_5\text{O}_2$
269	RCPHOT(IDMEK)	$\text{ACETOL} \rightarrow \text{CH}_3\text{CO}_3 + \text{HCHO} + \text{HO}_2$
270	RCPHOT(IDCHOCHO)	$\text{GLYOX} \rightarrow 1.9 \text{ CO} + 0.1 \text{ HCHO} + 0.5 \text{ HO}_2$
271	RCPHOT(IDRCOCHO)	$\text{MGLYOX} \rightarrow \text{CH}_3\text{CO}_3 + \text{CO} + \text{HO}_2$
272	RCPHOT(IDRCOCHO)	$\text{EGLYOX} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{CO} + \text{HO}_2$
273	RCPHOT(IDRCOCHO)	$\text{CH}_3\text{COCO}_2\text{H} \rightarrow 0.6 \text{ CH}_3\text{CHO} + 0.05 \text{ <CH}_3\text{COOH>} + 0.05 \text{ CO} + 0.35 \text{ CH}_3\text{CO}_3 + 0.35 \text{ HO}_2$
274	RCPHOT(IDCH3COY)	$\text{BIACET} \rightarrow 2 \text{ CH}_3\text{CO}_3$
275	RCPHOT(IDCH3COY)	$\text{BIACETOH} \rightarrow \text{CH}_3\text{CO}_3 + \text{HOCH}_2\text{CO}_3$
276	RCPHOT(IDCH3COY)	$\text{CO}_2\text{C}_3\text{CHO} \rightarrow \text{CH}_3\text{CO}_3 + 0.41 \text{ HO}_2 + 1.41 \text{ CO} + 0.58 \text{ OH}$
277	RCPHOT(IDRCOCHO)	$\text{CO}_2\text{C}_3\text{CHO} \rightarrow \text{CH}_3\text{CO}_3 + 2 \text{ CO} + \text{HO}_2$
278	$\text{RCPHOT}(\text{IDNO}_2) \times 0.2$	$\text{C}_5\text{DICARB} \rightarrow \text{C}_5\text{DICARBO}_2 + \text{HO}_2$
279	RCPHOT(IDCH3O2H)	$\text{CH}_3\text{OOH} \rightarrow \text{HCHO} + \text{OH} + \text{HO}_2$
280	RCPHOT(IDCH3O2H)	$\text{C}_2\text{H}_5\text{OOH} \rightarrow \text{HO}_2 + \text{CH}_3\text{CHO} + \text{OH}$
281	RCPHOT(IDCH3O2H)	$\text{BURO}_2\text{H} \rightarrow \text{OH} + 0.716 \text{ HO}_2 + 0.716 \text{ MEK} + 0.284 \text{ CH}_3\text{CHO} + 0.284 \text{ C}_2\text{H}_5\text{O}_2$
282	RCPHOT(IDCH3O2H)	$\text{ETRO}_2\text{H} \rightarrow \text{OH} + \text{HOCH}_2\text{CH}_2\text{O}$
283	RCPHOT(IDCH3O2H)	$\text{CH}_3\text{CO}_3\text{H} \rightarrow \text{CH}_3\text{O}_2 + \text{OH}$

EmChem19X (continued on next page)

	Rate coefficient	Reaction
284	RCPHOT(IDCH3O2H)	MEKO2H $\longrightarrow$ OH + 0.854 CH3CHO + 0.854 CH3CO3 + 0.146 C2H5CO3 + 0.146 HCHO
285	RCPHOT(IDMEK)	MEKO2H $\longrightarrow$ OH + 0.854 CH3CHO + 0.854 CH3CO3 + 0.146 C2H5CO3 + 0.146 HCHO
286	RCPHOT(IDCH3O2H)	HCOCH2OOH $\longrightarrow$ OH + HCHO + CO + HO2
287	RCPHOT(IDHCHO-H) $\times 0.6$	HCOCH2OOH $\longrightarrow$ OH + HCHO + CO + HO2
288	RCPHOT(IDCH3O2H)	CO2H3CO3H $\longrightarrow$ MGLYOX + HO2 + OH
289	RCPHOT(IDCH3O2H)	MVKO2H $\longrightarrow$ OH + 0.7 HOCH2CHO + 0.7 CH3CO3 + 0.3 HO2 + 0.3 HCHO + 0.3 MGLYOX
290	RCPHOT(IDHCHO-H) $\times 1.87$	MACROOH $\longrightarrow$ OH + ACETOL + CO + HO2
291	RCPHOT(IDCH3O2H)	ISRO2H $\longrightarrow$ OH + HO2 + HCHO + 0.16 MACR + 0.84 MVK
292	RCPHOT(IDCH3O2H)	OXYBPEROOH $\longrightarrow$ OH + HO2 + 0.35 BIACET + 0.325 C5DICARB + 0.325 MGLYOX + 0.675 BZFUONE + 0.325 EGLYOX
293	RCPHOT(IDCH3O2H)	OCATEC1OOH $\longrightarrow$ OH + OXCATEC1O
294	RCPHOT(IDCH3O2H)	DM123OOH $\longrightarrow$ OXY1O + OH
295	RCPHOT(IDCH3O2H)	OXNCATCOOH $\longrightarrow$ OH + CH3COCO2H + HO2 + NC4MDCO2H
296	RCPHOT(IDCH3O2H)	OXNNCATOOH $\longrightarrow$ OH + CH3COCO2H + NO2 + NC4MDCO2H
297	RCPHOT(IDCH3O2H)	NOXYOL1OOH $\longrightarrow$ OH + NOXYOL1O
298	RCPHOT(IDCH3O2H)	NOXYOLOOH $\longrightarrow$ OH + NO2 + GLYOX + CH3COCO2H + C3H6
299	RCPHOT(IDMEK) $\times 0.78$	NOXYOLOOH $\longrightarrow$ OH + NO2 + HO2 + GLYOX + CH3COCO2H + C3H6
300	RCPHOT(IDMEK) $\times 0.78$	SC4H9NO3 $\longrightarrow$ NO2 + 0.652 MEK + 0.652 HO2 + 0.348 CH3CHO + 0.348 C2H5O2
301	RCPHOT(IDMEK) $\times 8.3337$	NOA $\longrightarrow$ CH3CO3 + HCHO + NO2
302	RCPHOT(IDMEK) $\times 13$	MVKNO3 $\longrightarrow$ CH3CO3 + HOCH2CHO + NO2
303	RCPHOT(IDMEK) $\times 83$	CO2N3CHO $\longrightarrow$ GLYOX + CH3CO3 + NO2
304	RCPHOT(IDHCHO-H) $\times 0.1814$	ISON $\longrightarrow$ 0.333 MACR + 0.667 MVK + HCHO + NO2 + HO2
305	RCPHOT(IDMEK) $\times 133.34$	ISON2 $\longrightarrow$ ACETOL + 2 CO + HO2 + NO2

Notes:

"T" is temperature, "M" is third body, RCPHOT are photolysis rates.

Reaction coefficients are in units of s^{-1} for unimolecular reactions, $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for bimolecular reactions, and $\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-2}$ for termolecular reactions.

$$\text{FH2O} = 1.0 + 1.41 \times 10^{-21} e^{2200/T} \times [\text{H2O}]$$

$$\text{KAPHO2} = 3.14 \times 10^{-12} e^{580/T}$$

$$\text{KAPNO} = 7.5 \times 10^{-12} e^{290/T}$$

$$\text{KHO2RO2} = 2.91 \times 10^{-13} e^{1300/T}$$

$$\text{KMT05} = 1.44 \times 10^{-13} + [\text{M}] \times 3.43 \times 10^{-33}$$

$$\text{KNO3AL} = 1.4 \times 10^{-12} e^{-1860/T}$$

$$\text{KRO2NO} = 2.7 \times 10^{-12} e^{360/T}$$

$$\text{KRO2NO3} = 2.3 \times 10^{-12}$$

$$\text{K14ISOM1} = 3 \times 10^7 e^{-5300/T}$$

Some complex 3-body rate-expressions are given in Tables [G.3](#) and [G.4](#)

Table H.2: Gas-phase species in EmChem19X (note that most of the organic species represent a number of different compounds and in some cases their reactions have been adjusted (rates and/or products) to take this into account)

Model species	description
non-advected (short-lived) species	
OD	O(¹ D)
OP	O(³ P)
OH	OH
HO2	HO ₂
CH3O2	CH ₃ O ₂ , RO ₂
C2H5O2	C ₂ H ₅ O ₂ , RO ₂
C4H9O2	C ₄ H ₉ O ₂ , RO ₂
ISRO2	HOC ₅ H ₈ O ₂ , RO ₂
HCOCH2O2	HCOCH ₂ O ₂ , RO ₂
ETRO2	HOCH ₂ CH ₂ O ₂ , RO ₂
PRRO2	CH ₃ CHO ₂ CH ₂ OH, RO ₂
HMVKO2	HOCH ₂ CH(O ₂)C(O)CH ₃ and CH ₃ C(O)CH(OH)CH ₂ O ₂ , RO ₂
OXYBIPERO2	C ₈ H ₁₁ O ₅ , RO ₂
MACO3	CH ₂ C(CH ₃)C(O)O ₂ , RO ₂
MEKO2	CH ₃ COCHO ₂ CH ₃ and CH ₃ COCH ₂ CH ₂ O ₂ , RO ₂
C5DICARBO2	CH ₃ COCH(O ₂)CH(OH)CHO, RO ₂
DM123O2	2,3-(CH ₃) ₂ -C ₆ H ₃ O ₂ , RO ₂
OXCATEC1O2	2,3-(CH ₃) ₂ -6-OH-C ₆ H ₂ O ₂ , RO ₂
CH2O2CO3H	CH ₂ O ₂ CO ₃ H, RO ₂
MACRO2	O=CHC(O ₂)(CH ₃)CH ₂ OH, RO ₂
HOCH2CO3	HOCH ₂ C(O)O ₂ , RO ₂
CH3CO3	CH ₃ C(O)O ₂ , RO ₂
C2H5CO3	C ₂ H ₅ C(O)O ₂ , RO ₂
CO2H3CO3	CH ₃ C(O)CH(OH)C(O)O ₂ , RO ₂
IBUTOLBO2	HOCH ₂ C(CH ₃) ₂ O ₂ , RO ₂
TERPO2	C ₁₀ H ₁₇ O ₃ , RO ₂
HOCH2CH2O	HOCH ₂ CH ₂ O, oxy-radical
OXY1O	2,3-(CH ₃) ₂ -C ₆ H ₃ O, o-xyloxy radical
OXCATEC1O	2,3-(CH ₃) ₂ -6-OH-C ₆ H ₂ O, oxy-radical
advected species	
NRN9O2	CH ₃ C(O ₂)CH ₂ ONO ₂ and CH ₃ CH(CH ₂ O ₂)ONO ₂ , RO ₂ , OXN, organic nitrate
NISOPO2	CH ₂ (O ₂)CH=C(CH ₃)CH ₂ ONO ₂ , RO ₂ , OXN, organic nitrate
NC4CO3	C(O)(O ₂)CH=C(CH ₃)CH ₂ ONO ₂ , RO ₂ , OXN, organic nitrate
NOXYOLO2	C ₈ H ₁₀ NO ₈ , RO ₂ , OXN, organic nitrate
OXNCATECO2	C ₈ H ₁₀ NO ₉ , RO ₂ , OXN, nitro group
OXNNCATCO2	C ₈ H ₉ N ₂ O ₁₁ , RO ₂ , OXN, organic nitrate, nitro group
NOXYOL1O2	2,3-(CH ₃) ₂ -6-NO ₂ -C ₆ H ₂ O ₂ , RO ₂ , OXN, nitro group
NOXYOL1O	2,3-(CH ₃) ₂ -6-NO ₂ -C ₆ H ₂ O, oxy-radical, OXN, nitro group
O3	O ₃
NO	NO, NO _x , OXN
NO2	NO ₂ , NO _x , OXN
NO3	NO ₃ , OXN
N2O5	N ₂ O ₅ , OXN
H2	H ₂
H2O2	H ₂ O ₂
HONO	HONO, OXN
HNO3	HNO ₃ , OXN
<i>EmChem19X species (continued on next page)</i>	

Model species	description
HO2NO2	HO ₂ NO ₂ , OXN
CO	CO
CH4	CH ₄
C2H6	C ₂ H ₆
NC4H10	n-C ₄ H ₁₀
C2H4	C ₂ H ₄
C3H6	C ₃ H ₆
BENZENE	C ₆ H ₆
TOLUENE	C ₆ H ₅ CH ₃
OXYL	o-(CH ₃) ₂ -C ₆ H ₄
C5H8	CH ₂ =C(CH ₃)CH=CH ₂ , isoprene
APINENE	C ₁₀ H ₁₆ (α-pinene), monoterpene
CH3OH	CH ₃ OH
C2H5OH	C ₂ H ₅ OH
OXYLOL	2,3-(CH ₃) ₂ -C ₆ H ₃ OH
OXYCATECH	3,4-(CH ₃) ₂ -1,2-C ₆ H ₂ (OH) ₂
HCHO	HCHO, carbonyl
CH3CHO	CH ₃ CHO, carbonyl
MACR	CH ₂ =C(CH ₃)CHO, carbonyl
MEK	CH ₃ C(O)C ₂ H ₅ , carbonyl
MVK	CH ₃ C(=O)CH=CH ₂ , carbonyl
HOCH2CHO	HOCH ₂ CHO, carbonyl
HCOCH2OOH	HCOCH ₂ OOH, ROOH, carbonyl
ACETOL	CH ₃ C(O)CH ₂ OH, carbonyl
GLYOX	HCOHCO, glyoxal, carbonyl
MGLYOX	CH ₃ C(O)CHO, methyl glyoxal, carbonyl
EGLYOX	C ₂ H ₅ C(O)CHO, carbonyl
CO2H3CHO	CH ₃ C(O)CH(OH)CHO, carbonyl
CO23C3CHO	CH ₃ C(O)C(O)CHO, carbonyl
BIACET	CH ₃ C(O)C(O)CH ₃ , 2,3-butanedione, carbonyl
BIACETOH	CH ₃ C(O)C(O)CH ₂ OH, carbonyl
C5DICARB	CH ₃ C(O)CH=CHCHO, 4-oxopent-2-enal, carbonyl
BZFUONE	C ₄ H ₄ O ₂ , 2(5H)-Furanone, carbonyl
HOCH2CO2H	HOCH ₂ C(O)OH, acid
CH3COCO2H	CH ₃ C(O)C(O)OH, carbonyl, acid
MACO2H	CH ₂ =C(CH ₃)C(=O)OH, acid
CH3OOH	CH ₃ OOH, ROOH
C2H5OOH	C ₂ H ₅ OOH, ROOH
BURO2H	sec-C ₄ H ₉ OOH, ROOH
DM123OOH	2,3-(CH ₃) ₂ -C ₆ H ₃ OOH, ROOH
ETRO2H	HOCH ₂ CH ₂ OOH, ROOH
MEKO2H	CH ₃ C(O)CH(CH ₃)OOH, carbonyl, ROOH
ISRO2H	C ₃ H ₈ (OH)(OOH), hydroperoxides from isoprene (several isomers), ROOH
C5DICAROOH	CH ₃ COCH(OOH)CH(OH)CHO, ROOH, carbonyl
OCATEC1OOH	2,3-(CH ₃) ₂ -6-OH-C ₆ H ₂ OOH, ROOH
HPALD	HCOCH=C(CH ₃)CH ₂ OOH and HCOC(CH ₃)=CHCH ₂ OOH, ROOH, carbonyl
MVKO2H	HOCH ₂ CH(OOH)C(O)CH ₃ and CH ₃ C(O)CH(OH)CH ₂ OOH, ROOH, carbonyl
MACROOH	O=CHC(CH ₃)(OOH)CH ₂ OH, ROOH, carbonyl
OXYBPEROOH	C ₈ H ₁₂ O ₅ (multifunctional), ROOH
CH3CO3H	CH ₃ C(O)OOH, peroxyacid
CO2H3CO3H	CH ₃ C(O)CH(OH)C(O)OOH, peroxyacid, carbonyl
IEPOX	C ₃ H ₁₀ O ₃ (epoxide with two OH groups)
SC4H9NO3	sec-C ₄ H ₉ NO ₃ , OXN, organic nitrate
MVKNO3	CH ₃ CH(O)CH(ONO ₂)CH ₂ OH and CH ₃ CH(O)CH(OH)CH ₂ ONO ₂ , OXN, organic nitrate, carbonyl
OXY1OHNO2	2,3-(CH ₃) ₂ -6-NO ₂ -C ₆ H ₂ OH, OXN, nitro group
OXNCATECH	2,3-(OH) ₂ -3,4-(CH ₃) ₂ -C ₆ HNO ₂ , OXN nitro group
NOXYOL1OOH	3,4-(CH ₃) ₂ -2-OOH-C ₆ H ₂ NO ₂ , ROOH, OXN, nitro group
CO2N3CHO	HCOCH(ONO ₂)C(O)CH ₃ , carbonyl, OXN, organic nitrate

EmChem19X species (continued on next page)

Model species	description
NALD	$\text{O}_2\text{NOCH}_2\text{CHO}$, OXN, organic nitrate, carbonyl
NOA	$\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{ONO}_2$, carbonyl, OXN, organic nitrate
ISON	$\text{C}_5\text{H}_8(\text{OH})(\text{NO}_3)$ (lumped species, repr first-gen nitrates from isoprene degradation), OXN, organic nitrate
ISON2	$\text{HCOCH}=\text{C}(\text{CH}_3)\text{CH}_2\text{ONO}_2$, OXN, organic nitrate, carbonyl
NC4MDCO2H	$\text{C}(\text{O})\text{OHC}(\text{CH}_3)=\text{C}(\text{CHO})\text{NO}_2$, carbonyl, acid, OXN, nitro group
NOXYOLOOH	$\text{C}_8\text{H}_{11}\text{NO}_8$, ROOH, OXN, organic nitrate
OXNCATCOOH	$\text{C}_8\text{H}_{11}\text{NO}_9$, ROOH, OXN, nitro group
PAN	$\text{CH}_3\text{C}(\text{O})\text{OONO}_2$, OXN, PANs
PHAN	$\text{HOCH}_2\text{C}(\text{O})\text{OONO}_2$, OXN, PANs
PPN	$\text{C}_2\text{H}_5\text{C}(\text{O})\text{OONO}_2$, OXN, PANs
MPAN	$\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(=\text{O})\text{OONO}_2$, OXN, PANs
C4PAN6	$\text{CH}_3\text{C}(\text{O})\text{CH}(\text{OH})\text{C}(\text{O})\text{OONO}_2$, carbonyl, OXN, PANs
C5PAN18	$\text{O}_2\text{NOCH}_2\text{C}(\text{CH}_3)=\text{CHC}(\text{O})\text{OONO}_2$, OXN, PANs, organic nitrate
OXNNCATOOH	$\text{C}_8\text{H}_{10}\text{N}_2\text{O}_{11}$, ROOH, OXN, organic nitrate, nitro group
TERPOOH	$\text{C}_{10}\text{H}_{16}(\text{OH})(\text{OOH})$, ROOH
SO2	SO_2
NH3	NH_3

Notes:

RO_2 : organic peroxy radicals, carbonyl: aldehydes and/or ketones, ROOH: organic hydroperoxides,

OXN: species containing oxidised nitrogen, PANs: peroxyacyl nitrates, organic nitrate: species containing R-ONO2 (excl. PANs)

nitro group: species containing R-NO2

I. CRIv2R5Em mechanism

Table I.1: Gas Phase Chemistry of CRIv2R5Em

N	Rate coefficient	Reaction
1	$5.6 \times 10^{-34} \times (T/300)^{-2.6} \times O_2 \times N_2$	$OP \longrightarrow O_3$
2	$6.0 \times 10^{-34} \times (T/300)^{-2.6} \times O_2 \times O_2$	$OP \longrightarrow O_3$
3	$8.0 \times 10^{-12} e^{-2060/T}$	$OP + O_3 \longrightarrow$
4	KMT01	$OP + NO \longrightarrow NO_2$
5	$5.5 \times 10^{-12} e^{188/T}$	$OP + NO_2 \longrightarrow NO$
6	KMT02	$OP + NO_2 \longrightarrow NO_3$
7	$3.2 \times 10^{-11} e^{67/T} \times O_2$	$OD \longrightarrow OP$
8	$2.15 \times 10^{-11} e^{110/T} \times N_2$	$OD \longrightarrow OP$
9	$1.4 \times 10^{-12} e^{-1310/T}$	$NO + O_3 \longrightarrow NO_2$
10	$1.4 \times 10^{-13} e^{-2470/T}$	$NO_2 + O_3 \longrightarrow NO_3$
11	$3.3 \times 10^{-39} e^{530/T} \times O_2$	$NO + NO \longrightarrow 2 NO_2$
12	$1.8 \times 10^{-11} e^{110/T}$	$NO + NO_3 \longrightarrow 2 NO_2$
13	$4.5 \times 10^{-14} e^{-1260/T}$	$NO_2 + NO_3 \longrightarrow NO + NO_2$
14	KMT03	$NO_2 + NO_3 \longrightarrow N_2O_5$
15	KMT04	$N_2O_5 \longrightarrow NO_2 + NO_3$
16	$2.14 \times 10^{-10} \times H_2O$	$OD \longrightarrow 2 OH$
17	$1.7 \times 10^{-12} e^{-940/T}$	$OH + O_3 \longrightarrow HO_2$
18	$7.7 \times 10^{-12} e^{-2100/T}$	$OH + H_2 \longrightarrow HO_2$
19	KMT05	$OH + CO \longrightarrow HO_2$
20	$2.9 \times 10^{-12} e^{-160/T}$	$OH + H_2O_2 \longrightarrow HO_2$
21	$2.03 \times 10^{-16} \times (T/300)^{4.57} e^{693/T}$	$HO_2 + O_3 \longrightarrow OH$
22	$4.8 \times 10^{-11} e^{250/T}$	$OH + HO_2 \longrightarrow$
23	$2.2 \times 10^{-13} e^{600/T} \times KMT06$	$HO_2 + HO_2 \longrightarrow H_2O_2$
24	$1.9 \times 10^{-33} e^{980/T} \times KMT06 \times M$	$HO_2 + HO_2 \longrightarrow H_2O_2$
25	KMT07CRI	$OH + NO \longrightarrow HONO$
26	KMT08	$OH + NO_2 \longrightarrow HNO_3$
27	2.0×10^{-11}	$OH + NO_3 \longrightarrow HO_2 + NO_2$
28	$3.45 \times 10^{-12} e^{270/T}$	$HO_2 + NO \longrightarrow OH + NO_2$
29	KMT09	$HO_2 + NO_2 \longrightarrow HO_2NO_2$
30	KMT10	$HO_2NO_2 \longrightarrow HO_2 + NO_2$
31	$3.2 \times 10^{-13} e^{690/T}$	$OH + HO_2NO_2 \longrightarrow NO_2$
32	4.0×10^{-12}	$HO_2 + NO_3 \longrightarrow OH + NO_2$
33	$2.5 \times 10^{-12} e^{260/T}$	$OH + HONO \longrightarrow NO_2$
34	KMT3-OH-HNO3	$OH + HNO_3 \longrightarrow NO_3$
35	$6.38 \times 10^{-18} \times T^2 e^{144/T}$	$OH + CH_3OH \longrightarrow HO_2 + HCHO$
36	$6.7 \times 10^{-18} \times T^2 e^{511/T}$	$OH + C_2H_5OH \longrightarrow 0.95 CH_3CHO + 0.95 HO_2 + 0.05 HOCH_2CH_2O_2$

CRIv2R5Em (continued on next page)

	Rate coefficient	Reaction
37	$4.6 \times 10^{-12} e^{70/T}$	$\text{OH} + \text{NPROPOL} \longrightarrow 0.51 \text{ RN9O2} + 0.49 \text{ C2H5CHO} + 0.49 \text{ HO2}$
38	$2.6 \times 10^{-12} e^{200/T}$	$\text{OH} + \text{IPROPOL} \longrightarrow 0.861 \text{ CH3COCH3} + 0.861 \text{ HO2} + 0.139 \text{ RN9O2}$
39	$1.25 \times 10^{-17} \times T^2 e^{615/T}$	$\text{OH} + \text{HCHO} \longrightarrow \text{HO2} + \text{CO}$
40	$2. \times 10^{-12} e^{-2440/T}$	$\text{NO3} + \text{HCHO} \longrightarrow \text{HO2} + \text{CO} + \text{HNO3}$
41	$4.7 \times 10^{-12} e^{345/T}$	$\text{OH} + \text{CH3CHO} \longrightarrow \text{CH3CO3}$
42	KNO3AL	$\text{NO3} + \text{CH3CHO} \longrightarrow \text{CH3CO3} + \text{HNO3}$
43	$4.9 \times 10^{-12} e^{405/T}$	$\text{OH} + \text{C2H5CHO} \longrightarrow \text{C2H5CO3}$
44	$3.24 \times 10^{-12} e^{-1860/T}$	$\text{NO3} + \text{C2H5CHO} \longrightarrow \text{C2H5CO3} + \text{HNO3}$
45	$1.85 \times 10^{-20} \times T^{2.82} e^{-987/T}$	$\text{OH} + \text{CH4} \longrightarrow \text{CH3O2}$
46	$1.49 \times 10^{-17} \times T^2 e^{-499/T}$	$\text{OH} + \text{C2H6} \longrightarrow \text{C2H5O2}$
47	$1.65 \times 10^{-17} \times T^2 e^{-87/T}$	$\text{OH} + \text{C3H8} \longrightarrow 0.736 \text{ IC3H7O2} + 0.264 \text{ RN10O2}$
48	$9.8 \times 10^{-12} e^{-425/T}$	$\text{OH} + \text{NC4H10} \longrightarrow \text{RN13O2}$
49	KMT15	$\text{OH} + \text{C2H4} \longrightarrow \text{HOCH2CH2O2}$
50	$3.3 \times 10^{-12} e^{-2880/T}$	$\text{NO3} + \text{C2H4} \longrightarrow \text{NRN6O2}$
51	$6.82 \times 10^{-15} e^{-2500/T}$	$\text{O3} + \text{C2H4} \longrightarrow 1.139 \text{ HCHO} + 0.63 \text{ CO} + 0.13 \text{ HO2} + 0.13 \text{ OH} + 0.139 \text{ H2O2} + 0.231 \text{ HCOOH}$
52	KMT16	$\text{OH} + \text{C3H6} \longrightarrow \text{RN9O2}$
53	$4.6 \times 10^{-13} e^{-1155/T}$	$\text{NO3} + \text{C3H6} \longrightarrow \text{NRN9O2}$
54	$5.77 \times 10^{-15} e^{-1880/T}$	$\text{O3} + \text{C3H6} \longrightarrow 0.545 \text{ CH3CHO} + 0.545 \text{ HCHO} + 0.1 \text{ CH4} + 0.28 \text{ CH3O2} + 0.36 \text{ OH} + 0.09 \text{ H2O2} + 0.075 \text{ CH3CO2H} + 0.075 \text{ HCOOH} + 0.28 \text{ HO2} + 0.56 \text{ CO}$
55	$1.01 \times 10^{-11} e^{550/T}$	$\text{OH} + \text{TBUT2ENE} \longrightarrow \text{RN12O2}$
56	3.9×10^{-13}	$\text{NO3} + \text{TBUT2ENE} \longrightarrow \text{NRN12O2}$
57	$7.0 \times 10^{-15} e^{-1060/T}$	$\text{O3} + \text{TBUT2ENE} \longrightarrow 1.0675 \text{ CH3CHO} + 0.695 \text{ CH3O2} + 0.57 \text{ CO} + 0.57 \text{ OH} + 0.125 \text{ HO2} + 0.125 \text{ CH4} + 0.1125 \text{ CH3CO2H} + 0.0675 \text{ H2O2}$
58	KMT17	$\text{OH} + \text{C2H2} \longrightarrow 0.636 \text{ GLYOX} + 0.636 \text{ OH} + 0.364 \text{ HCOOH} + 0.364 \text{ CO} + 0.364 \text{ HO2}$
59	$2.3 \times 10^{-12} e^{-190/T}$	$\text{OH} + \text{BENZENE} \longrightarrow 0.53 \text{ AROH14} + 0.53 \text{ HO2} + 0.47 \text{ RA13O2}$
60	$1.8 \times 10^{-12} e^{340/T}$	$\text{OH} + \text{TOLUENE} \longrightarrow 0.82 \text{ RA16O2} + 0.18 \text{ AROH17} + 0.18 \text{ HO2}$
61	1.36×10^{-11}	$\text{OH} + \text{OXYL} \longrightarrow 0.7 \text{ RA19AO2} + 0.3 \text{ RA19CO2}$
62	2.63×10^{-11}	$\text{OH} + \text{AROH14} \longrightarrow \text{RAROH14}$
63	3.78×10^{-12}	$\text{NO3} + \text{AROH14} \longrightarrow \text{RAROH14} + \text{HNO3}$
64	9.0×10^{-13}	$\text{OH} + \text{ARNOH14} \longrightarrow \text{CARB13} + \text{NO2}$
65	9.0×10^{-14}	$\text{NO3} + \text{ARNOH14} \longrightarrow \text{CARB13} + \text{NO2} + \text{HNO3}$
66	4.65×10^{-11}	$\text{OH} + \text{AROH17} \longrightarrow \text{RAROH17}$
67	1.25×10^{-11}	$\text{NO3} + \text{AROH17} \longrightarrow \text{RAROH17} + \text{HNO3}$
68	1.53×10^{-12}	$\text{OH} + \text{ARNOH17} \longrightarrow \text{CARB16} + \text{NO2}$
69	3.13×10^{-13}	$\text{NO3} + \text{ARNOH17} \longrightarrow \text{CARB16} + \text{NO2} + \text{HNO3}$
70	$2.70 \times 10^{-11} e^{390/T}$	$\text{OH} + \text{C5H8} \longrightarrow 0.538 \text{ CRU14} + 0.4 \text{ TRU14} + 0.062 \text{ UCARB13} + 0.062 \text{ HO2}$
71	$2.95 \times 10^{-12} e^{-450/T}$	$\text{NO3} + \text{C5H8} \longrightarrow \text{NRU14O2}$
72	$1.03 \times 10^{-14} e^{-1995/T}$	$\text{O3} + \text{C5H8} \longrightarrow 0.825 \text{ HCHO} + 0.468 \text{ MACR} + 0.312 \text{ MVK} + 0.25 \text{ OH} + 0.364 \text{ CO} + 0.173 \text{ HO2} + 0.175 \text{ HCOOH} + 0.385 \text{ H2O2} + 0.019 \text{ CH3O2} + 0.154 \text{ CH3CO3} + 0.047 \text{ CH3CHO}$
73	$8.8 \times 10^{-12} e^{-1320/T} + 1.7 \times 10^{-14} e^{423/T}$	$\text{OH} + \text{CH3COCH3} \longrightarrow \text{RN8O2}$
74	$1.5 \times 10^{-12} e^{-90/T}$	$\text{OH} + \text{MEK} \longrightarrow \text{RN11O2}$
75	$1.34 \times 10^{-11} e^{410/T}$	$\text{OH} + \text{APINENE} \longrightarrow \text{RTN28O2}$
76	$1.20 \times 10^{-12} e^{490/T}$	$\text{NO3} + \text{APINENE} \longrightarrow \text{NRTN28O2}$
77	$8.22 \times 10^{-16} e^{-640/T}$	$\text{O3} + \text{APINENE} \longrightarrow 0.8 \text{ OH} + 0.8 \text{ RTN26O2} + 0.125 \text{ RCOOH25} + 0.075 \text{ TNCARB26} + 0.075 \text{ H2O2}$
78	$1.62 \times 10^{-11} e^{460/T}$	$\text{OH} + \text{BPINENE} \longrightarrow \text{RTX28O2}$
79	2.51×10^{-12}	$\text{NO3} + \text{BPINENE} \longrightarrow \text{NRTX28O2}$
80	$1.39 \times 10^{-15} e^{-1280/T}$	$\text{O3} + \text{BPINENE} \longrightarrow 0.45 \text{ HCHO} + 0.35 \text{ RTX24O2} + 0.35 \text{ OH} + 0.4 \text{ TX-CARB24} + 0.2 \text{ H2O2} + 0.25 \text{ TXCARB22} + 0.2 \text{ CO}$
81	$1.34 \times 10^{-11} e^{410/T} \times 3.22$	$\text{OH} + \text{XTERP} \longrightarrow \text{RTN28O2}$
82	$1.20 \times 10^{-12} e^{490/T} \times 2.5$	$\text{NO3} + \text{XTERP} \longrightarrow \text{NRTN28O2}$
83	$8.22 \times 10^{-16} e^{-640/T} \times 3.3$	$\text{O3} + \text{XTERP} \longrightarrow 0.8 \text{ OH} + 0.8 \text{ RTN26O2} + 0.125 \text{ RCOOH25} + 0.075 \text{ TNCARB26} + 0.075 \text{ H2O2}$

CRIV2R5Em (continued on next page)

	Rate coefficient	Reaction
84	4.5×10^{-13}	$\text{OH} + \text{HCOOH} \longrightarrow \text{HO}_2$
85	$4.0 \times 10^{-14} e^{850/T}$	$\text{OH} + \text{CH}_3\text{CO}_2\text{H} \longrightarrow \text{CH}_3\text{O}_2$
86	1.23×10^{-11}	$\text{OH} + \text{HCOCO}_2\text{H} \longrightarrow \text{CO} + \text{HO}_2$
87	6.65×10^{-12}	$\text{OH} + \text{RCOOH}_2\text{S} \longrightarrow \text{RTN}_2\text{SO}_2$
88	$8.0 \times 10^{-12} e^{380/T}$	$\text{OH} + \text{MACR} \longrightarrow 0.55 \text{ MACRO}_2 + 0.45 \text{ MACO}_3$
89	3.4×10^{-15}	$\text{NO}_3 + \text{MACR} \longrightarrow \text{MACO}_3 + \text{HNO}_3$
90	$1.4 \times 10^{-15} e^{-2100/T}$	$\text{O}_3 + \text{MACR} \longrightarrow 0.902 \text{ MGLYOX} + 0.652 \text{ CO} + 0.239 \text{ OH} + 0.141 \text{ HO}_2 + 0.242 \text{ HCHO} + 0.204 \text{ HCOOH} + 0.142 \text{ H}_2\text{O}_2 + 0.098 \text{ CH}_3\text{CO}_3$
91	$2.6 \times 10^{-12} e^{610/T}$	$\text{OH} + \text{MVK} \longrightarrow \text{RU10O}_2$
92	$8.5 \times 10^{-16} e^{-1520/T}$	$\text{O}_3 + \text{MVK} \longrightarrow 0.28 \text{ CH}_3\text{CO}_3 + 0.645 \text{ HCHO} + 0.36 \text{ OH} + 0.56 \text{ CO} + 0.1 \text{ CH}_3\text{CHO} + 0.62 \text{ MGLYOX} + 0.075 \text{ HCOOH} + 0.165 \text{ H}_2\text{O}_2 + 0.18 \text{ HO}_2$
93	$3.1 \times 10^{-12} e^{340/T}$	$\text{OH} + \text{GLYOX} \longrightarrow \text{HCOCO}$
94	4.0×10^{-16}	$\text{NO}_3 + \text{GLYOX} \longrightarrow \text{HCOCO} + \text{HNO}_3$
95	$1.9 \times 10^{-12} e^{575/T}$	$\text{OH} + \text{MGLYOX} \longrightarrow \text{CH}_3\text{CO}_3 + \text{CO}$
96	5.0×10^{-16}	$\text{NO}_3 + \text{MGLYOX} \longrightarrow \text{CH}_3\text{CO}_3 + \text{CO} + \text{HNO}_3$
97	$1.6 \times 10^{-12} e^{305/T}$	$\text{OH} + \text{ACETOL} \longrightarrow \text{MGLYOX} + \text{HO}_2$
98	8.0×10^{-12}	$\text{OH} + \text{HOCH}_2\text{CHO} \longrightarrow 0.8 \text{ HOCH}_2\text{CO}_3 + 0.2 \text{ GLYOX} + 0.2 \text{ HO}_2$
99	KNO_3AL	$\text{NO}_3 + \text{HOCH}_2\text{CHO} \longrightarrow \text{HOCH}_2\text{CO}_3 + \text{HNO}_3$
100	7.15×10^{-11}	$\text{OH} + \text{CO}_2\text{C}_3\text{CHO} \longrightarrow \text{CO}_2\text{C}_3\text{CO}_3$
101	$\text{KNO}_3\text{AL} \times 4$	$\text{CO}_2\text{C}_3\text{CHO} + \text{NO}_3 \longrightarrow \text{CO}_2\text{C}_3\text{CO}_3 + \text{HNO}_3$
102	2.4×10^{-13}	$\text{OH} + \text{CARB}_9 \longrightarrow \text{RN}_9\text{O}_2$
103	5.86×10^{-12}	$\text{OH} + \text{CARB}_{10} \longrightarrow \text{CARB}_9 + \text{HO}_2$
104	1.38×10^{-12}	$\text{OH} + \text{CARB}_{12} \longrightarrow \text{RN}_{12}\text{O}_2$
105	1.65×10^{-11}	$\text{OH} + \text{CARB}_{13} \longrightarrow \text{RN}_{13}\text{O}_2$
106	1.87×10^{-11}	$\text{OH} + \text{CARB}_{14} \longrightarrow \text{RN}_{14}\text{O}_2$
107	1.25×10^{-11}	$\text{OH} + \text{CARB}_{16} \longrightarrow \text{RN}_{16}\text{O}_2$
108	1.19×10^{-10}	$\text{OH} + \text{HCC}_7\text{CO} \longrightarrow \text{RN}_{17}\text{O}_2$
109	6.42×10^{-11}	$\text{OH} + \text{UCARB}_{12} \longrightarrow \text{RU}_{12}\text{O}_2$
110	$\text{KNO}_3\text{AL} \times 4.25$	$\text{NO}_3 + \text{UCARB}_{12} \longrightarrow \text{RU}_{12}\text{O}_2 + \text{HNO}_3$
111	2.4×10^{-17}	$\text{O}_3 + \text{UCARB}_{12} \longrightarrow 0.5 \text{ MGLYOX} + 0.5 \text{ GLYOX} + 0.25 \text{ ACETOL} + 0.25 \text{ HOCH}_2\text{CHO} + 0.75 \text{ CO} + 0.25 \text{ CH}_3\text{CO}_3 + 0.75 \text{ OH} + 0.5 \text{ HO}_2$
112	4.19×10^{-11}	$\text{OH} + \text{UCARB}_{13} \longrightarrow \text{RU}_{13}\text{O}_2$
113	1.19×10^{-17}	$\text{O}_3 + \text{UCARB}_{13} \longrightarrow 0.636 \text{ HCHO} + 0.607 \text{ CO}_2\text{C}_3\text{CHO} + 0.044 \text{ HCOOH} + 0.165 \text{ H}_2\text{O}_2 + 0.505 \text{ CO} + 0.389 \text{ HO}_2 + 0.508 \text{ OH} + 0.158 \text{ MGLYOX} + 0.158 \text{ GLYOX} + 0.158 \text{ CH}_3\text{CO}_3 + 0.077 \text{ RN}_8\text{O}_2$
114	5.78×10^{-11}	$\text{OH} + \text{HUCARB}_9 \longrightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2$
115	5.2×10^{-11}	$\text{OH} + \text{HPUCARB}_{12} \longrightarrow \text{HUCARB}_9 + \text{CO} + \text{OH}$
116	$\text{KNO}_3\text{AL} \times 4.25$	$\text{NO}_3 + \text{HPUCARB}_{12} \longrightarrow \text{HUCARB}_9 + \text{CO} + \text{OH} + \text{HNO}_3$
117	2.4×10^{-17}	$\text{O}_3 + \text{HPUCARB}_{12} \longrightarrow \text{GLYOX} + \text{MGLYOX} + 2 \text{ OH}$
118	3.42×10^{-11}	$\text{OH} + \text{DHCARB}_9 \longrightarrow \text{MGLYOX} + \text{HO}_2$
119	3.64×10^{-11}	$\text{OH} + \text{DHPCARB}_9 \longrightarrow \text{RN}_8\text{OOH} + \text{CO} + \text{OH}$
120	4.79×10^{-12}	$\text{OH} + \text{CCARB}_{12} \longrightarrow \text{RN}_{12}\text{O}_2$
121	5.2×10^{-11}	$\text{OH} + \text{UDCARB}_8 \longrightarrow 0.5 \text{ C}_2\text{H}_5\text{O}_2 + 0.5 \text{ ANHY} + 0.5 \text{ HO}_2$
122	5.58×10^{-11}	$\text{OH} + \text{UDCARB}_{11} \longrightarrow 0.55 \text{ RN}_{10}\text{O}_2 + 0.45 \text{ ANHY} + 0.45 \text{ CH}_3\text{O}_2$
123	7.0×10^{-11}	$\text{OH} + \text{UDCARB}_{14} \longrightarrow 0.55 \text{ RN}_{13}\text{O}_2 + 0.45 \text{ ANHY} + 0.45 \text{ C}_2\text{H}_5\text{O}_2$
124	1.0×10^{-10}	$\text{OH} + \text{TNCARB}_{10} \longrightarrow \text{RTN}_{10}\text{O}_2$
125	$\text{KNO}_3\text{AL} \times 5.5$	$\text{NO}_3 + \text{TNCARB}_{10} \longrightarrow \text{RTN}_{10}\text{O}_2 + \text{HNO}_3$
126	1.0×10^{-12}	$\text{OH} + \text{TNCARB}_{15} \longrightarrow \text{RN}_{15}\text{AO}_2$
127	4.2×10^{-11}	$\text{OH} + \text{TNCARB}_{26} \longrightarrow \text{RTN}_{26}\text{O}_2$
128	3.8×10^{-14}	$\text{NO}_3 + \text{TNCARB}_{26} \longrightarrow \text{RTN}_{26}\text{O}_2 + \text{HNO}_3$
129	4.55×10^{-12}	$\text{OH} + \text{TXCARB}_{22} \longrightarrow \text{RTX}_{22}\text{O}_2$
130	1.55×10^{-11}	$\text{OH} + \text{TXCARB}_{24} \longrightarrow \text{RTX}_{24}\text{O}_2$
131	4.16×10^{-11}	$\text{OH} + \text{NUCARB}_{12} \longrightarrow \text{NRU}_{12}\text{O}_2$
132	$5.3 \times 10^{-12} e^{190/T}$	$\text{OH} + \text{CH}_3\text{OOH} \longrightarrow 0.6 \text{ CH}_3\text{O}_2 + 0.4 \text{ HCHO} + 0.4 \text{ OH}$
133	1.36×10^{-11}	$\text{OH} + \text{C}_2\text{H}_5\text{OOH} \longrightarrow \text{CH}_3\text{CHO} + \text{OH}$
134	2.78×10^{-11}	$\text{OH} + \text{IC}_3\text{H}_7\text{OOH} \longrightarrow \text{CH}_3\text{COCH}_3 + \text{OH}$
135	2.13×10^{-11}	$\text{OH} + \text{HOC}_2\text{H}_4\text{OOH} \longrightarrow \text{HOCH}_2\text{CHO} + \text{OH}$
136	1.2×10^{-11}	$\text{OH} + \text{RN}_8\text{OOH} \longrightarrow \text{MGLYOX} + \text{OH}$

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	Rate coefficient	Reaction
137	2.5×10^{-11}	$\text{OH} + \text{RN9OOH} \rightarrow \text{ACETOL} + \text{OH}$
138	1.89×10^{-11}	$\text{OH} + \text{RN10OOH} \rightarrow \text{C2H5CHO} + \text{OH}$
139	2.5×10^{-11}	$\text{OH} + \text{RN11OOH} \rightarrow \text{CARB9} + \text{OH}$
140	3.25×10^{-11}	$\text{OH} + \text{RN12OOH} \rightarrow \text{CARB10} + \text{OH}$
141	3.57×10^{-11}	$\text{OH} + \text{RN13OOH} \rightarrow \text{MEK} + \text{OH}$
142	3.2×10^{-11}	$\text{OH} + \text{RN14OOH} \rightarrow \text{CARB12} + \text{OH}$
143	3.74×10^{-11}	$\text{OH} + \text{RN15OOH} \rightarrow \text{CARB13} + \text{OH}$
144	4.21×10^{-11}	$\text{OH} + \text{RN16OOH} \rightarrow \text{CARB14} + \text{OH}$
145	7.06×10^{-11}	$\text{OH} + \text{RN17OOH} \rightarrow \text{RN17O2}$
146	1.27×10^{-10}	$\text{OH} + \text{RN19OOH} \rightarrow \text{HCC7CO} + \text{OH}$
147	3.84×10^{-11}	$\text{OH} + \text{RU10OOH} \rightarrow \text{ACETOL} + \text{CO} + \text{OH}$
148	3.5×10^{-11}	$\text{OH} + \text{RU12OOH} \rightarrow \text{RU10OOH} + \text{CO} + \text{HO2}$
149	6.71×10^{-11}	$\text{OH} + \text{RU13OOH} \rightarrow \text{RN8OOH} + 2 \text{HCHO} + \text{HO2}$
150	7.14×10^{-11}	$\text{OH} + \text{RU14OOH} \rightarrow 0.85 \text{ IEPOX} + 0.09 \text{ UCARB12} + 0.94 \text{ OH} + 0.06 \text{ BRU14O2}$
151	9.77×10^{-11}	$\text{OH} + \text{RA13OOH} \rightarrow \text{GLYOX} + \text{UDCARB8} + \text{OH}$
152	9.64×10^{-11}	$\text{OH} + \text{RA16OOH} \rightarrow \text{GLYOX} + \text{UDCARB11} + \text{OH}$
153	7.62×10^{-11}	$\text{OH} + \text{RA19OOH} \rightarrow \text{RA19AO2}$
154	4.23×10^{-12}	$\text{OH} + \text{RTN10OOH} \rightarrow \text{RTN10O2}$
155	8.69×10^{-11}	$\text{OH} + \text{RTN14OOH} \rightarrow \text{RTN14O2}$
156	2.05×10^{-11}	$\text{OH} + \text{RTN23OOH} \rightarrow \text{RTN23O2}$
157	1.05×10^{-11}	$\text{OH} + \text{RTN24OOH} \rightarrow \text{RTN24O2}$
158	1.66×10^{-11}	$\text{OH} + \text{RTN25OOH} \rightarrow \text{RTN25O2}$
159	1.2×10^{-11}	$\text{OH} + \text{RTN26OOH} \rightarrow \text{RTN26O2}$
160	2.38×10^{-11}	$\text{OH} + \text{RTN28OOH} \rightarrow \text{TNCARB26} + \text{OH}$
161	7.5×10^{-11}	$\text{OH} + \text{RTX22OOH} \rightarrow \text{CH3COCH3} + \text{CCARB12} + \text{OH}$
162	8.59×10^{-11}	$\text{OH} + \text{RTX24OOH} \rightarrow \text{TXCARB22} + \text{OH}$
163	2.0×10^{-11}	$\text{OH} + \text{RTX28OOH} \rightarrow \text{RTX28O2}$
164	5.64×10^{-11}	$\text{OH} + \text{DHPR12OOH} \rightarrow \text{DHPCARB9} + \text{CO} + \text{OH}$
165	5.22×10^{-12}	$\text{OH} + \text{NRN6OOH} \rightarrow 2 \text{HCHO} + \text{NO2} + \text{OH}$
166	6.5×10^{-12}	$\text{OH} + \text{NRN9OOH} \rightarrow \text{CH3CHO} + \text{HCHO} + \text{NO2} + \text{OH}$
167	7.15×10^{-12}	$\text{OH} + \text{NRN12OOH} \rightarrow 2 \text{CH3CHO} + \text{NO2} + \text{OH}$
168	2.65×10^{-11}	$\text{OH} + \text{NRU12OOH} \rightarrow \text{NOA} + \text{GLYOX} + \text{HO2}$
169	1.03×10^{-10}	$\text{OH} + \text{NRU14OOH} \rightarrow \text{NUCARB12} + \text{OH}$
170	9.5×10^{-12}	$\text{OH} + \text{NRTN28OOH} \rightarrow \text{TNCARB26} + \text{NO2} + \text{OH}$
171	9.58×10^{-12}	$\text{OH} + \text{NRTX28OOH} \rightarrow \text{NRTX28O2}$
172	3.7×10^{-12}	$\text{OH} + \text{CH3CO3H} \rightarrow \text{CH3CO3}$
173	4.42×10^{-12}	$\text{OH} + \text{C2H5CO3H} \rightarrow \text{C2H5CO3}$
174	6.19×10^{-12}	$\text{OH} + \text{HOCH2CO3H} \rightarrow \text{HOCH2CO3}$
175	1.58×10^{-11}	$\text{OH} + \text{HCOCO3H} \rightarrow \text{HCOCO3}$
176	4.18×10^{-12}	$\text{OH} + \text{CO2C3CO3H} \rightarrow \text{CO2C3CO3}$
177	1.16×10^{-11}	$\text{OH} + \text{IEPOX} \rightarrow \text{RU12O2}$
178	1.5×10^{-12}	$\text{OH} + \text{ANH2} \rightarrow \text{HOCH2CH2O2}$
179	4.33×10^{-12}	$\text{OH} + \text{HMML} \rightarrow 0.7 \text{ MGLYOX} + 0.3 \text{ HCOOH} + 0.7 \text{ OH} + 0.3 \text{ CH3CO3}$
180	$4.0 \times 10^{-13} e^{-845/T}$	$\text{OH} + \text{CH3NO3} \rightarrow \text{HCHO} + \text{NO2}$
181	$6.7 \times 10^{-13} e^{-395/T}$	$\text{OH} + \text{C2H5NO3} \rightarrow \text{CH3CHO} + \text{NO2}$
182	$6.2 \times 10^{-13} e^{-230/T}$	$\text{OH} + \text{IC3H7NO3} \rightarrow \text{CH3COCH3} + \text{NO2}$
183	6.7×10^{-13}	$\text{OH} + \text{NOA} \rightarrow \text{MGLYOX} + \text{NO2}$
184	1.09×10^{-12}	$\text{OH} + \text{HOC2H4NO3} \rightarrow \text{HOCH2CHO} + \text{NO2}$
185	1.31×10^{-12}	$\text{OH} + \text{RN9NO3} \rightarrow \text{ACETOL} + \text{NO2}$
186	5.8×10^{-13}	$\text{OH} + \text{RN10NO3} \rightarrow \text{C2H5CHO} + \text{NO2}$
187	1.79×10^{-12}	$\text{OH} + \text{RN12NO3} \rightarrow \text{CARB10} + \text{NO2}$
188	9.2×10^{-13}	$\text{OH} + \text{RN13NO3} \rightarrow \text{MEK} + \text{NO2}$
189	1.03×10^{-11}	$\text{OH} + \text{RN15NO3} \rightarrow \text{CARB13} + \text{NO2}$
190	1.85×10^{-12}	$\text{OH} + \text{RN16NO3} \rightarrow \text{CARB14} + \text{NO2}$
191	9.6×10^{-11}	$\text{OH} + \text{RN19NO3} \rightarrow \text{HCC7CO} + \text{NO2}$
192	5.26×10^{-13}	$\text{OH} + \text{RU10NO3} \rightarrow \text{ACETOL} + \text{CO} + \text{NO2}$
193	2.5×10^{-12}	$\text{OH} + \text{RU12NO3} \rightarrow \text{ACETOL} + \text{GLYOX} + \text{NO2}$

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	Rate coefficient	Reaction
194	1.6×10^{-12}	$\text{OH} + \text{RU13NO}_3 \longrightarrow \text{NOA} + 2 \text{HCHO} + \text{HO}_2$
195	3.0×10^{-11}	$\text{OH} + \text{RU14NO}_3 \longrightarrow 0.34 \text{UCARB12} + 0.34 \text{NO}_2 + 0.48 \text{RU10NO}_3 + 0.48 \text{HCHO} + 0.18 \text{RU12NO}_3 + 0.66 \text{HO}_2$
196	7.3×10^{-11}	$\text{OH} + \text{RA13NO}_3 \longrightarrow \text{GLYOX} + \text{UDCARB8} + \text{NO}_2$
197	7.16×10^{-11}	$\text{OH} + \text{RA16NO}_3 \longrightarrow \text{GLYOX} + \text{UDCARB11} + \text{NO}_2$
198	8.31×10^{-11}	$\text{OH} + \text{RA19NO}_3 \longrightarrow \text{MGLYOX} + \text{UDCARB11} + \text{NO}_2$
199	2.88×10^{-12}	$\text{OH} + \text{RTN25NO}_3 \longrightarrow \text{CH}_3\text{COCH}_3 + \text{TNCARB15} + \text{NO}_2$
200	4.35×10^{-12}	$\text{OH} + \text{RTN28NO}_3 \longrightarrow \text{TNCARB26} + \text{NO}_2$
201	4.74×10^{-12}	$\text{OH} + \text{RTX22NO}_3 \longrightarrow \text{CH}_3\text{COCH}_3 + \text{CCARB12} + \text{NO}_2$
202	6.48×10^{-12}	$\text{OH} + \text{RTX24NO}_3 \longrightarrow \text{TXCARB22} + \text{NO}_2$
203	3.53×10^{-12}	$\text{OH} + \text{RTX28NO}_3 \longrightarrow \text{TXCARB24} + \text{HCHO} + \text{NO}_2$
204	3.0×10^{-14}	$\text{OH} + \text{PAN} \longrightarrow \text{HCHO} + \text{CO} + \text{NO}_2$
205	1.12×10^{-12}	$\text{OH} + \text{PHAN} \longrightarrow \text{HCHO} + \text{CO} + \text{NO}_2$
206	1.27×10^{-12}	$\text{OH} + \text{PPN} \longrightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{NO}_2$
207	5.93×10^{-13}	$\text{OH} + \text{CO}_2\text{C}_3\text{PAN} \longrightarrow \text{MGLYOX} + \text{CO} + \text{NO}_2$
208	2.9×10^{-11}	$\text{OH} + \text{MPAN} \longrightarrow 0.22 \text{ACETOL} + 0.22 \text{CO} + 0.78 \text{HMML} + \text{NO}_3$
209	3.66×10^{-12}	$\text{OH} + \text{RTN26PAN} \longrightarrow \text{CH}_3\text{COCH}_3 + \text{CARB16} + \text{NO}_2$
210	$3.18 \times 10^{-12} \times \text{O}_2$	$\text{CRU14} \longrightarrow \text{CRU14O}_2$
211	$2.31 \times 10^{16} e^{-10420/T}$	$\text{CRU14O}_2 \longrightarrow \text{CRU14}$
212	$3.11 \times 10^{-12} \times \text{O}_2$	$\text{CRU14} \longrightarrow \text{BRU14O}_2$
213	$7.9 \times 10^{15} e^{-11370/T}$	$\text{BRU14O}_2 \longrightarrow \text{CRU14}$
214	$2.5 \times 10^{-12} e^{-480/T} \times \text{O}_2$	$\text{TRU14} \longrightarrow \text{TRU14O}_2$
215	$5.95 \times 10^{14} e^{-9465/T}$	$\text{TRU14O}_2 \longrightarrow \text{TRU14}$
216	$3.02 \times 10^{-12} \times \text{O}_2$	$\text{TRU14} \longrightarrow \text{BRU14O}_2$
217	$6.34 \times 10^{15} e^{-10760/T}$	$\text{BRU14O}_2 \longrightarrow \text{TRU14}$
218	$1.78 \times 10^{10} e^{-8483/T} \times \text{EXP}(10^8/T^3)$	$\text{CRU14O}_2 \longrightarrow 0.5 \text{DHPR12O}_2 + 0.5 \text{HPUCARB12} + 0.5 \text{HO}_2$
219	$1.38 \times 10^{11} e^{-9750/T}$	$\text{BRU14O}_2 \longrightarrow 0.6 \text{MVK} + 0.4 \text{MACR} + \text{HCHO} + \text{OH}$
220	$7.0 \times 10^{11} e^{-3160/T}$	$\text{HCOCO} \longrightarrow 2 \text{CO} + \text{HO}_2$
221	$5.0 \times 10^{-12} \times \text{O}_2$	$\text{HCOCO} \longrightarrow 2 \text{CO} + \text{HO}_2$
222	$5.0 \times 10^{-12} \times \text{O}_2 \times 3.2 \times (1 - e^{-550/T})$	$\text{HCOCO} \longrightarrow \text{CO} + \text{OH}$
223	$5.0 \times 10^{-12} \times \text{O}_2 \times 3.2 e^{-550/T}$	$\text{HCOCO} \longrightarrow \text{HCOCO}_3$
224	K14ISOM1	$\text{DHPR12O}_2 \longrightarrow \text{DHPCARB9} + \text{CO} + \text{OH}$
225	K14ISOM1 $\times 0.008$	$\text{RU12O}_2 \longrightarrow \text{DHCARB9} + \text{CO} + \text{OH}$
226	K14ISOM1 $\times 0.85$	$\text{MACRO}_2 \longrightarrow \text{ACETOL} + \text{CO} + \text{OH}$
227	2.08×10^{-12}	$\text{RAROH14} + \text{NO}_2 \longrightarrow \text{ARNOH14}$
228	2.08×10^{-12}	$\text{RAROH17} + \text{NO}_2 \longrightarrow \text{ARNOH17}$
229	KFPAN	$\text{CH}_3\text{CO}_3 + \text{NO}_2 \longrightarrow \text{PAN}$
230	KBPAN	$\text{PAN} \longrightarrow \text{CH}_3\text{CO}_3 + \text{NO}_2$
231	KFPAN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \longrightarrow \text{PPN}$
232	KBPAN	$\text{PPN} \longrightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$
233	KFPAN	$\text{MACO}_3 + \text{NO}_2 \longrightarrow \text{MPAN}$
234	$1.6 \times 10^{16} e^{-13500/T}$	$\text{MPAN} \longrightarrow \text{MACO}_3 + \text{NO}_2$
235	KFPAN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \longrightarrow \text{PHAN}$
236	KBPAN	$\text{PHAN} \longrightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$
237	KFPAN	$\text{HCOCO}_3 + \text{NO}_2 \longrightarrow \text{HO}_2 + \text{CO} + \text{NO}_3$
238	KFPAN	$\text{CO}_2\text{C}_3\text{CO}_3 + \text{NO}_2 \longrightarrow \text{CO}_2\text{C}_3\text{PAN}$
239	KBPAN	$\text{CO}_2\text{C}_3\text{PAN} \longrightarrow \text{CO}_2\text{C}_3\text{CO}_3 + \text{NO}_2$
240	KFPAN $\times 0.722$	$\text{RTN26O}_2 + \text{NO}_2 \longrightarrow \text{RTN26PAN}$
241	KBPAN	$\text{RTN26PAN} \longrightarrow \text{RTN26O}_2 + \text{NO}_2$
242	$2.3 \times 10^{-12} e^{360/T}$	$\text{CH}_3\text{O}_2 + \text{NO} \longrightarrow 0.999 \text{HCHO} + 0.999 \text{HO}_2 + 0.999 \text{NO}_2 + 0.001 \text{CH}_3\text{NO}_3$
243	$2.55 \times 10^{-12} e^{380/T}$	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \longrightarrow 0.967 \text{CH}_3\text{CHO} + 0.967 \text{HO}_2 + 0.967 \text{NO}_2 + 0.033 \text{C}_2\text{H}_5\text{NO}_3$
244	$2.9 \times 10^{-12} e^{350/T}$	$\text{RN10O}_2 + \text{NO} \longrightarrow 0.98 \text{C}_2\text{H}_5\text{CHO} + 0.98 \text{HO}_2 + 0.98 \text{NO}_2 + 0.02 \text{RN10NO}_3$
245	$2.7 \times 10^{-12} e^{360/T}$	$\text{IC}_3\text{H}_7\text{O}_2 + \text{NO} \longrightarrow 0.965 \text{CH}_3\text{COCH}_3 + 0.965 \text{HO}_2 + 0.965 \text{NO}_2 + 0.035 \text{IC}_3\text{H}_7\text{NO}_3$
246	KRO2NO	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \longrightarrow 0.995 \text{NO}_2 + 0.995 \text{HO}_2 + 1.544 \text{HCHO} + 0.223 \text{HOCH}_2\text{CHO} + 0.005 \text{HOC}_2\text{H}_4\text{NO}_3$

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	Rate coefficient	Reaction
247	KRO2NO	MACRO2 + NO $\longrightarrow$ 0.987 ACETOL + 0.987 CO + 0.987 HO2 + 0.013 RU10NO3 + 0.987 NO2
248	KRO2NO	RN8O2 + NO $\longrightarrow$ CH3CO3 + HCHO + NO2
249	KRO2NO	RN9O2 + NO $\longrightarrow$ 0.979 CH3CHO + 0.979 HCHO + 0.979 HO2 + 0.979 NO2 + 0.021 RN9NO3
250	KRO2NO	RN11O2 + NO $\longrightarrow$ CH3CO3 + CH3CHO + NO2
251	KRO2NO	RN12O2 + NO $\longrightarrow$ 1.918 CH3CHO + 0.959 HO2 + 0.959 NO2 + 0.041 RN12NO3
252	KRO2NO	RN13O2 + NO $\longrightarrow$ 0.917 NO2 + 0.552 MEK + 0.552 HO2 + 0.365 CH3CHO + 0.365 C2H5O2 + 0.083 RN13NO3
253	KRO2NO	RN14O2 + NO $\longrightarrow$ C2H5CO3 + CH3CHO + NO2
254	KRO2NO	RN15O2 + NO $\longrightarrow$ 0.936 C2H5CHO + 0.936 CH3CHO + 0.936 HO2 + 0.936 NO2 + 0.064 RN15NO3
255	KRO2NO	RN16O2 + NO $\longrightarrow$ 0.877 RN15AO2 + 0.877 NO2 + 0.123 RN16NO3
256	KRO2NO	RN17O2 + NO $\longrightarrow$ RN16AO2 + NO2
257	KRO2NO	RN19O2 + NO $\longrightarrow$ 0.722 HCC7CO + 0.722 NO2 + 0.722 HO2 + 0.278 RN19NO3
258	KRO2NO	RN13AO2 + NO $\longrightarrow$ RN12O2 + NO2
259	KRO2NO	RN15AO2 + NO $\longrightarrow$ 0.975 CARB13 + 0.975 HO2 + 0.975 NO2 + 0.025 RN15NO3
260	KRO2NO	RN16AO2 + NO $\longrightarrow$ RN15O2 + NO2
261	KRO2NO	RU10O2 + NO $\longrightarrow$ 0.295 MGLYOX + 0.295 HCHO + 0.67 CH3CO3 + 0.67 HOCH2CHO + 0.295 HO2 + 0.035 RU10NO3 + 0.965 NO2
262	KRO2NO	RU12O2 + NO $\longrightarrow$ 0.558 ACETOL + 0.407 HOCH2CHO + 0.388 GLYOX + 0.407 MGLYOX + 0.17 HOCH2CO3 + 0.795 HO2 + 0.035 RU12NO3 + 0.965 NO2
263	KRO2NO	RU13O2 + NO $\longrightarrow$ 0.949 CO2C3CHO + 0.949 HCHO + 0.949 HO2 + 0.949 NO2 + 0.051 RU13NO3
264	KRO2NO	CRU14O2 + NO $\longrightarrow$ 0.908 UCARB12 + 0.908 HO2 + 0.908 NO2 + 0.092 RU14NO3
265	KRO2NO	TRU14O2 + NO $\longrightarrow$ 0.908 UCARB12 + 0.908 HO2 + 0.908 NO2 + 0.092 RU14NO3
266	KRO2NO	BRU14O2 + NO $\longrightarrow$ 0.889 HCHO + 0.889 HO2 + 0.889 NO2 + 0.593 MVK + 0.296 MACR + 0.111 RU14NO3
267	KRO2NO	RA13O2 + NO $\longrightarrow$ 0.918 GLYOX + 0.918 UDCARB8 + 0.918 HO2 + 0.918 NO2 + 0.082 RA13NO3
268	KRO2NO	RA16O2 + NO $\longrightarrow$ 0.889 NO2 + 0.889 HO2 + 0.622 GLYOX + 0.622 UDCARB11 + 0.267 MGLYOX + 0.267 UDCARB8 + 0.111 RA16NO3
269	KRO2NO	RA19AO2 + NO $\longrightarrow$ 0.862 GLYOX + 0.862 UDCARB14 + 0.862 HO2 + 0.862 NO2 + 0.138 RA19NO3
270	KRO2NO	RA19CO2 + NO $\longrightarrow$ 0.862 CARB9 + 0.862 UDCARB8 + 0.862 HO2 + 0.862 NO2 + 0.138 RA19NO3
271	KRO2NO	RTN10O2 + NO $\longrightarrow$ RN8O2 + CO + NO2
272	KRO2NO	RTN14O2 + NO $\longrightarrow$ HCHO + TNCARB10 + HO2 + NO2
273	KRO2NO	RTN23O2 + NO $\longrightarrow$ CH3COCH3 + RTN14O2 + NO2
274	KRO2NO	RTN24O2 + NO $\longrightarrow$ RTN23O2 + NO2
275	KRO2NO	RTN25O2 + NO $\longrightarrow$ 0.84 RTN24O2 + 0.84 NO2 + 0.16 RTN25NO3
276	KRO2NO	RTN28O2 + NO $\longrightarrow$ 0.767 NO2 + 0.233 RTN28NO3 + 0.702 TNCARB26 + 0.702 HO2 + 0.065 CH3COCH3 + 0.065 RN19O2
277	KRO2NO	RTX22O2 + NO $\longrightarrow$ 0.7 CH3COCH3 + 0.7 RN13O2 + 0.7 NO2 + 0.3 RTX22NO3
278	KRO2NO	RTX24O2 + NO $\longrightarrow$ 0.843 NO2 + 0.506 TXCARB22 + 0.506 HO2 + 0.337 CH3COCH3 + 0.337 RN13AO2 + 0.337 HCHO + 0.157 RTX24NO3
279	KRO2NO	RTX28O2 + NO $\longrightarrow$ 0.767 NO2 + 0.233 RTX28NO3 + 0.702 TXCARB24 + 0.702 HCHO + 0.702 HO2 + 0.065 CH3COCH3 + 0.065 RN19O2
280	KRO2NO	DHPRI2O2 + NO $\longrightarrow$ GLYOX + RN8OOH + OH + NO2
281	KRO2NO	NRN6O2 + NO $\longrightarrow$ 2 HCHO + 2 NO2
282	KRO2NO	NRN9O2 + NO $\longrightarrow$ CH3CHO + HCHO + 2 NO2

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	Rate coefficient	Reaction
283	KRO2NO	NRN12O2 + NO $\longrightarrow$ 2 CH3CHO + 2 NO2
284	KRO2NO	NRU12O2 + NO $\longrightarrow$ NOA + 0.5 GLYOX + 0.5 CO + HO2 + NO2
285	KRO2NO	NRU14O2 + NO $\longrightarrow$ NUCARB12 + HO2 + NO2
286	KRO2NO	NRTN28O2 + NO $\longrightarrow$ TNCARB26 + 2 NO2
287	KRO2NO	NRTX28O2 + NO $\longrightarrow$ TXCARB24 + HCHO + 2 NO2
288	KAPNO	CH3CO3 + NO $\longrightarrow$ CH3O2 + NO2
289	KAPNO	C2H5CO3 + NO $\longrightarrow$ C2H5O2 + NO2
290	$8.7 \times 10^{-12} e^{290/T}$	MACO3 + NO $\longrightarrow$ 0.35 CH3CO3 + 0.65 CH3O2 + 0.65 CO + HCHO + NO2
291	KAPNO	HOCH2CO3 + NO $\longrightarrow$ HO2 + HCHO + NO2
292	KAPNO	HCOCO3 + NO $\longrightarrow$ HO2 + CO + NO2
293	KAPNO	CO2C3CO3 + NO $\longrightarrow$ RN8O2 + NO2
294	KAPNO	RTN26O2 + NO $\longrightarrow$ RTN25O2 + NO2
295	KRO2NO3 $\times 0.4$	CH3O2 + NO3 $\longrightarrow$ HCHO + HO2 + NO2
296	KRO2NO3	C2H5O2 + NO3 $\longrightarrow$ CH3CHO + HO2 + NO2
297	KRO2NO3	IC3H7O2 + NO3 $\longrightarrow$ CH3COCH3 + HO2 + NO2
298	KRO2NO3	HOCH2CH2O2 + NO3 $\longrightarrow$ 1.552 HCHO + HO2 + NO2 + 0.224 HOCH2CHO
299	KRO2NO3	MACRO2 + NO3 $\longrightarrow$ ACETOL + CO + HO2 + NO2
300	KRO2NO3	RN8O2 + NO3 $\longrightarrow$ CH3CO3 + HCHO + NO2
301	KRO2NO3	RN9O2 + NO3 $\longrightarrow$ CH3CHO + HCHO + HO2 + NO2
302	KRO2NO3	RN10O2 + NO3 $\longrightarrow$ C2H5CHO + HO2 + NO2
303	KRO2NO3	RN11O2 + NO3 $\longrightarrow$ CH3CO3 + CH3CHO + NO2
304	KRO2NO3	RN12O2 + NO3 $\longrightarrow$ 2 CH3CHO + HO2 + NO2
305	KRO2NO3	RN13O2 + NO3 $\longrightarrow$ NO2 + 0.602 MEK + 0.602 HO2 + 0.398 CH3CHO + 0.398 C2H5O2
306	KRO2NO3	RN14O2 + NO3 $\longrightarrow$ C2H5CO3 + CH3CHO + NO2
307	KRO2NO3	RN15O2 + NO3 $\longrightarrow$ C2H5CHO + CH3CHO + HO2 + NO2
308	KRO2NO3	RN16O2 + NO3 $\longrightarrow$ RN15AO2 + NO2
309	KRO2NO3	RN17O2 + NO3 $\longrightarrow$ RN16AO2 + NO2
310	KRO2NO3	RN19O2 + NO3 $\longrightarrow$ HCC7CO + NO2 + HO2
311	KRO2NO3	RN13AO2 + NO3 $\longrightarrow$ RN12O2 + NO2
312	KRO2NO3	RN15AO2 + NO3 $\longrightarrow$ CARB13 + HO2 + NO2
313	KRO2NO3	RN16AO2 + NO3 $\longrightarrow$ RN15O2 + NO2
314	KRO2NO3	RU10O2 + NO3 $\longrightarrow$ 0.3 MGLYOX + 0.3 HCHO + 0.7 CH3CO3 + 0.7 HOCH2CHO + 0.3 HO2 + NO2
315	KRO2NO3	RU12O2 + NO3 $\longrightarrow$ 0.585 ACETOL + 0.415 HOCH2CHO + 0.415 GLYOX + 0.415 MGLYOX + 0.17 HOCH2CO3 + 0.83 HO2 + NO2
316	KRO2NO3	RU13O2 + NO3 $\longrightarrow$ CO2C3CHO + HCHO + HO2 + NO2
317	KRO2NO3	CRU14O2 + NO3 $\longrightarrow$ UCARB12 + HO2 + NO2
318	KRO2NO3	TRU14O2 + NO3 $\longrightarrow$ UCARB12 + HO2 + NO2
319	KRO2NO3	BRU14O2 + NO3 $\longrightarrow$ 0.667 MVK + 0.333 MACR + HCHO + HO2 + NO2
320	KRO2NO3	RA13O2 + NO3 $\longrightarrow$ GLYOX + UDCARB8 + HO2 + NO2
321	KRO2NO3	RA16O2 + NO3 $\longrightarrow$ 0.7 GLYOX + 0.7 UDCARB11 + 0.3 MGLYOX + 0.3 UDCARB8 + HO2 + NO2
322	KRO2NO3	RA19AO2 + NO3 $\longrightarrow$ GLYOX + UDCARB14 + HO2 + NO2
323	KRO2NO3	RA19CO2 + NO3 $\longrightarrow$ CARB9 + UDCARB8 + HO2 + NO2
324	KRO2NO3	RTN10O2 + NO3 $\longrightarrow$ RN8O2 + CO + NO2
325	KRO2NO3	RTN14O2 + NO3 $\longrightarrow$ HCHO + TNCARB10 + HO2 + NO2
326	KRO2NO3	RTN23O2 + NO3 $\longrightarrow$ CH3COCH3 + RTN14O2 + NO2
327	KRO2NO3	RTN24O2 + NO3 $\longrightarrow$ RTN23O2 + NO2
328	KRO2NO3	RTN25O2 + NO3 $\longrightarrow$ RTN24O2 + NO2
329	KRO2NO3	RTN28O2 + NO3 $\longrightarrow$ TNCARB26 + HO2 + NO2
330	KRO2NO3	RTX22O2 + NO3 $\longrightarrow$ CH3COCH3 + RN13O2 + NO2
331	KRO2NO3	RTX24O2 + NO3 $\longrightarrow$ TXCARB22 + HO2 + NO2
332	KRO2NO3	RTX28O2 + NO3 $\longrightarrow$ TXCARB24 + HCHO + HO2 + NO2
333	KRO2NO3	DHPR12O2 + NO3 $\longrightarrow$ GLYOX + RN8OOH + OH + NO2
334	KRO2NO3	NRN6O2 + NO3 $\longrightarrow$ 2 HCHO + 2 NO2
335	KRO2NO3	NRN9O2 + NO3 $\longrightarrow$ CH3CHO + HCHO + 2 NO2
336	KRO2NO3	NRN12O2 + NO3 $\longrightarrow$ 2 CH3CHO + 2 NO2

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	Rate coefficient	Reaction
337	KRO2NO3	NRU12O2 + NO3 → NOA + 0.5 GLYOX + 0.5 CO + HO2 + NO2
338	KRO2NO3	NRU14O2 + NO3 → NUCARB12 + HO2 + NO2
339	KRO2NO3	NRTN28O2 + NO3 → TNCARB26 + 2 NO2
340	KRO2NO3	NRTX28O2 + NO3 → TXCARB24 + HCHO + 2 NO2
341	KRO2NO3 × 1.6	CH3CO3 + NO3 → CH3O2 + NO2
342	KRO2NO3 × 1.6	C2H5CO3 + NO3 → C2H5O2 + NO2
343	KRO2NO3 × 1.74	MACO3 + NO3 → 0.35 CH3CO3 + 0.65 CH3O2 + 0.65 CO + HCHO + NO2
344	KRO2NO3 × 1.6	HOCH2CO3 + NO3 → HO2 + HCHO + NO2
345	KRO2NO3 × 1.74	HCOCO3 + NO3 → HO2 + CO + NO2
346	KRO2NO3 × 1.74	CO2C3CO3 + NO3 → RN8O2 + NO2
347	KRO2NO3 × 1.6	RTN26O2 + NO3 → RTN25O2 + NO2
348	$3.8 \times 10^{-13} e^{780/T}$	CH3O2 + HO2 → 0.9 CH3OOH + 0.1 HCHO
349	$6.4 \times 10^{-13} e^{710/T}$	C2H5O2 + HO2 → C2H5OOH
350	KRO2HO2 × 0.52	IC3H7O2 + HO2 → IC3H7OOH
351	$2.03 \times 10^{-13} e^{1250/T}$	HOCH2CH2O2 + HO2 → HOC2H4OOH
352	KRO2HO2 × 0.625	MACRO2 + HO2 → RU10OOH
353	KRO2HO2 × 0.52	RN8O2 + HO2 → RN8OOH
354	KRO2HO2 × 0.52	RN9O2 + HO2 → RN9OOH
355	KRO2HO2 × 0.52	RN10O2 + HO2 → RN10OOH
356	KRO2HO2 × 0.625	RN11O2 + HO2 → RN11OOH
357	KRO2HO2 × 0.625	RN12O2 + HO2 → RN12OOH
358	KRO2HO2 × 0.625	RN13O2 + HO2 → RN13OOH
359	KRO2HO2 × 0.706	RN14O2 + HO2 → RN14OOH
360	KRO2HO2 × 0.706	RN15O2 + HO2 → RN15OOH
361	KRO2HO2 × 0.706	RN16O2 + HO2 → RN16OOH
362	KRO2HO2 × 0.77	RN17O2 + HO2 → RN17OOH
363	KRO2HO2 × 0.77	RN19O2 + HO2 → RN19OOH
364	KRO2HO2 × 0.625	RN13AO2 + HO2 → RN13OOH
365	KRO2HO2 × 0.706	RN15AO2 + HO2 → RN15OOH
366	KRO2HO2 × 0.706	RN16AO2 + HO2 → RN16OOH
367	KRO2HO2 × 0.625	RU10O2 + HO2 → RU10OOH
368	KRO2HO2 × 0.706	RU12O2 + HO2 → RU12OOH
369	KRO2HO2 × 0.706	RU13O2 + HO2 → RU13OOH
370	KRO2HO2 × 0.706	CRU14O2 + HO2 → RU14OOH
371	KRO2HO2 × 0.706	TRU14O2 + HO2 → RU14OOH
372	KRO2HO2 × 0.706	BRU14O2 + HO2 → RU14OOH
373	KRO2HO2 × 0.77	RA13O2 + HO2 → RA13OOH
374	KRO2HO2 × 0.82	RA16O2 + HO2 → RA16OOH
375	KRO2HO2 × 0.859	RA19AO2 + HO2 → RA19OOH
376	KRO2HO2 × 0.859	RA19CO2 + HO2 → RA19OOH
377	KRO2HO2 × 0.706	RTN10O2 + HO2 → RTN10OOH
378	KRO2HO2 × 0.77	RTN14O2 + HO2 → RTN14OOH
379	KRO2HO2 × 0.89	RTN23O2 + HO2 → RTN23OOH
380	KRO2HO2 × 0.89	RTN24O2 + HO2 → RTN24OOH
381	KRO2HO2 × 0.89	RTN25O2 + HO2 → RTN25OOH
382	KRO2HO2 × 0.914	RTN28O2 + HO2 → RTN28OOH
383	KRO2HO2 × 0.914	RTX28O2 + HO2 → RTX28OOH
384	KRO2HO2 × 0.89	RTX24O2 + HO2 → RTX24OOH
385	KRO2HO2 × 0.89	RTX22O2 + HO2 → RTX22OOH
386	KRO2HO2 × 0.706	DHPR12O2 + HO2 → DHPR12OOH
387	KRO2HO2 × 0.387	NRN6O2 + HO2 → NRN6OOH
388	KRO2HO2 × 0.52	NRN9O2 + HO2 → NRN9OOH
389	KRO2HO2 × 0.625	NRN12O2 + HO2 → NRN12OOH
390	KRO2HO2 × 0.706	NRU12O2 + HO2 → NRU12OOH
391	KRO2HO2 × 0.706	NRU14O2 + HO2 → NRU14OOH
392	KRO2HO2 × 0.914	NRTN28O2 + HO2 → NRTN28OOH
393	KRO2HO2 × 0.914	NRTX28O2 + HO2 → NRTX28OOH

CRIv2R5Em (continued on next page)

	Rate coefficient	Reaction
394	$3.14 \times 10^{-12} e^{580/T}$	$\text{CH}_3\text{CO}_3 + \text{HO}_2 \longrightarrow 0.454 \text{ CH}_3\text{O}_2 + 0.454 \text{ OH} + 0.384 \text{ CH}_3\text{CO}_3\text{H} + 0.162 \text{ O}_3 + 0.162 \text{ CH}_3\text{CO}_2\text{H}$
395	$3.14 \times 10^{-12} e^{580/T}$	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \longrightarrow 0.56 \text{ C}_2\text{H}_5\text{CO}_3\text{H} + 0.44 \text{ C}_2\text{H}_5\text{O}_2 + 0.44 \text{ OH}$
396	$3.14 \times 10^{-12} e^{580/T}$	$\text{MACO}_3 + \text{HO}_2 \longrightarrow 0.56 \text{ RU100OH} + 0.154 \text{ CH}_3\text{CO}_3 + 0.286 \text{ CH}_3\text{O}_2 + 0.286 \text{ CO} + 0.44 \text{ HCHO} + 0.44 \text{ OH}$
397	$3.14 \times 10^{-12} e^{580/T}$	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \longrightarrow 0.56 \text{ HOCH}_2\text{CO}_3\text{H} + 0.44 \text{ HCHO} + 0.44 \text{ HO}_2 + 0.44 \text{ OH}$
398	$3.14 \times 10^{-12} e^{580/T}$	$\text{HCOCO}_3 + \text{HO}_2 \longrightarrow 0.44 \text{ HO}_2 + 0.44 \text{ CO} + 0.44 \text{ OH} + 0.41 \text{ HCOCO}_3\text{H} + 0.15 \text{ HCOCO}_2\text{H} + 0.15 \text{ O}_3$
399	$3.14 \times 10^{-12} e^{580/T}$	$\text{CO}_2\text{C}_3\text{CO}_3 + \text{HO}_2 \longrightarrow 0.44 \text{ RN8O}_2 + 0.44 \text{ OH} + 0.56 \text{ CO}_2\text{C}_3\text{CO}_3\text{H}$
400	$3.14 \times 10^{-12} e^{580/T}$	$\text{RTN26O}_2 + \text{HO}_2 \longrightarrow 0.56 \text{ RTN26OOH} + 0.44 \text{ RTN25O}_2 + 0.44 \text{ OH}$
401	$7.4 \times 10^{-13} e^{-520/T} \times 2$	$\text{CH}_3\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{HCHO} + \text{HO}_2$
402	$2.06 \times 10^{-13} e^{365/T} - 1.48 \times 10^{-12} e^{-520/T}$	$\text{CH}_3\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.5 \text{ HCHO} + 0.5 \text{ CH}_3\text{OH}$
403	3.1×10^{-13}	$\text{C}_2\text{H}_5\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.8 \text{ CH}_3\text{CHO} + 0.6 \text{ HO}_2 + 0.2 \text{ C}_2\text{H}_5\text{OH}$
404	4.0×10^{-14}	$\text{IC}_3\text{H}_7\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.8 \text{ CH}_3\text{COCH}_3 + 0.6 \text{ HO}_2 + 0.2 \text{ IPROPOL}$
405	2.0×10^{-12}	$\text{HOCH}_2\text{CH}_2\text{O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 1.552 \text{ HCHO} + \text{HO}_2 + 0.224 \text{ HOCH}_2\text{CHO}$
406	3.6×10^{-13}	$\text{MACRO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{ACETOL} + \text{CO} + \text{HO}_2$
407	1.4×10^{-12}	$\text{RN8O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CH}_3\text{CO}_3 + \text{HCHO}$
408	8.8×10^{-13}	$\text{RN9O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$
409	6.0×10^{-13}	$\text{RN10O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.8 \text{ C}_2\text{H}_5\text{CHO} + 0.6 \text{ HO}_2 + 0.2 \text{ NPROPOL}$
410	1.4×10^{-12}	$\text{RN11O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CH}_3\text{CO}_3 + \text{CH}_3\text{CHO}$
411	8.8×10^{-13}	$\text{RN12O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2$
412	2.5×10^{-13}	$\text{RN13O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.602 \text{ MEK} + 0.602 \text{ HO}_2 + 0.398 \text{ CH}_3\text{CHO} + 0.398 \text{ C}_2\text{H}_5\text{O}_2$
413	1.4×10^{-12}	$\text{RN14O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{CH}_3\text{CHO}$
414	8.8×10^{-13}	$\text{RN15O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{C}_2\text{H}_5\text{CHO} + \text{CH}_3\text{CHO} + \text{HO}_2$
415	2.5×10^{-13}	$\text{RN16O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RN15AO}_2$
416	1.4×10^{-12}	$\text{RN17O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RN16AO}_2$
417	2.5×10^{-13}	$\text{RN19O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{HCC7CO} + 0.75 \text{ HO}_2$
418	8.8×10^{-13}	$\text{RN13AO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RN12O}_2$
419	8.8×10^{-13}	$\text{RN15AO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CARB13} + \text{HO}_2$
420	8.8×10^{-13}	$\text{RN16AO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RN15O}_2$
421	1.22×10^{-12}	$\text{RU10O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.3 \text{ MGLYOX} + 0.3 \text{ HCHO} + 0.7 \text{ CH}_3\text{CO}_3 + 0.7 \text{ HOCH}_2\text{CHO} + 0.3 \text{ HO}_2$
422	4.2×10^{-13}	$\text{RU12O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.585 \text{ ACETOL} + 0.415 \text{ HOCH}_2\text{CHO} + 0.415 \text{ GLYOX} + 0.415 \text{ MGLYOX} + 0.17 \text{ HOCH}_2\text{CO}_3 + 0.83 \text{ HO}_2$
423	6.0×10^{-13}	$\text{RU13O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CO}_2\text{C}_3\text{CHO} + \text{HCHO} + \text{HO}_2$
424	2.4×10^{-12}	$\text{CRU14O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{UCARB12} + \text{HO}_2$
425	2.4×10^{-12}	$\text{TRU14O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{UCARB12} + \text{HO}_2$
426	1.26×10^{-12}	$\text{BRU14O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.333 \text{ MVK} + 0.667 \text{ MACR} + \text{HCHO} + \text{HO}_2$
427	8.8×10^{-13}	$\text{RA13O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{GLYOX} + \text{UDCARB8} + \text{HO}_2$
428	8.8×10^{-13}	$\text{RA16O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 0.7 \text{ GLYOX} + 0.7 \text{ UDCARB11} + \text{HO}_2 + 0.3 \text{ MGLYOX} + 0.3 \text{ UDCARB8}$
429	8.8×10^{-13}	$\text{RA19AO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{GLYOX} + \text{UDCARB14} + \text{HO}_2$
430	8.8×10^{-13}	$\text{RA19CO}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{GLYOX} + \text{UDCARB14} + \text{HO}_2$
431	2.0×10^{-12}	$\text{RTN10O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RN8O}_2 + \text{CO}$
432	8.8×10^{-13}	$\text{RTN14O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{HCHO} + \text{TNCARB10} + \text{HO}_2$
433	6.7×10^{-15}	$\text{RTN23O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CH}_3\text{COCH}_3 + \text{RTN14O}_2$
434	6.7×10^{-15}	$\text{RTN24O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RTN23O}_2$
435	1.3×10^{-12}	$\text{RTN25O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{RTN24O}_2$
436	2.85×10^{-13}	$\text{RTN28O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{TNCARB26} + \text{HO}_2$
437	2.5×10^{-13}	$\text{RTX22O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CH}_3\text{COCH}_3 + \text{RN13O}_2$
438	2.5×10^{-13}	$\text{RTX24O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{TXCARB22} + \text{HO}_2$
439	2.0×10^{-12}	$\text{RTX28O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{TXCARB24} + \text{HCHO} + \text{HO}_2$
440	7.6×10^{-13}	$\text{DHPR12O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{GLYOX} + \text{RN8OOH} + \text{OH}$
441	6.0×10^{-13}	$\text{NRN6O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow 2 \text{ HCHO} + \text{NO}_2$
442	2.3×10^{-13}	$\text{NRN9O}_2 + [\text{RO}_2\text{POOL}] \longrightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{NO}_2$

CRIV2R5Em (continued on next page)

	Rate coefficient	Reaction
443	2.5×10^{-13}	$\text{NRN12O2} + [\text{RO2POOL}] \rightarrow 2 \text{CH3CHO} + \text{NO2}$
444	9.6×10^{-13}	$\text{NRU12O2} + [\text{RO2POOL}] \rightarrow \text{NOA} + 0.5 \text{GLYOX} + 0.5 \text{CO} + \text{HO2}$
445	1.3×10^{-12}	$\text{NRU14O2} + [\text{RO2POOL}] \rightarrow \text{NUCARB12} + \text{HO2}$
446	1.0×10^{-13}	$\text{NRTN28O2} + [\text{RO2POOL}] \rightarrow \text{TNCARB26} + \text{NO2}$
447	9.2×10^{-14}	$\text{NRTX28O2} + [\text{RO2POOL}] \rightarrow \text{TXCARB24} + \text{HCHO} + \text{NO2}$
448	1.0×10^{-11}	$\text{CH3CO3} + [\text{RO2POOL}] \rightarrow \text{CH3O2}$
449	1.0×10^{-11}	$\text{C2H5CO3} + [\text{RO2POOL}] \rightarrow \text{C2H5O2}$
450	1.0×10^{-11}	$\text{MACO3} + [\text{RO2POOL}] \rightarrow 0.35 \text{CH3CO3} + 0.65 \text{CH3O2} + 0.65 \text{CO} + \text{HCHO}$
451	1.0×10^{-11}	$\text{HOCH2CO3} + [\text{RO2POOL}] \rightarrow \text{HCHO} + \text{HO2}$
452	1.0×10^{-11}	$\text{HCOCO3} + [\text{RO2POOL}] \rightarrow 0.7 \text{CO} + 0.7 \text{HO2} + 0.3 \text{HCOCO2H}$
453	1.0×10^{-11}	$\text{CO2C3CO3} + [\text{RO2POOL}] \rightarrow \text{RN8O2}$
454	1.0×10^{-11}	$\text{RTN26O2} + [\text{RO2POOL}] \rightarrow \text{RTN25O2}$
455	RCPHOT(IDO3-O1D)	$\text{O3} \rightarrow \text{OD}$
456	RCPHOT(IDO3-O3P)	$\text{O3} \rightarrow \text{OP}$
457	RCPHOT(IDH2O2)	$\text{H2O2} \rightarrow 2 \text{OH}$
458	RCPHOT(IDNO2)	$\text{NO2} \rightarrow \text{NO} + \text{OP}$
459	RCPHOT(IDNO3-NO)	$\text{NO3} \rightarrow \text{NO}$
460	RCPHOT(IDNO3-NO2)	$\text{NO3} \rightarrow \text{NO2} + \text{OP}$
461	RCPHOT(IDHONO)	$\text{HONO} \rightarrow \text{OH} + \text{NO}$
462	RCPHOT(IDHNO3)	$\text{HNO3} \rightarrow \text{OH} + \text{NO2}$
463	RCPHOT(IDHCHO-H)	$\text{HCHO} \rightarrow \text{CO} + 2 \text{HO2}$
464	RCPHOT(IDHCHO-H2)	$\text{HCHO} \rightarrow \text{H2} + \text{CO}$
465	RCPHOT(IDCH3CHO)	$\text{CH3CHO} \rightarrow \text{CH3O2} + \text{HO2} + \text{CO}$
466	RCPHOT(IDMEK) $\times 5.2$	$\text{C2H5CHO} \rightarrow \text{C2H5O2} + \text{CO} + \text{HO2}$
467	RCPHOT(IDACETON)	$\text{CH3COCH3} \rightarrow \text{CH3CO3} + \text{CH3O2}$
468	RCPHOT(IDMEK)	$\text{MEK} \rightarrow \text{CH3CO3} + \text{C2H5O2}$
469	RCPHOT(IDRCOCHO)	$\text{HCOCO2H} \rightarrow 2 \text{HO2} + \text{CO}$
470	RCPHOT(IDHCHO-H2) $\times 0.0474$	$\text{MACR} \rightarrow 0.5 \text{MACO3} + \text{HO2} + 0.825 \text{CO} + 0.5 \text{HCHO} + 0.325 \text{CH3O2} + 0.175 \text{CH3CO3}$
471	RCPHOT(IDHCHO-H2) $\times 0.078$	$\text{MVK} \rightarrow 0.5 \text{CH3CO3} + 0.5 \text{HCHO} + \text{CO} + 0.5 \text{HO2} + 0.5 \text{C3H6}$
472	RCPHOT(IDRCOCHO) $\times 0.46$	$\text{GLYOX} \rightarrow 2 \text{CO} + \text{H2}$
473	RCPHOT(IDRCOCHO) $\times 0.07$	$\text{GLYOX} \rightarrow \text{HCHO} + \text{CO}$
474	RCPHOT(IDCH3O2H) $\times 4.79$	$\text{GLYOX} \rightarrow 2 \text{CO} + 2 \text{HO2}$
475	RCPHOT(IDRCOCHO)	$\text{MGLYOX} \rightarrow \text{CH3CO3} + \text{CO} + \text{HO2}$
476	RCPHOT(IDMEK)	$\text{ACETOL} \rightarrow \text{CH3CO3} + \text{HCHO} + \text{HO2}$
477	RCPHOT(IDHCHO-H) $\times 0.6$	$\text{HOCH2CHO} \rightarrow \text{HCHO} + \text{CO} + 2 \text{HO2}$
478	RCPHOT(IDHCHO-H) $\times 0.6$	$\text{CO2C3CHO} \rightarrow \text{RN8O2} + \text{HCHO}$
479	RCPHOT(IDCH3COY)	$\text{CARB9} \rightarrow 2 \text{CH3CO3}$
480	RCPHOT(IDMEK)	$\text{CARB10} \rightarrow \text{CH3CO3} + \text{CH3CHO} + \text{HO2}$
481	RCPHOT(IDCH3COY)	$\text{CARB12} \rightarrow \text{CH3CO3} + \text{RN8O2}$
482	RCPHOT(IDMEK) $\times 3$	$\text{CARB13} \rightarrow \text{RN8O2} + \text{CH3CHO} + \text{HO2}$
483	RCPHOT(IDMEK) $\times 4.74$	$\text{CARB14} \rightarrow \text{CH3CO3} + \text{RN10O2}$
484	RCPHOT(IDMEK) $\times 3.35$	$\text{CARB16} \rightarrow \text{RN8O2} + \text{C2H5CHO} + \text{HO2}$
485	RCPHOT(IDHCHO-H2) $\times 0.0474$	$\text{UCARB12} \rightarrow 0.5 \text{RU12O2} + 1.25 \text{HO2} + 0.75 \text{CO} + 0.25 \text{CH3CO3} + 0.25 \text{HOCH2CHO} + 0.25 \text{ACETOL}$
486	RCPHOT(IDMEK)	$\text{UCARB13} \rightarrow \text{CH3CO3} + \text{RN8O2}$
487	RCPHOT(IDHCHO-H2) $\times 6$	$\text{HUCARB9} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO2} + \text{OH}$
488	RCPHOT(IDHCHO-H2) $\times 12$	$\text{HPUCARB12} \rightarrow 0.5 \text{HUCARB9} + 1.5 \text{OH} + 0.425 \text{ACETOL} + 0.425 \text{HO2} + 0.075 \text{CH3CO3} + 0.075 \text{HOCH2CHO} + 1.425 \text{CO}$
489	RCPHOT(IDHCHO-H) $\times 1.67$	$\text{DHCARB9} \rightarrow \text{ACETOL} + \text{CO} + 2 \text{HO2}$
490	RCPHOT(IDHCHO-H) $\times 0.6$	$\text{DHPCARB9} \rightarrow \text{RN8OOH} + \text{CO} + \text{HO2} + \text{OH}$
491	RCPHOT(IDCH3O2H) $\times 2$	$\text{DHPCARB9} \rightarrow \text{MGLYOX} + \text{HCHO} + 2 \text{OH}$
492	RCPHOT(IDNO2) $\times \text{JSF19}$	$\text{UDCARB8} \rightarrow \text{C2H5O2} + \text{HO2}$
493	RCPHOT(IDNO2) $\times \text{JSF16}$	$\text{UDCARB8} \rightarrow \text{ANHY} + 2 \text{HO2}$
494	RCPHOT(IDNO2) $\times \text{JSF17}$	$\text{UDCARB11} \rightarrow \text{ANHY} + \text{HO2} + \text{CH3O2}$
495	RCPHOT(IDNO2) $\times \text{JSF18}$	$\text{UDCARB11} \rightarrow \text{RN10O2} + \text{HO2}$
496	RCPHOT(IDNO2) $\times \text{JSF17}$	$\text{UDCARB14} \rightarrow \text{ANHY} + \text{HO2} + \text{C2H5O2}$
497	RCPHOT(IDNO2) $\times \text{JSF18}$	$\text{UDCARB14} \rightarrow \text{RN13O2} + \text{HO2}$

CRIV2R5Em (continued on next page)

	Rate coefficient	Reaction
498	RCPHOT(IDCH3COY)×0.5	TNCARB10 → 2 CH3CO3 + CO
499	RCPHOT(IDHCHO-H)×0.6	TNCARB26 → RTN26O2 + HO2
500	RCPHOT(IDMEK)×132.76	NUCARB12 → 0.5 ACETOL + 0.5 HUCARB9 + 1.5 CO + 0.5 OH + 0.5 HO2 + NO2
501	RCPHOT(IDCH3O2H)	CH3OOH → HCHO + HO2 + OH
502	RCPHOT(IDCH3O2H)	C2H5OOH → CH3CHO + HO2 + OH
503	RCPHOT(IDCH3O2H)	IC3H7OOH → CH3COCH3 + HO2 + OH
504	RCPHOT(IDCH3O2H)	HOC2H4OOH → 2 HCHO + HO2 + OH
505	RCPHOT(IDCH3O2H)	RN8OOH → CH3CO3 + HCHO + OH
506	RCPHOT(IDMEK)	RN8OOH → CH3CO3 + HCHO + OH
507	RCPHOT(IDCH3O2H)	RN9OOH → CH3CHO + HCHO + HO2 + OH
508	RCPHOT(IDCH3O2H)	RN10OOH → C2H5CHO + HO2 + OH
509	RCPHOT(IDCH3O2H)	RN11OOH → RN10O2 + OH
510	RCPHOT(IDCH3O2H)	RN12OOH → 2 CH3CHO + HO2 + OH
511	RCPHOT(IDCH3O2H)	RN13OOH → 0.398 CH3CHO + 0.398 C2H5O2 + 0.602 MEK + 0.602 HO2 + OH
512	RCPHOT(IDCH3O2H)	RN14OOH → RN13O2 + OH
513	RCPHOT(IDCH3O2H)	RN15OOH → C2H5CHO + CH3CHO + HO2 + OH
514	RCPHOT(IDCH3O2H)	RN16OOH → RN15AO2 + OH
515	RCPHOT(IDCH3O2H)	RN17OOH → RN16O2 + OH
516	RCPHOT(IDCH3O2H)	RN19OOH → HCC7CO + OH + HO2
517	RCPHOT(IDCH3O2H)	RU10OOH → 0.226 MGLYOX + 0.376 HCHO + 0.52 CH3CO3 + 0.467 HOCH2CHO + 0.383 HO2 + 0.254 CO + 0.097 CH3O2 + 0.157 ACETOL + OH
518	RCPHOT(IDCH3O2H)	RU12OOH → 0.585 ACETOL + 0.415 HOCH2CHO + 0.415 GLYOX + 0.415 MGLYOX + 0.17 HOCH2CO3 + 0.83 HO2 + OH
519	RCPHOT(IDCH3O2H)	RU13OOH → CO2C3CHO + HCHO + HO2 + OH
520	RCPHOT(IDMEK)	RU13OOH → CO2C3CHO + HCHO + HO2 + OH
521	RCPHOT(IDCH3O2H)	RA13OOH → GLYOX + UDCARB8 + HO2 + OH
522	RCPHOT(IDCH3O2H)	RA16OOH → GLYOX + UDCARB11 + HO2 + OH
523	RCPHOT(IDCH3O2H)	RA19OOH → MGLYOX + UDCARB11 + HO2 + OH
524	RCPHOT(IDCH3O2H)	RTN10OOH → RN8O2 + CO + OH
525	RCPHOT(IDCH3O2H)	RTN14OOH → TNCARB10 + HCHO + HO2 + OH
526	RCPHOT(IDCH3O2H)	RTN23OOH → CH3COCH3 + RTN14O2 + OH
527	RCPHOT(IDCH3O2H)	RTN24OOH → RTN23O2 + OH
528	RCPHOT(IDCH3O2H)	RTN25OOH → RTN24O2 + OH
529	RCPHOT(IDCH3O2H)	RTN26OOH → RTN25O2 + OH
530	RCPHOT(IDCH3O2H)	RTN28OOH → TNCARB26 + HO2 + OH
531	RCPHOT(IDCH3O2H)	RTX22OOH → CH3COCH3 + RN13O2 + OH
532	RCPHOT(IDCH3O2H)	RTX24OOH → TXCARB22 + HO2 + OH
533	RCPHOT(IDCH3O2H)	RTX28OOH → TXCARB24 + HCHO + HO2 + OH
534	RCPHOT(IDHCHO-H)×1.67	DHPR12OOH → DHPCARB9 + CO + OH + HO2
535	RCPHOT(IDCH3O2H)×3	DHPR12OOH → GLYOX + RN8OOH + 2 OH
536	RCPHOT(IDCH3O2H)	NRN6OOH → 2 HCHO + NO2 + OH
537	RCPHOT(IDCH3O2H)	NRN9OOH → CH3CHO + HCHO + NO2 + OH
538	RCPHOT(IDCH3O2H)	NRN12OOH → 2 CH3CHO + NO2 + OH
539	RCPHOT(IDCH3O2H)	NRU12OOH → NOA + GLYOX + HO2 + OH
540	RCPHOT(IDCH3O2H)	NRU14OOH → NUCARB12 + HO2 + OH
541	RCPHOT(IDCH3O2H)	NRTN28OOH → TNCARB26 + NO2 + OH
542	RCPHOT(IDCH3O2H)	NRTX28OOH → TXCARB24 + HCHO + NO2 + OH
543	RCPHOT(IDCH3O2H)	CH3CO3H → CH3O2 + OH
544	RCPHOT(IDCH3O2H)	C2H5CO3H → C2H5O2 + OH
545	RCPHOT(IDCH3O2H)	HOCH2CO3H → HCHO + HO2 + OH
546	RCPHOT(IDCH3O2H)	HCOCO3H → HO2 + CO + OH
547	RCPHOT(IDHCHO-H)×0.6	HCOCO3H → HO2 + CO + OH
548	RCPHOT(IDCH3O2H)	CO2C3CO3H → RN8O2 + OH
549	RCPHOT(IDMEK)	CO2C3CO3H → RN8O2 + OH
550	RCPHOT(IDMEK)×0.293	CH3NO3 → HCHO + HO2 + NO2

CRIV2R5Em (continued on next page)

	Rate coefficient	Reaction
551	$\text{RCPHOT}(\text{IDHNO}_3) \times 1.932$	$\text{C}_2\text{H}_5\text{NO}_3 \longrightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$
552	$\text{RCPHOT}(\text{IDMEK}) \times 0.778$	$\text{IC}_3\text{H}_7\text{NO}_3 \longrightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$
553	$\text{RCPHOT}(\text{IDMEK}) \times 8.3$	$\text{NOA} \longrightarrow \text{CH}_3\text{CO}_3 + \text{HCHO} + \text{NO}_2$
554	$\text{RCPHOT}(\text{IDHNO}_3) \times 2.62$	$\text{RN10NO}_3 \longrightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{NO}_2$
555	$\text{RCPHOT}(\text{IDMEK}) \times 0.778$	$\text{RN13NO}_3 \longrightarrow 0.398 \text{ CH}_3\text{CHO} + 0.398 \text{ C}_2\text{H}_5\text{O}_2 + 0.602 \text{ MEK} + 0.602 \text{ HO}_2 + \text{NO}_2$
556	$\text{RCPHOT}(\text{IDHNO}_3) \times 2.62$	$\text{RN16NO}_3 \longrightarrow \text{RN15O}_2 + \text{NO}_2$
557	$\text{RCPHOT}(\text{IDMEK}) \times 0.778$	$\text{RN19NO}_3 \longrightarrow \text{HCC}_7\text{CO} + \text{NO}_2 + \text{HO}_2$
558	$\text{RCPHOT}(\text{IDMEK}) \times 13.3$	$\text{RU10NO}_3 \longrightarrow \text{CH}_3\text{CO}_3 + \text{HOCH}_2\text{CHO} + \text{NO}_2$
559	$\text{RCPHOT}(\text{IDMEK}) \times 83$	$\text{RU12NO}_3 \longrightarrow \text{MGLYOX} + \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$
560	$\text{RCPHOT}(\text{IDMEK})$	$\text{RU13NO}_3 \longrightarrow \text{CO}_2\text{C}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$
561	$\text{RCPHOT}(\text{IDHNO}_3) \times 2.62$	$\text{RU14NO}_3 \longrightarrow 0.333 \text{ MVK} + 0.667 \text{ MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$
562	$\text{RCPHOT}(\text{IDMEK}) \times 0.778$	$\text{RA13NO}_3 \longrightarrow \text{GLYOX} + \text{UDCARB}_8 + \text{HO}_2 + \text{NO}_2$
563	$\text{RCPHOT}(\text{IDMEK}) \times 0.778$	$\text{RA16NO}_3 \longrightarrow \text{GLYOX} + \text{UDCARB}_{11} + \text{HO}_2 + \text{NO}_2$
564	$\text{RCPHOT}(\text{IDHCHO-H}) \times 0.234$	$\text{RA19NO}_3 \longrightarrow \text{MGLYOX} + \text{UDCARB}_{11} + \text{HO}_2 + \text{NO}_2$
565	$\text{RCPHOT}(\text{IDMEK}) \times 0.778$	$\text{RTX24NO}_3 \longrightarrow \text{TXCARB}_{22} + \text{HO}_2 + \text{NO}_2$

Notes:

"T" is temperature, "M" is third body, RCPHOT are photolysis rates.

Reaction coefficients are in units of s^{-1} for unimolecular reactions, $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for bimolecular reactions, and $\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-2}$ for termolecular reactions.

$$\text{JSF16 } 7.2 \times 10^{-3}$$

$$\text{JSF17 } 9 \times 10^{-3}$$

$$\text{JSF18 } 1.1 \times 10^{-2}$$

$$\text{JSF19 } 1.28 \times 10^{-2}$$

$$\text{KAPHO}_2 = 3.14 \times 10^{-12} \text{e}^{580/T}$$

$$\text{KAPNO} = 7.5 \times 10^{-12} \text{e}^{290/T}$$

$$\text{KMT05} = 1.44 \times 10^{-13} + [\text{M}] \times 3.43 \times 10^{-33}$$

$$\text{KMT06} = 1 + (1.4 \times 10^{-21} \text{e}^{2200/T} \times [\text{H}_2\text{O}])$$

$$\text{KNO}_3\text{AL} = 1.4 \times 10^{-12} \text{e}^{-1860/T}$$

$$\text{KRO}_2\text{HO}_2 = 2.91 \times 10^{-13} \text{e}^{1300/T}$$

$$\text{KRO}_2\text{NO} = 2.7 \times 10^{-12} \text{e}^{360/T}$$

$$\text{KRO}_2\text{NO}_3 = 2.3 \times 10^{-12}$$

$$\text{K14ISOM1} = 3 \times 10^7 \text{e}^{-5300/T}$$

Some complex 3-body rate-expressions are given in Tables [G.3](#) and [G.4](#)

J. CB6r2Em mechanism

Table J.1: Gas Phase Chemistry of CB6r2Em (adapted from CB6r2)

N	Rate coefficient	Reaction
1	$5.68 \times 10^{-34} \times (T/300)^{-2.6}$	$OP + \langle O_2 \rangle + \langle M \rangle \longrightarrow O_3$
2	$1.4 \times 10^{-12} e^{-1310/T}$	$O_3 + NO \longrightarrow NO_2$
3	$1 \times 10^{-31} \times (T/300)^{-1.6}$	$OP + NO + \langle M \rangle \longrightarrow NO_2$
4	$5.5 \times 10^{-12} e^{188/T}$	$OP + NO_2 \longrightarrow NO$
5	K-6	$OP + NO_2 \longrightarrow NO_3$
6	$8 \times 10^{-12} e^{-2060/T}$	$OP + O_3 \longrightarrow$
7	$2.23 \times 10^{-11} e^{115/T}$	$OD + \langle M \rangle \longrightarrow OP$
8	2.14×10^{-10}	$OD + \langle H_2O \rangle \longrightarrow 2 OH$
9	$1.7 \times 10^{-12} e^{-940/T}$	$O_3 + OH \longrightarrow HO_2$
10	$2.03 \times 10^{-16} \times (T/300)^{4.57} e^{693/T}$	$O_3 + HO_2 \longrightarrow OH$
11	$2.4 \times 10^{-11} e^{110/T}$	$OH + OP \longrightarrow HO_2$
12	$2.7 \times 10^{-11} e^{224/T}$	$HO_2 + OP \longrightarrow OH$
13	$6.2 \times 10^{-14} \times (T/298)^{2.6} e^{945/T}$	$OH + OH \longrightarrow OP$
14	K-17	$OH + OH \longrightarrow H_2O_2$
15	$4.8 \times 10^{-11} e^{250/T}$	$OH + HO_2 \longrightarrow$
16	$2.2 \times 10^{-13} e^{600/T} + \dots$ $1.9 \times 10^{-33} e^{980/T} * M$	$HO_2 + HO_2 \longrightarrow H_2O_2$
17	$3.08 \times 10^{-34} e^{2800/T} + \dots$ $+ 2.66 \times 10^{-54} e^{3180/T} * M$	$HO_2 + HO_2 + \langle H_2O \rangle \longrightarrow H_2O_2$
18	$2.9 \times 10^{-12} e^{-160/T}$	$H_2O_2 + OH \longrightarrow HO_2$
19	$1.4 \times 10^{-12} e^{-2000/T}$	$H_2O_2 + OP \longrightarrow OH + HO_2$
20	$3.3 \times 10^{-39} e^{530/T}$	$NO + NO + \langle O_2 \rangle \longrightarrow 2 NO_2$
21	$3.45 \times 10^{-12} e^{270/T}$	$HO_2 + NO \longrightarrow OH + NO_2$
22	$1.4 \times 10^{-13} e^{-2470/T}$	$NO_2 + O_3 \longrightarrow NO_3$
23	$1.8 \times 10^{-11} e^{110/T}$	$NO_3 + NO \longrightarrow 2 NO_2$
24	$4.5 \times 10^{-14} e^{-1260/T}$	$NO_3 + NO_2 \longrightarrow NO + NO_2$
25	1.7×10^{-11}	$NO_3 + OP \longrightarrow NO_2$
26	2×10^{-11}	$NO_3 + OH \longrightarrow HO_2 + NO_2$
27	4×10^{-12}	$NO_3 + HO_2 \longrightarrow OH + NO_2$
28	1×10^{-17}	$NO_3 + O_3 \longrightarrow NO_2$
29	$8.5 \times 10^{-13} e^{-2450/T}$	$NO_3 + NO_3 \longrightarrow 2 NO_2$
30	K-36	$NO_3 + NO_2 \longrightarrow N_2O_5$
31	K-37	$N_2O_5 \longrightarrow NO_3 + NO_2$
32	1×10^{-22}	$N_2O_5 + \langle H_2O \rangle \longrightarrow 2 HNO_3$
33	K-40	$NO + OH \longrightarrow HONO$
34	5×10^{-40}	$NO + NO_2 + \langle H_2O \rangle \longrightarrow 2 HONO$

CB6r2Em (continued on next page)

	Rate coefficient	Reaction
35	1×10^{-20}	$\text{HONO} + \text{HONO} \longrightarrow \text{NO} + \text{NO}_2$
36	$2.5 \times 10^{-12} e^{260/T}$	$\text{HONO} + \text{OH} \longrightarrow \text{NO}_2$
37	K-45	$\text{NO}_2 + \text{OH} \longrightarrow \text{HNO}_3$
38	K-46	$\text{HNO}_3 + \text{OH} \longrightarrow \text{NO}_3$
39	K-48	$\text{HO}_2 + \text{NO}_2 \longrightarrow \text{PNA}$
40	K-49	$\text{PNA} \longrightarrow \text{HO}_2 + \text{NO}_2$
41	$3.2 \times 10^{-13} e^{690/T}$	$\text{PNA} + \text{OH} \longrightarrow \text{NO}_2$
42	$7.5 \times 10^{-12} e^{290/T}$	$\text{C}_2\text{O}_3 + \text{NO} \longrightarrow \text{NO}_2 + \text{MEO}_2 + \text{RO}_2$
43	K-54	$\text{C}_2\text{O}_3 + \text{NO}_2 \longrightarrow \text{PAN}$
44	K-55	$\text{PAN} \longrightarrow \text{NO}_2 + \text{C}_2\text{O}_3$
45	K-57	$\text{C}_2\text{O}_3 + \text{HO}_2 \longrightarrow 0.41 \text{ PACD} + 0.15 \text{ AACD} + 0.15 \text{ O}_3 + 0.44 \text{ MEO}_2 + 0.44 \text{ RO}_2 + 0.44 \text{ OH}$
46	K-58	$\text{C}_2\text{O}_3 + \text{RO}_2 \longrightarrow \text{C}_2\text{O}_3$
47	K-59	$\text{C}_2\text{O}_3 + \text{C}_2\text{O}_3 \longrightarrow 2 \text{ MEO}_2 + 2 \text{ RO}_2$
48	$2.9 \times 10^{-12} e^{500/T}$	$\text{C}_2\text{O}_3 + \text{CXO}_3 \longrightarrow \text{MEO}_2 + \text{ALD}_2 + \text{XO}_2\text{H} + 2 \text{ RO}_2$
49	$6.7 \times 10^{-12} e^{340/T}$	$\text{CXO}_3 + \text{NO} \longrightarrow \text{NO}_2 + \text{ALD}_2 + \text{XO}_2\text{H} + \text{RO}_2$
50	K-54	$\text{CXO}_3 + \text{NO}_2 \longrightarrow \text{PANX}$
51	K-55	$\text{PANX} \longrightarrow \text{NO}_2 + \text{CXO}_3$
52	$5.2 \times 10^{-13} e^{980/T}$	$\text{CXO}_3 + \text{HO}_2 \longrightarrow 0.41 \text{ PACD} + 0.15 \text{ AACD} + 0.15 \text{ O}_3 + 0.44 \text{ ALD}_2 + 0.44 \text{ XO}_2\text{H} + 0.44 \text{ RO}_2 + 0.44 \text{ OH}$
53	$8.9 \times 10^{-13} e^{800/T}$	$\text{CXO}_3 + \text{RO}_2 \longrightarrow 0.8 \text{ ALD}_2 + 0.8 \text{ XO}_2\text{H} + 0.8 \text{ RO}_2$
54	$3.2 \times 10^{-12} e^{500/T}$	$\text{CXO}_3 + \text{CXO}_3 \longrightarrow 2 \text{ ALD}_2 + 2 \text{ XO}_2\text{H} + 2 \text{ RO}_2$
55	$2.4 \times 10^{-12} e^{360/T}$	$\text{RO}_2 + \text{NO} \longrightarrow \text{NO}$
56	$4.8 \times 10^{-13} e^{800/T}$	$\text{RO}_2 + \text{HO}_2 \longrightarrow \text{HO}_2$
57	K-70	$\text{RO}_2 + \text{RO}_2 \longrightarrow$
58	$2.3 \times 10^{-12} e^{360/T}$	$\text{MEO}_2 + \text{NO} \longrightarrow \text{FORM} + \text{HO}_2 + \text{NO}_2$
59	$3.8 \times 10^{-13} e^{780/T}$	$\text{MEO}_2 + \text{HO}_2 \longrightarrow 0.9 \text{ CH}_3\text{OOH} + 0.1 \text{ FORM}$
60	$2 \times 10^{-12} e^{500/T}$	$\text{MEO}_2 + \text{C}_2\text{O}_3 \longrightarrow \text{FORM} + 0.9 \text{ HO}_2 + 0.9 \text{ MEO}_2 + 0.1 \text{ AACD} + 0.9 \text{ RO}_2$
61	K-70	$\text{MEO}_2 + \text{RO}_2 \longrightarrow 0.685 \text{ FORM} + 0.315 \text{ MEOH} + 0.37 \text{ HO}_2 + \text{RO}_2$
62	K-75	$\text{XO}_2\text{H} + \text{NO} \longrightarrow \text{NO}_2 + \text{HO}_2$
63	$6.8 \times 10^{-13} e^{800/T}$	$\text{XO}_2\text{H} + \text{HO}_2 \longrightarrow \text{ROOH}$
64	K-58	$\text{XO}_2\text{H} + \text{C}_2\text{O}_3 \longrightarrow 0.8 \text{ HO}_2 + 0.8 \text{ MEO}_2 + 0.2 \text{ AACD} + 0.8 \text{ RO}_2$
65	K-70	$\text{XO}_2\text{H} + \text{RO}_2 \longrightarrow 0.6 \text{ HO}_2 + \text{RO}_2$
66	K-75	$\text{XO}_2 + \text{NO} \longrightarrow \text{NO}_2$
67	K-76	$\text{XO}_2 + \text{HO}_2 \longrightarrow \text{ROOH}$
68	K-58	$\text{XO}_2 + \text{C}_2\text{O}_3 \longrightarrow 0.8 \text{ MEO}_2 + 0.2 \text{ AACD} + 0.8 \text{ RO}_2$
69	K-70	$\text{XO}_2 + \text{RO}_2 \longrightarrow \text{RO}_2$
70	K-75	$\text{XO}_2\text{N} + \text{NO} \longrightarrow 0.5 \text{ NTR}_1 + 0.5 \text{ NTR}_2$
71	K-76	$\text{XO}_2\text{N} + \text{HO}_2 \longrightarrow \text{ROOH}$
72	K-58	$\text{XO}_2\text{N} + \text{C}_2\text{O}_3 \longrightarrow 0.8 \text{ HO}_2 + 0.8 \text{ MEO}_2 + 0.2 \text{ AACD} + 0.8 \text{ RO}_2$
73	K-70	$\text{XO}_2\text{N} + \text{RO}_2 \longrightarrow \text{RO}_2$
74	$5.3 \times 10^{-12} e^{190/T}$	$\text{CH}_3\text{OOH} + \text{OH} \longrightarrow 0.6 \text{ MEO}_2 + 0.6 \text{ RO}_2 + 0.4 \text{ FORM} + 0.4 \text{ OH}$
75	$5.3 \times 10^{-12} e^{190/T}$	$\text{ROOH} + \text{OH} \longrightarrow 0.54 \text{ XO}_2\text{H} + 0.06 \text{ XO}_2\text{N} + 0.6 \text{ RO}_2 + 0.4 \text{ OH}$
76	2×10^{-12}	$\text{NTR}_1 + \text{OH} \longrightarrow \text{NTR}_2$
77	4.5×10^{-13}	$\text{FACD} + \text{OH} \longrightarrow \text{HO}_2$
78	$4 \times 10^{-14} e^{850/T}$	$\text{AACD} + \text{OH} \longrightarrow \text{MEO}_2 + \text{RO}_2$
79	$5.3 \times 10^{-12} e^{190/T}$	$\text{PACD} + \text{OH} \longrightarrow \text{C}_2\text{O}_3$
80	$5.4 \times 10^{-12} e^{135/T}$	$\text{FORM} + \text{OH} \longrightarrow \text{HO}_2 + \text{CO}$
81	$3.4 \times 10^{-11} e^{-1600/T}$	$\text{FORM} + \text{OP} \longrightarrow \text{OH} + \text{HO}_2 + \text{CO}$
82	5.5×10^{-16}	$\text{FORM} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{HO}_2 + \text{CO}$
83	$9.7 \times 10^{-15} e^{625.0/T}$	$\text{FORM} + \text{HO}_2 \longrightarrow \text{HCO}_3$
84	$2.4 \times 10^{12} e^{-7000/T}$	$\text{HCO}_3 \longrightarrow \text{FORM} + \text{HO}_2$
85	5.6×10^{-12}	$\text{HCO}_3 + \text{NO} \longrightarrow \text{FACD} + \text{NO}_2 + \text{HO}_2$
86	$5.6 \times 10^{-15} e^{2300/T}$	$\text{HCO}_3 + \text{HO}_2 \longrightarrow 0.5 \text{ CH}_3\text{OOH} + 0.5 \text{ FACD} + 0.2 \text{ OH} + 0.2 \text{ HO}_2$
87	$1.8 \times 10^{-11} e^{-1100/T}$	$\text{ALD}_2 + \text{OP} \longrightarrow \text{C}_2\text{O}_3 + \text{OH}$
88	$4.7 \times 10^{-12} e^{345/T}$	$\text{ALD}_2 + \text{OH} \longrightarrow \text{C}_2\text{O}_3$
89	$1.4 \times 10^{-12} e^{-1860/T}$	$\text{ALD}_2 + \text{NO}_3 \longrightarrow \text{C}_2\text{O}_3 + \text{HNO}_3$
90	$1.3 \times 10^{-11} e^{-870/T}$	$\text{ALDX} + \text{OP} \longrightarrow \text{CXO}_3 + \text{OH}$
91	$4.9 \times 10^{-12} e^{405/T}$	$\text{ALDX} + \text{OH} \longrightarrow \text{CXO}_3$

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	Rate coefficient	Reaction
92	6.3×10^{-15}	$\text{ALDX} + \text{NO}_3 \longrightarrow \text{CXO}_3 + \text{HNO}_3$
93	8×10^{-12}	$\text{GLYD} + \text{OH} \longrightarrow 0.2 \text{ GLY} + 0.2 \text{ HO}_2 + 0.8 \text{ C}_2\text{O}_3$
94	$1.4 \times 10^{-12} e^{-1860/T}$	$\text{GLYD} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{C}_2\text{O}_3$
95	$3.1 \times 10^{-12} e^{340/T}$	$\text{GLY} + \text{OH} \longrightarrow 1.8 \text{ CO} + 0.2 \text{ XO}_2 + 0.2 \text{ RO}_2 + \text{HO}_2$
96	$1.4 \times 10^{-12} e^{-1860/T}$	$\text{GLY} + \text{NO}_3 \longrightarrow \text{HNO}_3 + 1.5 \text{ CO} + 0.5 \text{ XO}_2 + 0.5 \text{ RO}_2 + \text{HO}_2$
97	$1.4 \times 10^{-12} e^{-1860/T}$	$\text{MGLY} + \text{NO}_3 \longrightarrow \text{HNO}_3 + \text{C}_2\text{O}_3 + \text{XO}_2 + \text{RO}_2$
98	$1.9 \times 10^{-12} e^{575/T}$	$\text{MGLY} + \text{OH} \longrightarrow \text{C}_2\text{O}_3 + \text{CO}$
99	$7.7 \times 10^{-12} e^{-2100/T}$	$\text{H}_2 + \text{OH} \longrightarrow \text{HO}_2$
100	$1.44 \times 10^{-13} + 3.43 \times 10^{-33} * \text{M}$	$\text{CO} + \text{OH} \longrightarrow \text{HO}_2$
101	$1.85 \times 10^{-12} e^{-1690/T}$	$\text{CH}_4 + \text{OH} \longrightarrow \text{MEO}_2 + \text{RO}_2$
102	$6.9 \times 10^{-12} e^{-1000/T}$	$\text{ETHA} + \text{OH} \longrightarrow 0.991 \text{ ALD}_2 + 0.991 \text{ XO}_2\text{H} + 0.009 \text{ XO}_2\text{N} + \text{RO}_2$
103	$2.85 \times 10^{-12} e^{-345/T}$	$\text{MEOH} + \text{OH} \longrightarrow \text{FORM} + \text{HO}_2$
104	$3 \times 10^{-12} e^{20/T}$	$\text{ETOH} + \text{OH} \longrightarrow 0.95 \text{ ALD}_2 + 0.9 \text{ HO}_2 + 0.1 \text{ XO}_2\text{H} + 0.1 \text{ RO}_2 + 0.078 \text{ FORM} + 0.011 \text{ GLYD}$
105	$1.41 \times 10^{-12} e^{-620.6/T}$	$\text{ACET} + \text{OH} \longrightarrow \text{FORM} + \text{C}_2\text{O}_3 + \text{XO}_2 + \text{RO}_2$
106	$7.6 \times 10^{-12} e^{-585/T}$	$\text{PRPA} + \text{OH} \longrightarrow 0.71 \text{ ACET} + 0.26 \text{ ALDX} + 0.26 \text{ PAR} + 0.97 \text{ XO}_2\text{H} + 0.03 \text{ XO}_2\text{N} + \text{RO}_2$
107	8.1×10^{-13}	$\text{PAR} + \text{OH} \longrightarrow 0.11 \text{ ALDX} + 0.76 \text{ ROR} + 0.13 \text{ XO}_2\text{N} + 0.11 \text{ XO}_2\text{H} + 0.76 \text{ XO}_2 + \text{RO}_2 + 0.11 \text{ PARLOSS}$
108	$5.7 \times 10^{12} e^{-5780/T}$	$\text{ROR} \longrightarrow 0.2 \text{ KET} + 0.42 \text{ ACET} + 0.74 \text{ ALD}_2 + 0.37 \text{ ALDX} + 0.04 \text{ XO}_2\text{N} + 0.94 \text{ XO}_2\text{H} + 0.98 \text{ RO}_2 + 0.02 \text{ ROR} + 2.7 \text{ PARLOSS}$
109	$1.5 \times 10^{-14} e^{-200/T}$	$\text{ROR} + \text{O}_2 \longrightarrow \text{KET} + \text{HO}_2$
110	$8.6 \times 10^{-12} e^{400/T}$	$\text{ROR} + \text{NO}_2 \longrightarrow \text{NTR}_1$
111	K-136	$\text{ETHY} + \text{OH} \longrightarrow 0.7 \text{ GLY} + 0.7 \text{ OH} + 0.3 \text{ FACD} + 0.3 \text{ CO} + 0.3 \text{ HO}_2$
112	$1.04 \times 10^{-11} e^{-792/T}$	$\text{ETH} + \text{OP} \longrightarrow \text{FORM} + \text{HO}_2 + \text{CO} + 0.7 \text{ XO}_2\text{H} + 0.7 \text{ RO}_2 + 0.3 \text{ OH}$
113	K-138	$\text{ETH} + \text{OH} \longrightarrow \text{XO}_2\text{H} + \text{RO}_2 + 1.56 \text{ FORM} + 0.22 \text{ GLYD}$
114	$9.1 \times 10^{-15} e^{-2580/T}$	$\text{ETH} + \text{O}_3 \longrightarrow \text{FORM} + 0.51 \text{ CO} + 0.16 \text{ HO}_2 + 0.16 \text{ OH} + 0.37 \text{ FACD}$
115	$3.3 \times 10^{-12} e^{-2880/T}$	$\text{ETH} + \text{NO}_3 \longrightarrow 0.5 \text{ NO}_2 + 0.5 \text{ NTR}_1 + 0.5 \text{ XO}_2\text{H} + 0.5 \text{ XO}_2 + \text{RO}_2 + 1.125 \text{ FORM}$
116	$1 \times 10^{-11} e^{-280/T}$	$\text{OLE} + \text{OP} \longrightarrow 0.2 \text{ ALD}_2 + 0.3 \text{ ALDX} + 0.1 \text{ HO}_2 + 0.2 \text{ XO}_2\text{H} + 0.2 \text{ CO} + 0.2 \text{ FORM} + 0.01 \text{ XO}_2\text{N} + 0.21 \text{ RO}_2 + 0.2 \text{ PAR} + 0.1 \text{ OH}$
117	K-142	$\text{OLE} + \text{OH} \longrightarrow 0.781 \text{ FORM} + 0.488 \text{ ALD}_2 + 0.488 \text{ ALDX} + 0.976 \text{ XO}_2\text{H} + 0.195 \text{ XO}_2 + 0.024 \text{ XO}_2\text{N} + 1.195 \text{ RO}_2 + 0.73 \text{ PARLOSS}$
118	$5.5 \times 10^{-15} e^{-1880/T}$	$\text{OLE} + \text{O}_3 \longrightarrow 0.295 \text{ ALD}_2 + 0.555 \text{ FORM} + 0.27 \text{ ALDX} + 0.15 \text{ XO}_2\text{H} + 0.15 \text{ RO}_2 + 0.334 \text{ OH} + 0.08 \text{ HO}_2 + 0.378 \text{ CO} + 0.075 \text{ GLY} + 0.075 \text{ MGLY} + 0.09 \text{ FACD} + 0.13 \text{ AACD} + 0.04 \text{ H}_2\text{O}_2 + 0.79 \text{ PARLOSS}$
119	$4.6 \times 10^{-13} e^{-1155/T}$	$\text{OLE} + \text{NO}_3 \longrightarrow 0.5 \text{ NO}_2 + 0.5 \text{ NTR}_1 + 0.48 \text{ XO}_2 + 0.48 \text{ XO}_2\text{H} + 0.04 \text{ XO}_2\text{N} + \text{RO}_2 + 0.5 \text{ FORM} + 0.25 \text{ ALD}_2 + 0.375 \text{ ALDX} + \text{PARLOSS}$
120	2.3×10^{-11}	$\text{IOLE} + \text{OP} \longrightarrow 1.24 \text{ ALD}_2 + 0.66 \text{ ALDX} + 0.1 \text{ XO}_2\text{H} + 0.1 \text{ RO}_2 + 0.1 \text{ CO} + 0.1 \text{ PAR}$
121	$1.05 \times 10^{-11} e^{519/T}$	$\text{IOLE} + \text{OH} \longrightarrow 1.3 \text{ ALD}_2 + 0.7 \text{ ALDX} + \text{XO}_2\text{H} + \text{RO}_2$
122	$4.7 \times 10^{-15} e^{-1013/T}$	$\text{IOLE} + \text{O}_3 \longrightarrow 0.732 \text{ ALD}_2 + 0.442 \text{ ALDX} + 0.128 \text{ FORM} + 0.245 \text{ CO} + 0.5 \text{ OH} + 0.3 \text{ XO}_2\text{H} + 0.3 \text{ RO}_2 + 0.24 \text{ GLY} + 0.06 \text{ MGLY} + 0.29 \text{ PAR} + 0.08 \text{ AACD} + 0.08 \text{ H}_2\text{O}_2$
123	3.7×10^{-13}	$\text{IOLE} + \text{NO}_3 \longrightarrow 0.5 \text{ NO}_2 + 0.5 \text{ NTR}_1 + 0.48 \text{ XO}_2 + 0.48 \text{ XO}_2\text{H} + 0.04 \text{ XO}_2\text{N} + \text{RO}_2 + 0.5 \text{ ALD}_2 + 0.625 \text{ ALDX} + \text{PAR}$
124	$2.7 \times 10^{-11} e^{390/T}$	$\text{C}_5\text{H}_8 + \text{OH} \longrightarrow \text{ISO}_2 + \text{RO}_2$
125	3×10^{-11}	$\text{C}_5\text{H}_8 + \text{OP} \longrightarrow 0.75 \text{ ISPD} + 0.5 \text{ FORM} + 0.25 \text{ XO}_2 + 0.25 \text{ RO}_2 + 0.25 \text{ HO}_2 + 0.25 \text{ CXO}_3 + 0.25 \text{ PAR}$
126	$2.39 \times 10^{-12} e^{365/T}$	$\text{ISO}_2 + \text{NO} \longrightarrow 0.1 \text{ INTR} + 0.9 \text{ NO}_2 + 0.673 \text{ FORM} + 0.9 \text{ ISPD} + 0.818 \text{ HO}_2 + 0.082 \text{ XO}_2\text{H} + 0.082 \text{ RO}_2$
127	$7.43 \times 10^{-13} e^{700/T}$	$\text{ISO}_2 + \text{HO}_2 \longrightarrow 0.88 \text{ ISPX} + 0.12 \text{ OH} + 0.12 \text{ HO}_2 + 0.12 \text{ FORM} + 0.12 \text{ ISPD}$
128	K-58	$\text{ISO}_2 + \text{C}_2\text{O}_3 \longrightarrow 0.598 \text{ FORM} + \text{ISPD} + 0.728 \text{ HO}_2 + 0.072 \text{ XO}_2\text{H} + 0.8 \text{ MEO}_2 + 0.2 \text{ AACD} + 0.872 \text{ RO}_2$
129	K-70	$\text{ISO}_2 + \text{RO}_2 \longrightarrow 0.598 \text{ FORM} + \text{ISPD} + 0.728 \text{ HO}_2 + 0.072 \text{ XO}_2\text{H} + 0.072 \text{ RO}_2$
130	$3.3 \times 10^9 e^{-8300/T}$	$\text{ISO}_2 \longrightarrow \text{HO}_2 + \text{HPLD}$
131	$1.03 \times 10^{-14} e^{-1995/T}$	$\text{C}_5\text{H}_8 + \text{O}_3 \longrightarrow 0.6 \text{ FORM} + 0.65 \text{ ISPD} + 0.15 \text{ ALDX} + 0.2 \text{ CXO}_3 + 0.35 \text{ PAR} + 0.266 \text{ OH} + 0.2 \text{ XO}_2 + 0.2 \text{ RO}_2 + 0.066 \text{ HO}_2 + 0.066 \text{ CO}$
132	$3.03 \times 10^{-12} e^{-448/T}$	$\text{C}_5\text{H}_8 + \text{NO}_3 \longrightarrow 0.35 \text{ NO}_2 + 0.65 \text{ NTR}_2 + 0.64 \text{ XO}_2\text{H} + 0.33 \text{ XO}_2 + 0.03 \text{ XO}_2\text{N} + \text{RO}_2 + 0.35 \text{ FORM} + 0.35 \text{ ISPD}$
133	$5.58 \times 10^{-12} e^{511/T}$	$\text{ISPD} + \text{OH} \longrightarrow 0.022 \text{ XO}_2\text{N} + 0.521 \text{ XO}_2 + 0.115 \text{ MGLY} + 0.115 \text{ MEO}_2 + 0.269 \text{ GLYD} + 0.269 \text{ C}_2\text{O}_3 + 0.457 \text{ OPO}_3 + 0.117 \text{ PAR} + 0.137 \text{ ACET} + 0.137 \text{ CO} + 0.137 \text{ HO}_2 + 0.658 \text{ RO}_2$

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	Rate coefficient	Reaction
134	$3.88 \times 10^{-15} e^{-1770/T}$	ISPD + O3 $\rightarrow$ 0.04 ALD2 + 0.231 FORM + 0.531 MGLY + 0.17 GLY + 0.17 ACET + 0.543 CO + 0.461 OH + 0.15 FACD + 0.398 HO2 + 0.143 C2O3
135	$4.1 \times 10^{-12} e^{-1860/T}$	ISPD + NO3 $\rightarrow$ 0.717 HNO3 + 0.142 NTR2 + 0.142 NO2 + 0.142 XO2 + 0.142 XO2H + 0.113 GLYD + 0.113 MGLY + 0.717 PAR + 0.717 CXO3 + 0.284 RO2
136	$2.23 \times 10^{-11} e^{372/T}$	ISPX + OH $\rightarrow$ 0.904 EPOX + 0.933 OH + 0.067 ISO2 + 0.067 RO2 + 0.029 IOLE + 0.029 ALDX
137	$6 \times 10^{-12} e^{-1860/T}$	HPLD + NO3 $\rightarrow$ HNO3 + ISPD
138	$5.78 \times 10^{-11} e^{-400/T}$	EPOX + OH $\rightarrow$ EPX2 + RO2
139	$7.43 \times 10^{-13} e^{700/T}$	EPX2 + HO2 $\rightarrow$ 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 1.125 OH + 0.825 HO2 + 0.375 FORM + 0.074 FACD + 0.251 CO + 2.175 PAR
140	$2.39 \times 10^{-12} e^{365/T}$	EPX2 + NO $\rightarrow$ 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 0.125 OH + 0.825 HO2 + 0.375 FORM + NO2 + 0.251 CO + 2.175 PAR
141	K-58	EPX2 + C2O3 $\rightarrow$ 0.22 GLYD + 0.22 GLY + 0.22 MGLY + 0.1 OH + 0.66 HO2 + 0.3 FORM + 0.2 CO + 1.74 PAR + 0.8 MEO2 + 0.2 AACD + 0.8 RO2
142	K-70	EPX2 + RO2 $\rightarrow$ 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 0.125 OH + 0.825 HO2 + 0.375 FORM + 0.251 CO + 2.175 PAR + RO2
143	3.1×10^{-11}	INTR + OH $\rightarrow$ 0.63 XO2 + 0.37 XO2H + RO2 + 0.444 NO2 + 0.185 NO3 + 0.104 INTR + 0.592 FORM + 0.331 GLYD + 0.185 FACD + 2.7 PAR + 0.098 OLE + 0.078 ALDX + 0.266 NTR2
144	3.6×10^{-11}	TERP + OP $\rightarrow$ 0.15 ALDX + 5.12 PAR
145	$1.5 \times 10^{-11} e^{449/T}$	TERP + OH $\rightarrow$ 0.75 XO2H + 0.5 XO2 + 0.25 XO2N + 1.5 RO2 + 0.28 FORM + 1.66 PAR + 0.47 ALDX
146	$1.2 \times 10^{-15} e^{-821/T}$	TERP + O3 $\rightarrow$ 0.57 OH + 0.07 XO2H + 0.69 XO2 + 0.18 XO2N + 0.94 RO2 + 0.24 FORM + 0.001 CO + 7 PAR + 0.21 ALDX + 0.39 CXO3
147	$3.7 \times 10^{-12} e^{175/T}$	TERP + NO3 $\rightarrow$ 0.47 NO2 + 0.28 XO2H + 0.75 XO2 + 0.25 XO2N + 1.28 RO2 + 0.47 ALDX + 0.53 NTR2
148	$2.3 \times 10^{-12} e^{-190/T}$	BENZ + OH $\rightarrow$ 0.53 CRES + 0.352 BZO2 + 0.352 RO2 + 0.118 OPEN + 0.118 OH + 0.53 HO2
149	$2.7 \times 10^{-12} e^{360/T}$	BZO2 + NO $\rightarrow$ 0.918 NO2 + 0.082 NTR2 + 0.918 GLY + 0.918 OPEN + 0.918 HO2
150	K-58	BZO2 + C2O3 $\rightarrow$ GLY + OPEN + HO2 + MEO2 + RO2
151	$1.9 \times 10^{-13} e^{1300/T}$	BZO2 + HO2 $\rightarrow$
152	K-70	BZO2 + RO2 $\rightarrow$ GLY + OPEN + HO2 + RO2
153	$1.8 \times 10^{-12} e^{340/T}$	TOL + OH $\rightarrow$ 0.18 CRES + 0.65 TO2 + 0.72 RO2 + 0.1 OPEN + 0.1 OH + 0.07 XO2H + 0.18 HO2
154	$2.7 \times 10^{-12} e^{360/T}$	TO2 + NO $\rightarrow$ 0.86 NO2 + 0.14 NTR2 + 0.417 GLY + 0.443 MGLY + 0.66 OPEN + 0.2 XOPN + 0.86 HO2
155	K-58	TO2 + C2O3 $\rightarrow$ 0.48 GLY + 0.52 MGLY + 0.77 OPEN + 0.23 XOPN + HO2 + MEO2 + RO2
156	$1.9 \times 10^{-13} e^{1300/T}$	TO2 + HO2 $\rightarrow$
157	K-70	TO2 + RO2 $\rightarrow$ 0.48 GLY + 0.52 MGLY + 0.77 OPEN + 0.23 XOPN + HO2 + RO2
158	1.85×10^{-11}	XYL + OH $\rightarrow$ 0.155 CRES + 0.544 XLO2 + 0.602 RO2 + 0.244 XOPN + 0.244 OH + 0.058 XO2H + 0.155 HO2
159	$2.7 \times 10^{-12} e^{360/T}$	XLO2 + NO $\rightarrow$ 0.86 NO2 + 0.14 NTR2 + 0.221 GLY + 0.675 MGLY + 0.3 OPEN + 0.56 XOPN + 0.86 HO2
160	$1.9 \times 10^{-13} e^{1300/T}$	XLO2 + HO2 $\rightarrow$
161	K-58	XLO2 + C2O3 $\rightarrow$ 0.26 GLY + 0.77 MGLY + 0.35 OPEN + 0.65 XOPN + HO2 + MEO2 + RO2
162	K-70	XLO2 + RO2 $\rightarrow$ 0.26 GLY + 0.77 MGLY + 0.35 OPEN + 0.65 XOPN + HO2 + RO2
163	$1.7 \times 10^{-12} e^{950/T}$	CRES + OH $\rightarrow$ 0.025 GLY + 0.025 OPEN + HO2 + 0.2 CRO + 0.732 CAT1 + 0.02 XO2N + 0.02 RO2
164	1.4×10^{-11}	CRES + NO3 $\rightarrow$ 0.3 CRO + HNO3 + 0.48 XO2 + 0.12 XO2H + 0.24 GLY + 0.24 MGLY + 0.48 OPO3 + 0.1 XO2N + 0.7 RO2
165	2.1×10^{-12}	CRO + NO2 $\rightarrow$ CRON
166	5.5×10^{-12}	CRO + HO2 $\rightarrow$ CRES
167	1.53×10^{-12}	CRON + OH $\rightarrow$ NTR2 + 0.5 CRO
168	3.8×10^{-12}	CRON + NO3 $\rightarrow$ NTR2 + 0.5 CRO + HNO3
169	9×10^{-11}	XOPN + OH $\rightarrow$ MGLY + 0.4 GLY + 2 XO2H + 2 RO2
170	$1.08 \times 10^{-16} e^{-500/T}$	XOPN + O3 $\rightarrow$ 1.2 MGLY + 0.5 OH + 0.6 C2O3 + 0.1 ALD2 + 0.5 CO + 0.3 XO2H + 0.3 RO2
171	3×10^{-12}	XOPN + NO3 $\rightarrow$ 0.5 NO2 + 0.5 NTR2 + 0.45 XO2H + 0.45 XO2 + 0.1 XO2N + RO2 + 0.25 OPEN + 0.25 MGLY
172	4.4×10^{-11}	OPEN + OH $\rightarrow$ 0.6 OPO3 + 0.4 XO2H + 0.4 RO2 + 0.4 GLY

CB6r2Em (continued on next page)

	Rate coefficient	Reaction
173	$5.4 \times 10^{-17} e^{-500/T}$	$\text{OPEN} + \text{O}_3 \longrightarrow 1.4 \text{ GLY} + 0.24 \text{ MGLY} + 0.5 \text{ OH} + 0.12 \text{ C}_2\text{O}_3 + 0.08 \text{ FORM} + 0.02 \text{ ALD}_2 + 1.98 \text{ CO} + 0.56 \text{ HO}_2$
174	3.8×10^{-12}	$\text{OPEN} + \text{NO}_3 \longrightarrow \text{OPO}_3 + \text{HNO}_3$
175	5×10^{-11}	$\text{CAT}_1 + \text{OH} \longrightarrow 0.14 \text{ FORM} + 0.2 \text{ HO}_2 + 0.5 \text{ CRO}$
176	1.7×10^{-10}	$\text{CAT}_1 + \text{NO}_3 \longrightarrow \text{CRO} + \text{HNO}_3$
177	1×10^{-11}	$\text{OPO}_3 + \text{NO} \longrightarrow \text{NO}_2 + 0.5 \text{ GLY} + 0.5 \text{ CO} + 0.8 \text{ HO}_2 + 0.2 \text{ CXO}_3$
178	K-54	$\text{OPO}_3 + \text{NO}_2 \longrightarrow \text{OPAN}$
179	K-55	$\text{OPAN} \longrightarrow \text{OPO}_3 + \text{NO}_2$
180	K-57	$\text{OPO}_3 + \text{HO}_2 \longrightarrow 0.41 \text{ PACD} + 0.15 \text{ AACD} + 0.15 \text{ O}_3 + 0.44 \text{ ALDX} + 0.44 \text{ XO}_2\text{H} + 0.44 \text{ RO}_2 + 0.44 \text{ OH}$
181	K-59	$\text{OPO}_3 + \text{C}_2\text{O}_3 \longrightarrow \text{MEO}_2 + \text{XO}_2 + \text{ALDX} + 2 \text{ RO}_2$
182	K-58	$\text{OPO}_3 + \text{RO}_2 \longrightarrow 0.8 \text{ XO}_2\text{H} + 0.8 \text{ ALDX} + 1.8 \text{ RO}_2 + 0.2 \text{ AACD}$
183	3.6×10^{-11}	$\text{OPAN} + \text{OH} \longrightarrow 0.5 \text{ NO}_2 + 0.5 \text{ GLY} + \text{CO} + 0.5 \text{ NTR}_2$
184	3×10^{-12}	$\text{PANX} + \text{OH} \longrightarrow \text{ALD}_2 + \text{NO}_2$
185	2.3×10^{-5}	$\text{NTR}_2 \longrightarrow \text{HNO}_3$
186	$1.85 \times 10^{-12} e^{-1690/T}$	$\text{ECH}_4 + \text{OH} \longrightarrow \text{MEO}_2 + \text{RO}_2$
187	1×10^{-9}	$\text{PARLOSS} + \text{PAR} \longrightarrow$
188	RCPHOT(IDNO ₂)	$\text{NO}_2 \longrightarrow \text{NO} + \text{OP}$
189	RCPHOT(IDO ₃ -O ₃ P)	$\text{O}_3 \longrightarrow \text{OP}$
190	RCPHOT(IDO ₃ -O ₁ D)	$\text{O}_3 \longrightarrow \text{OD}$
191	RCPHOT(IDH ₂ O ₂)	$\text{H}_2\text{O}_2 \longrightarrow 2 \text{ OH}$
192	RCPHOT(IDNO ₃)	$\text{NO}_3 \longrightarrow 0.113 \text{ NO} + 0.887 \text{ NO}_2 + 0.887 \text{ OP}$
193	RCPHOT(IDN ₂ O ₅)	$\text{N}_2\text{O}_5 \longrightarrow \text{NO}_2 + \text{NO}_3$
194	RCPHOT(IDHONO)	$\text{HONO} \longrightarrow \text{NO} + \text{OH}$
195	RCPHOT(IDHNO ₃)	$\text{HNO}_3 \longrightarrow \text{OH} + \text{NO}_2$
196	RCPHOT(IDHO ₂ NO ₂)	$\text{PNA} \longrightarrow 0.59 \text{ HO}_2 + 0.59 \text{ NO}_2 + 0.41 \text{ OH} + 0.41 \text{ NO}_3$
197	RCPHOT(IDHO ₂ NO ₂) $\times 0.14$	$\text{PAN} \longrightarrow 0.6 \text{ NO}_2 + 0.6 \text{ C}_2\text{O}_3 + 0.4 \text{ NO}_3 + 0.4 \text{ MEO}_2 + 0.4 \text{ RO}_2$
198	RCPHOT(IDHO ₂ NO ₂) $\times 0.14$	$\text{PANX} \longrightarrow 0.6 \text{ NO}_2 + 0.6 \text{ CXO}_3 + 0.4 \text{ NO}_3 + 0.4 \text{ ALD}_2 + 0.4 \text{ XO}_2\text{H} + 0.4 \text{ RO}_2$
199	RCPHOT(IDCH ₃ O ₂ H)	$\text{CH}_3\text{OOH} \longrightarrow \text{MEO}_2 + \text{RO}_2 + \text{OH}$
200	RCPHOT(IDCH ₃ O ₂ H)	$\text{ROOH} \longrightarrow \text{HO}_2 + \text{OH}$
201	RCPHOT(IDHCHO-H)	$\text{FORM} \longrightarrow 2 \text{ HO}_2 + \text{CO}$
202	RCPHOT(IDHCHO-H ₂)	$\text{FORM} \longrightarrow \text{CO} + \text{H}_2$
203	RCPHOT(IDCH ₃ CHO)	$\text{ALD}_2 \longrightarrow \text{MEO}_2 + \text{RO}_2 + \text{CO} + \text{HO}_2$
204	RCPHOT(IDMEK) $\times 5.4$	$\text{ALDX} \longrightarrow \text{ALD}_2 + \text{XO}_2\text{H} + \text{RO}_2 + \text{CO} + \text{HO}_2$
205	RCPHOT(IDACETON) $\times 10$.	$\text{GLYD} \longrightarrow 0.74 \text{ FORM} + 0.89 \text{ CO} + 1.4 \text{ HO}_2 + 0.15 \text{ MEOH} + 0.19 \text{ OH} + 0.11 \text{ GLY} + 0.11 \text{ XO}_2\text{H} + 0.11 \text{ RO}_2$
206	RCPHOT(IDCHOCHO)	$\text{GLY} \longrightarrow 2 \text{ HO}_2 + 2 \text{ CO}$
207	RCPHOT(IDRCOCHO)	$\text{MGLY} \longrightarrow \text{C}_2\text{O}_3 + \text{HO}_2 + \text{CO}$
208	RCPHOT(IDACETON) $\times 1.5$	$\text{KET} \longrightarrow 0.5 \text{ ALD}_2 + 0.5 \text{ C}_2\text{O}_3 + 0.5 \text{ XO}_2\text{H} + 0.5 \text{ CXO}_3 + 0.5 \text{ MEO}_2 + \text{RO}_2 + 2.5 \text{ PARLOSS}$
209	RCPHOT(IDACETON)	$\text{ACET} \longrightarrow 0.38 \text{ CO} + 1.38 \text{ MEO}_2 + 1.38 \text{ RO}_2 + 0.62 \text{ C}_2\text{O}_3$
210	RCPHOT(IDHCHO-H ₂) $\times 0.62$	$\text{ISPD} \longrightarrow 0.76 \text{ HO}_2 + 0.34 \text{ XO}_2\text{H} + 0.16 \text{ XO}_2 + 0.34 \text{ MEO}_2 + 0.208 \text{ C}_2\text{O}_3 + 0.26 \text{ FORM} + 0.24 \text{ OLE} + 0.24 \text{ PAR} + 0.17 \text{ ACET} + 0.128 \text{ GLYD} + 0.84 \text{ RO}_2$
211	RCPHOT(IDCHOCHO) $\times 7.2$	$\text{HPLD} \longrightarrow \text{OH} + \text{ISPD}$
212	RCPHOT(IDHONO) $\times 0.076$	$\text{CRON} \longrightarrow \text{HONO} + \text{HO}_2 + \text{FORM} + \text{OPEN}$
213	RCPHOT(IDNO ₂) $\times 0.087$	$\text{XOPN} \longrightarrow 0.4 \text{ GLY} + \text{XO}_2\text{H} + 0.7 \text{ HO}_2 + 0.7 \text{ CO} + 0.3 \text{ C}_2\text{O}_3$
214	RCPHOT(IDNO ₂) $\times 0.087$	$\text{OPEN} \longrightarrow \text{OPO}_3 + \text{HO}_2 + \text{CO}$

Notes:

"T" is temperature, "M" is third body, RCPHOT are photolysis rates.

Reaction coefficients are in units of s^{-1} for unimolecular reactions, $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for bimolecular reactions, and $\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-2}$ for termolecular reactions.

$$\text{K-57} = 5.2 \times 10^{-13} e^{980/T}$$

$$\text{K-58} = 8.9 \times 10^{-13} e^{800/T}$$

$$\text{K-59} = 2.9 \times 10^{-12} e^{500/T}$$

$$\text{K-70} = 6.5 \times 10^{-14} e^{500/T}$$

$$\text{K-75} = 2.7 \times 10^{-12} e^{360/T}$$

$$\text{K-76} = 6.8 \times 10^{-13} e^{800/T}$$

Some pressure dependent rate-coefficients are given in Table J.2

Table J.2: Rate coefficients for pressure dependent reactions in the CB6r2Em mechanism.

$K_{0,6}$	$1.3 \times 10^{-31} \times (T/300)^{-1.5}$
$K_{\infty,6}$	$2.3 \times 10^{-11} \times (T/300)^{0.24}$
G_6	$1.0 / (1.0 + \log_{10}(K_{0,6} \times [M] / K_{\infty,6})^2)$
$K-6$	$K_{0,6} \times [M] / (1.0 + K_{0,6} \times [M] / K_{\infty,6}) \times 0.6^{G_6}$
$K_{0,17}$	$6.9 \times 10^{-31} \times (T/300)^{-0.8}$
$K_{\infty,17}$	2.6×10^{-11}
G_{17}	$1.0 / (1.0 + (\log_{10}(K_{0,17} \times [M] / K_{\infty,17}) / 1.13)^2)$
$K-17$	$K_{0,17} \times [M] / (1.0 + K_{0,17} \times [M] / K_{\infty,17}) \times 0.5^{G_{17}}$
$K_{0,36}$	$3.6 \times 10^{-30} \times (T/300)^{-4.1}$
$K_{\infty,36}$	$1.9 \times 10^{-12} \times (T/300)^{0.2}$
G_{36}	$1.0 / (1.0 + (\log_{10}(K_{0,36} \times [M] / K_{\infty,36}) / 1.33)^2)$
$K-36$	$K_{0,36} \times [M] / (1.0 + K_{0,36} \times [M] / K_{\infty,36}) \times 0.35^{G_{36}}$
$K_{0,37}$	$0.0013 \times (T/300)^{-3.5} e^{-11000/T}$
$K_{\infty,37}$	$9.7 \times 10^{14} \times (T/300)^{0.1} e^{-11080/T}$
G_{37}	$1.0 / (1.0 + (\log_{10}(K_{0,37} \times [M] / K_{\infty,37}) / 1.33)^2)$
$K-37$	$K_{0,37} \times [M] / (1.0 + K_{0,37} \times [M] / K_{\infty,37}) \times 0.35^{G_{37}}$
$K_{0,40}$	$7.4 \times 10^{-31} \times (T/300)^{-2.4}$
$K_{\infty,40}$	$3.3 \times 10^{-11} \times (T/300)^{-0.3}$
G_{40}	$1.0 / (1.0 + (\log_{10}(K_{0,40} \times [M] / K_{\infty,40}) / 0.87)^2)$
$K-40$	$K_{0,40} \times [M] / (1.0 + K_{0,40} \times [M] / K_{\infty,40}) \times 0.81^{G_{40}}$
$K_{0,45}$	$1.8 \times 10^{-30} \times (T/300)^{-3.0}$
$K_{\infty,45}$	2.8×10^{-11}
G_{45}	$1.0 / (1.0 + \log_{10}(K_{0,45} \times [M] / K_{\infty,45})^2)$
$K-45$	$K_{0,45} \times [M] / (1.0 + K_{0,45} \times [M] / K_{\infty,45}) \times 0.6^{G_{45}}$
$K_{0,46}$	$2.4 \times 10^{-14} e^{460/T}$
$K_{2,46}$	$2.7 \times 10^{-17} e^{2199/T}$
$K_{3,46}$	$6.5 \times 10^{-34} e^{1335/T}$
$K-46$	$K_{0,46} + K_{3,46} \times [M] / (1.0 + K_{3,46} \times [M] / K_{2,46})$
$K_{0,48}$	$1.8 \times 10^{-31} \times (T/300)^{-3.2}$
$K_{\infty,48}$	4.7×10^{-12}
G_{48}	$1.0 / (1.0 + \log_{10}(K_{0,48} \times [M] / K_{\infty,48})^2)$
$K-48$	$K_{0,48} \times [M] / (1.0 + K_{0,48} \times [M] / K_{\infty,48}) \times 0.6^{G_{48}}$
$K_{0,49}$	$4.1 \times 10^{-5} e^{-10650/T}$
$K_{\infty,49}$	$4.8 \times 10^{15} e^{-11170/T}$
G_{49}	$1.0 / (1.0 + \log_{10}(K_{0,49} \times [M] / K_{\infty,49})^2)$
$K-49$	$K_{0,49} \times [M] / (1.0 + K_{0,49} \times [M] / K_{\infty,49}) \times 0.6^{G_{49}}$
$K_{0,54}$	$2.7 \times 10^{-28} \times (T/300)^{-7.1}$
$K_{\infty,54}$	$1.2 \times 10^{-11} \times (T/300)^{-0.9}$
G_{54}	$1.0 / (1.0 + (\log_{10}(K_{0,54} \times [M] / K_{\infty,54}) / 1.41)^2)$
$K-54$	$K_{0,54} \times [M] / (1.0 + K_{0,54} \times [M] / K_{\infty,54}) \times 0.3^{G_{54}}$
$K_{0,55}$	$0.0049 e^{-12100/T}$
$K_{\infty,55}$	$5.4 \times 10^{16} e^{-13830/T}$
G_{55}	$1.0 / (1.0 + (\log_{10}(K_{0,55} \times [M] / K_{\infty,55}) / 1.41)^2)$
$K-55$	$K_{0,55} \times [M] / (1.0 + K_{0,55} \times [M] / K_{\infty,55}) \times 0.3^{G_{55}}$
$K_{0,136}$	$5 \times 10^{-30} \times (T/300)^{-1.5}$
$K_{\infty,136}$	1×10^{-12}
G_{136}	$1.0 / (1.0 + (\log_{10}(K_{0,136} \times [M] / K_{\infty,136}) / 1.3)^2)$
$K-136$	$K_{0,136} \times [M] / (1.0 + K_{0,136} \times [M] / K_{\infty,136}) \times 0.37^{G_{136}}$
$K_{0,138}$	$8.6 \times 10^{-29} \times (T/300)^{-3.1}$
$K_{\infty,138}$	$9 \times 10^{-12} \times (T/300)^{-0.85}$
G_{138}	$1.0 / (1.0 + (\log_{10}(K_{0,138} \times [M] / K_{\infty,138}) / 1.15)^2)$
$K-138$	$K_{0,138} \times [M] / (1.0 + K_{0,138} \times [M] / K_{\infty,138}) \times 0.48^{G_{138}}$
$K_{0,142}$	$8 \times 10^{-27} \times (T/300)^{-3.5}$
$K_{\infty,142}$	$3 \times 10^{-11} \times 300/T$
G_{142}	$1.0 / (1.0 + (\log_{10}(K_{0,142} \times [M] / K_{\infty,142}) / 1.13)^2)$
$K-142$	$K_{0,142} \times [M] / (1.0 + K_{0,142} \times [M] / K_{\infty,142}) \times 0.5^{G_{142}}$

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