MOZART-GEOS5 Chemical Mechanism (MOZCART) Documentation

Generated from KPP Files

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1 Introduction

This document describes the MOZART-GEOS5 chemical mechanism (MOZCART) as implemented in the Kinetic PreProcessor (KPP) format. The MOZCART mechanism is a tropospheric gas-phase chemical mechanism that includes comprehensive treatment of hydrocarbon chemistry, nitrogen oxides, and sulfur chemistry.

The mechanism includes 83 variable species and represents atmospheric chemistry processes including:

- Photolysis reactions
- Gas-phase radical reactions
- Volatile organic compound (VOC) oxidation
- Nitrogen oxide chemistry
- Sulfur chemistry
- Aerosol precursor formation

2 Chemical Species

2.1 Variable Species

The mechanism includes 83 variable chemical species that are transported and undergo chemical transformations. These species are defined with the IGNORE flag, indicating they are calculated by the chemical solver.

Species	**Description**	**Category**
O3	Ozone	Oxidant
O	Atomic oxygen	Radical
O1D_CB4	Excited oxygen atom O(^{1}D)	Radical
N2O	Nitrous oxide	Nitrogen oxide
NO	Nitric oxide	Nitrogen oxide
NO2	Nitrogen dioxide	Nitrogen oxide
NO3	Nitrate radical	Nitrogen oxide
NH3	Ammonia	Nitrogen compound
HNO3	Nitric acid	Nitrogen oxide
HO2NO2	Peroxynitric acid	Nitrogen oxide
N2O5	Dinitrogen pentoxide	Nitrogen oxide
H2	Hydrogen	Inorganic
OH	Hydroxyl radical	Radical
HO2	Hydroperoxyl radical	Radical
H2O2	Hydrogen peroxide	Peroxide
CH4	Methane	Hydrocarbon
CO	Carbon monoxide	Carbon oxide
CH3O2	Methyl peroxy radical	Peroxy radical
CH3OOH	Methyl hydroperoxide	Peroxide

Species	Description	Category
CH2O	Formaldehyde	Aldehyde
CH3OH	Methanol	Alcohol
C2H4	Ethene	Alkene
EO	Ethoxy radical	Radical
EO2	Ethylperoxy radical	Peroxy radical
CH3CHO	Acetaldehyde	Aldehyde
CH3COOH	Acetic acid	Organic acid
CH3COCH3	Acetone	Ketone
CH3COCHO	Methylglyoxal	Dicarbonyl
CH3CO3	Acetyl peroxy radical	Peroxy radical
CH3COOOH	Peracetic acid	Peroxide
GLYOXAL	Glyoxal	Dicarbonyl
PO2	Propylperoxy radical	Peroxy radical
POOH	Propyl hydroperoxide	Peroxide
PAN	Peroxyacetyl nitrate	Organic nitrate
MPAN	Methacryloyl peroxynitrate	Organic nitrate
MCO3	Methacryloyl peroxy radical	Peroxy radical
MACR	Methacrolein	Aldehyde
MACRO2	Methacrolein peroxy radical	Peroxy radical
MACROOH	Methacrolein hydroperoxide	Peroxide
MVK	Methyl vinyl ketone	Ketone
C2H6	Ethane	Alkane
C3H6	Propene	Alkene
C3H8	Propane	Alkane
C2H5OH	Ethanol	Alcohol
C2H5OOH	Ethyl hydroperoxide	Peroxide
C3H7O2	Propyl peroxy radical	Peroxy radical
C3H7OOH	Propyl hydroperoxide	Peroxide
C10H16	α-Pinene (monoterpene)	Biogenic VOC
RO2	Generic peroxy radical	Peroxy radical
ROOH	Generic hydroperoxide	Peroxide
ONIT	Organic nitrate	Organic nitrate
ONITR	Alkyl nitrate	Organic nitrate
ISOP	Isoprene	Biogenic VOC
ISOPO2	Isoprene peroxy radical	Peroxy radical
ISOPOOH	Isoprene hydroperoxide	Peroxide
ISOPNO3	Isoprene nitrate	Organic nitrate
HYAC	Hydroxyacetone	Ketone
GLYALD	Glycolaldehyde	Aldehyde
HYDRALD	Hydroxyaldehyde	Aldehyde
ENEO2	Lumped alkene peroxy radical	Peroxy radical
MEK	Butanone (methyl ethyl ketone)	Ketone
MEKO2	Butanone peroxy radical	Peroxy radical
C2H5O2	Ethyl peroxy radical	Peroxy radical
BIGENE	Lumped alkenes	Alkene
BIGALD	Lumped aldehydes	Aldehyde
BIGALK	Lumped alkanes	Alkane

Species	Description	Category
ALKO2	Alkane peroxy radical	Peroxy radical
ALKOOH	Alkane hydroperoxide	Peroxide
MEKOOH	Butanone hydroperoxide	Peroxide
TOLUENE	Toluene	Aromatic
TOLO2	Toluene peroxy radical	Peroxy radical
TOLOOH	Toluene hydroperoxide	Peroxide
TERPO2	Monoterpene peroxy radical	Peroxy radical
TERPOOH	Monoterpene hydroperoxide	Peroxide
CRESOL	Cresol	Aromatic
DMS	Dimethyl sulfide	Sulfur compound
SO2	Sulfur dioxide	Sulfur compound
SO4	Sulfate	Sulfur compound
XO2	Generic peroxy radical	Peroxy radical
XOH	Generic hydroxyl compound	Radical
XOOH	Generic hydroperoxide	Peroxide

2.2 Fixed Species

The mechanism includes two fixed species that are held constant:

- **H2O**: Water vapor - concentration determined by meteorological conditions
- **M**: Total air density - represents third-body collisions in pressure-dependent reactions

3 Chemical Reactions

The MOZCART mechanism consists of 197 chemical reactions divided into two main categories:

3.1 Photolysis Reactions (J01-J38)

Photolysis reactions represent the breakdown of molecules by solar radiation. These reactions are typically first-order with rate constants that depend on solar zenith angle, overhead ozone column, and atmospheric conditions.

Key photolysis processes include:

3.1.1 Inorganic Photolysis

- O2 photolysis: $O2 + h\nu \rightarrow O + O$
- Ozone photolysis: $O3 + h\nu \rightarrow O(^1D) + O2$ or $O + O2$
- NO2 photolysis: $NO2 + h\nu \rightarrow O + NO$
- N2O5 photolysis: $N2O5 + h\nu \rightarrow NO2 + NO3$

3.1.2 Organic Photolysis

- Formaldehyde: CH2O + hν → HO2 + HO2 + CO or CO + H2
- Acetaldehyde: CH3CHO + hν → CH3O2 + CO + HO2
- Peroxides: ROOH + hν → RO + OH
- PAN: PAN + hν → CH3CO3 + NO2 (branching ratios apply)

3.2 Gas-Phase Reactions (001-157)

Gas-phase reactions include bimolecular and termolecular reactions with temperature and pressure dependencies.

3.2.1 Oxygen Chemistry

Key reactions controlling ozone formation and destruction:

$$\mathrm{O + O2 + M \rightarrow O3 + M} \quad (1)$$
$$\mathrm{O + O3 \rightarrow 2O2} \quad (2)$$
$$\mathrm{O(^1D) + M \rightarrow O + M} \quad (3)$$
$$\mathrm{O(^1D) + H2O \rightarrow 2OH} \quad (4)$$

3.2.2 HOx Chemistry

Reactions involving OH and HO2 radicals:

$$\mathrm{OH + CO \rightarrow HO2 + CO2} \quad (5)$$
$$\mathrm{HO2 + HO2 \rightarrow H2O2 + O2} \quad (6)$$
$$\mathrm{OH + HO2 \rightarrow H2O + O2} \quad (7)$$
$$\mathrm{H2O2 + OH \rightarrow HO2 + H2O} \quad (8)$$

3.2.3 NOx Chemistry

Nitrogen oxide reactions:

$$\mathrm{NO + HO2 \rightarrow NO2 + OH} \quad (9)$$
$$\mathrm{NO + O3 \rightarrow NO2 + O2} \quad (10)$$
$$\mathrm{NO2 + OH + M \rightarrow HNO3 + M} \quad (11)$$
$$\mathrm{NO2 + NO3 + M \rightarrow N2O5 + M} \quad (12)$$

3.2.4 Hydrocarbon Oxidation

Methane and higher hydrocarbons:

$$\mathrm{CH4 + OH \rightarrow CH3O2 + H2O} \quad (13)$$
$$\mathrm{CH3O2 + NO \rightarrow CH2O + NO2 + HO2} \quad (14)$$
$$\mathrm{C2H4 + OH + M \rightarrow EO2 + M} \quad (15)$$
$$\mathrm{ISOP + OH \rightarrow ISOPO2} \quad (16)$$

4 Rate Expressions

The mechanism uses several types of rate expressions:

4.1 Arrhenius Rate Constants

Simple temperature-dependent rate constants:

$$k(T) = A \exp\left(-\frac{E_a}{RT}\right) \tag{17}$$

Implemented as `ARR2(A, Ea, TEMP)` where E_a is in Kelvin.

4.2 Pressure-Dependent Reactions

Three-body reactions using Troe formalism:

$$k(T, M) = \frac{k_0[M]}{1 + k_0[M]/k_\infty} F_c^{\left(1+[\log_{10}(k_0[M]/k_\infty)]^2\right)^{-1}} \tag{18}$$

Implemented as `TROE(k0_300K, n, kinf_300K, m, TEMP, C_M)`.

4.3 User-Defined Functions

Several complex reactions use custom rate functions:

- **usr5**: OH + HNO3 reaction with complex pressure dependence
- **usr8**: CO + OH reaction with water vapor enhancement
- **usr9**: HO2 + HO2 reaction with water vapor catalysis
- **usr23**: SO2 + OH reaction using updated parameterization
- **usr24**: DMS + OH reaction with branching ratios

5 Ozone Chemistry and Formation Mechanisms

Ozone (O3) is a central species in tropospheric chemistry, serving both as an important greenhouse gas and air quality indicator. The MOZCART mechanism includes comprehensive treatment of ozone formation and destruction pathways through both inorganic and organic reaction chains.

5.1 Fundamental Ozone Reactions

5.1.1 Ozone Formation

The primary mechanism for tropospheric ozone formation involves the photochemical oxidation of volatile organic compounds (VOCs) in the presence of nitrogen oxides (NOx). The key reactions include:

Chapman Cycle:

$$\mathrm{O2} + \mathrm{h}\nu\ (\lambda < 242\ \mathrm{nm}) \rightarrow \mathrm{O} + \mathrm{O} \quad \text{(J01)} \tag{19}$$
$$\mathrm{O} + \mathrm{O2} + \mathrm{M} \rightarrow \mathrm{O3} + \mathrm{M} \quad \text{(001)} \tag{20}$$
$$\mathrm{O3} + \mathrm{h}\nu \rightarrow \mathrm{O}(^1\mathrm{D}) + \mathrm{O2} \quad \text{(J02)} \tag{21}$$
$$\mathrm{O3} + \mathrm{h}\nu \rightarrow \mathrm{O}(^3\mathrm{P}) + \mathrm{O2} \quad \text{(J03)} \tag{22}$$

Catalytic Ozone Production: The net production of ozone occurs through VOC oxidation in the presence of NOx:

$$\mathrm{VOC} + \mathrm{OH} \rightarrow \mathrm{RO2} + \mathrm{H2O} \tag{23}$$
$$\mathrm{RO2} + \mathrm{NO} \rightarrow \mathrm{RO} + \mathrm{NO2} \tag{24}$$
$$\mathrm{RO} + \mathrm{O2} \rightarrow \mathrm{RCHO} + \mathrm{HO2} \tag{25}$$
$$\mathrm{HO2} + \mathrm{NO} \rightarrow \mathrm{OH} + \mathrm{NO2} \tag{26}$$
$$2(\mathrm{NO2} + \mathrm{h}\nu) \rightarrow 2(\mathrm{NO} + \mathrm{O}) \tag{27}$$
$$2(\mathrm{O} + \mathrm{O2} + \mathrm{M}) \rightarrow 2(\mathrm{O3} + \mathrm{M}) \tag{28}$$

Net reaction: $\mathrm{VOC} + 4\mathrm{O2} + 2\mathrm{h}\nu \rightarrow \mathrm{RCHO} + \mathrm{H2O} + 2\mathrm{O3}$

5.1.2 Ozone Destruction

Ozone destruction occurs through several pathways:

Direct photolysis and O(^{1}D) reactions:

$$\mathrm{O3} + \mathrm{h}\nu \rightarrow \mathrm{O}(^1\mathrm{D}) + \mathrm{O2} \quad \text{(J02)} \tag{29}$$
$$\mathrm{O}(^1\mathrm{D}) + \mathrm{H2O} \rightarrow 2\mathrm{OH} \quad \text{(004)} \tag{30}$$
$$\mathrm{O}(^1\mathrm{D}) + \mathrm{M} \rightarrow \mathrm{O}(^3\mathrm{P}) + \mathrm{M} \quad \text{(003)} \tag{31}$$

Reaction with radicals:

$$\mathrm{O3} + \mathrm{OH} \rightarrow \mathrm{HO2} + \mathrm{O2} \quad \text{(009)} \tag{32}$$
$$\mathrm{O3} + \mathrm{HO2} \rightarrow \mathrm{OH} + 2\mathrm{O2} \quad \text{(010)} \tag{33}$$
$$\mathrm{O3} + \mathrm{NO} \rightarrow \mathrm{NO2} + \mathrm{O2} \quad \text{(019)} \tag{34}$$

Reaction with alkenes (ozonolysis):

$$\mathrm{O3} + \mathrm{C2H4} \rightarrow \mathrm{CH2O} + \text{products} \quad \text{(044)} \tag{35}$$
$$\mathrm{O3} + \mathrm{C3H6} \rightarrow \mathrm{CH2O} + \mathrm{CH3CHO} + \text{products} \quad \text{(056)} \tag{36}$$
$$\mathrm{O3} + \mathrm{ISOP} \rightarrow \mathrm{MACR} + \mathrm{MVK} + \text{products} \quad \text{(098)} \tag{37}$$

5.2 Detailed VOC Oxidation Pathways

Volatile organic compound oxidation is the primary driver of tropospheric ozone formation. The MOZCART mechanism includes detailed treatment of various VOC classes.

5.2.1 Alkane Oxidation

Methane Oxidation: Methane (CH4) is the most abundant hydrocarbon in the atmosphere:

$$\mathrm{CH4 + OH \rightarrow CH3O2 + H2O} \quad (034) \tag{38}$$

$$\mathrm{CH4 + O(^1D) \rightarrow 0.75\ CH3O2 + 0.75\ OH + products} \quad (035) \tag{39}$$

$$\mathrm{CH3O2 + NO \rightarrow CH2O + NO2 + HO2} \quad (036) \tag{40}$$

$$\mathrm{CH3O2 + HO2 \rightarrow CH3OOH + O2} \quad (038) \tag{41}$$

The methyl peroxy radical (CH3O2) can also undergo self-reaction:

$$\mathrm{CH3O2 + CH3O2 \rightarrow 2CH2O + 2HO2} \quad (036) \tag{42}$$

$$\mathrm{CH3O2 + CH3O2 \rightarrow CH2O + CH3OH} \quad (037) \tag{43}$$

Ethane Oxidation:

$$\mathrm{C2H6 + OH \rightarrow C2H5O2 + H2O} \quad (050) \tag{44}$$

$$\mathrm{C2H5O2 + NO \rightarrow CH3CHO + HO2 + NO2} \quad (051) \tag{45}$$

$$\mathrm{C2H5O2 + HO2 \rightarrow C2H5OOH + O2} \quad (052) \tag{46}$$

Propane Oxidation:

$$\mathrm{C3H8 + OH \rightarrow C3H7O2 + H2O} \quad (070) \tag{47}$$

$$\mathrm{C3H7O2 + NO \rightarrow 0.82\ CH3COCH3 + 0.27\ CH3CHO + NO2 + HO2} \quad (071) \tag{48}$$

Higher Alkanes (BIGALK): Large alkanes are represented by the lumped species BIGALK:

$$\mathrm{BIGALK + OH \rightarrow ALKO2} \quad (083) \tag{49}$$

$$\mathrm{ALKO2 + NO \rightarrow products + NO2 + HO2} \quad (084) \tag{50}$$

5.2.2 Alkene Oxidation

Ethene Oxidation:

$$\mathrm{C2H4 + OH + M \rightarrow EO2 + M} \quad (043) \tag{51}$$

$$\mathrm{C2H4 + O3 \rightarrow CH2O + products} \quad (044) \tag{52}$$

$$\mathrm{EO2 + NO \rightarrow EO + NO2} \quad (047) \tag{53}$$

$$\mathrm{EO \rightarrow 2CH2O + HO2} \quad (049) \tag{54}$$

Propene Oxidation:

$$\mathrm{C3H6 + OH + M \rightarrow PO2 + M} \quad (055) \tag{55}$$

$$\mathrm{C3H6 + O3 \rightarrow products} \quad (056) \tag{56}$$

$$\mathrm{C3H6 + NO3 \rightarrow ONIT} \quad (057) \tag{57}$$

$$\mathrm{PO2 + NO \rightarrow CH3CHO + CH2O + HO2 + NO2} \quad (058) \tag{58}$$

Lumped Alkenes (BIGENE):

$$\mathrm{BIGENE + OH \rightarrow ENEO2} \quad (080) \tag{59}$$

$$\mathrm{ENEO2 + NO \rightarrow products + NO2 + HO2} \quad (081) \tag{60}$$

5.2.3 Aromatic VOC Oxidation

Toluene Oxidation: Aromatic compounds undergo complex oxidation forming both ring-opening and ring-retaining products:

$$\text{TOLUENE} + \text{OH} \rightarrow 0.25\ \text{CRESOL} + 0.25\ \text{HO2} + 0.7\ \text{TOLO2} \quad (091) \tag{61}$$

$$\text{TOLO2} + \text{NO} \rightarrow 0.45\ \text{GLYOXAL} + 0.45\ \text{CH3COCHO} + 0.9\ \text{BIGALD} + \text{products} \quad (094) \tag{62}$$

$$\text{CRESOL} + \text{OH} \rightarrow \text{XOH} \quad (092) \tag{63}$$

$$\text{XOH} + \text{NO2} \rightarrow 0.7\ \text{NO2} + 0.7\ \text{BIGALD} + 0.7\ \text{HO2} \quad (093) \tag{64}$$

5.2.4 Biogenic VOC Oxidation

Isoprene Oxidation: Isoprene (C5H8) is the most abundant non-methane biogenic VOC:

OH-initiated oxidation:

$$\text{ISOP} + \text{OH} \rightarrow \text{ISOPO2} \quad (097) \tag{65}$$

$$\text{ISOPO2} + \text{NO} \rightarrow 0.08\ \text{ONITR} + 0.92\ \text{NO2} + \text{products} \quad (099) \tag{66}$$

$$\text{ISOPO2} + \text{HO2} \rightarrow \text{ISOPOOH} \quad (101) \tag{67}$$

$$\text{ISOPOOH} + \text{OH} \rightarrow 0.5\ \text{XO2} + 0.5\ \text{ISOPO2} \quad (102) \tag{68}$$

Ozonolysis:

$$\text{ISOP} + \text{O3} \rightarrow 0.4\ \text{MACR} + 0.2\ \text{MVK} + \text{products} \quad (098) \tag{69}$$

NO3-initiated oxidation:

$$\text{ISOP} + \text{NO3} \rightarrow \text{ISOPNO3} \quad (130) \tag{70}$$

$$\text{ISOPNO3} + \text{NO} \rightarrow \text{products} + \text{ONITR} \quad (131) \tag{71}$$

Monoterpene Oxidation: Monoterpenes (C10H16) represent larger biogenic VOCs:

$$\text{C10H16} + \text{OH} \rightarrow \text{TERPO2} \quad (123) \tag{72}$$

$$\text{C10H16} + \text{O3} \rightarrow 0.7\ \text{OH} + \text{MVK} + \text{MACR} + \text{HO2} \quad (124) \tag{73}$$

$$\text{C10H16} + \text{NO3} \rightarrow \text{TERPO2} + \text{NO2} \quad (125) \tag{74}$$

$$\text{TERPO2} + \text{NO} \rightarrow \text{products} + \text{NO2} \quad (126) \tag{75}$$

5.2.5 Oxidation of Secondary Products

Formaldehyde (CH2O): Formaldehyde is a key intermediate in VOC oxidation:

$$\text{CH2O} + \text{OH} \rightarrow \text{CO} + \text{HO2} + \text{H2O} \quad (041) \tag{76}$$

$$\text{CH2O} + \text{NO3} \rightarrow \text{CO} + \text{HO2} + \text{HNO3} \quad (040) \tag{77}$$

$$\text{CH2O} + \text{h}\nu \rightarrow \text{HO2} + \text{HO2} + \text{CO} \quad (J12) \tag{78}$$

$$\text{CH2O} + \text{h}\nu \rightarrow \text{CO} + \text{H2} \quad (J13) \tag{79}$$

Acetaldehyde (CH3CHO):

$$\text{CH3CHO} + \text{OH} \rightarrow \text{CH3CO3} + \text{H2O} \quad (061) \tag{80}$$
$$\text{CH3CHO} + \text{NO3} \rightarrow \text{CH3CO3} + \text{HNO3} \quad (062) \tag{81}$$
$$\text{CH3CHO} + \text{h}\nu \rightarrow \text{CH3O2} + \text{CO} + \text{HO2} \quad (\text{J15}) \tag{82}$$

Acetone (CH3COCH3):

$$\text{CH3COCH3} + \text{OH} \rightarrow \text{RO2} + \text{H2O} \quad (075) \tag{83}$$
$$\text{CH3COCH3} + \text{h}\nu \rightarrow \text{CH3CO3} + \text{CH3O2} \quad (\text{J25}) \tag{84}$$

5.3 PAN Chemistry

Peroxyacetyl nitrate (PAN) and related compounds serve as temporary reservoirs for NOx and play crucial roles in ozone formation:

PAN Formation and Destruction:

$$\text{CH3CO3} + \text{NO2} + \text{M} \rightarrow \text{PAN} + \text{M} \quad (064) \tag{85}$$
$$\text{PAN} + \text{M} \rightarrow \text{CH3CO3} + \text{NO2} + \text{M} \quad (068) \tag{86}$$
$$\text{PAN} + \text{OH} \rightarrow \text{CH2O} + \text{NO3} + \text{CO2} \quad (149) \tag{87}$$
$$\text{PAN} + \text{h}\nu \rightarrow 0.6\ \text{CH3CO3} + 0.6\ \text{NO2} + \text{products} \quad (\text{J18}) \tag{88}$$

MPAN (Methacryloyl PAN):

$$\text{MCO3} + \text{NO2} + \text{M} \rightarrow \text{MPAN} + \text{M} \quad (121) \tag{89}$$
$$\text{MPAN} + \text{M} \rightarrow \text{MCO3} + \text{NO2} + \text{M} \quad (122) \tag{90}$$
$$\text{MPAN} + \text{OH} \rightarrow \text{products} \quad (148) \tag{91}$$

5.4 Ozone Production Efficiency

The ozone production efficiency depends on the VOC/NOx ratio and the reactivity of the VOC mixture. Different VOC classes contribute differently to ozone formation:

- **High reactivity**: Alkenes (C2H4, C3H6), isoprene, monoterpenes
- **Medium reactivity**: Aromatics (toluene), aldehydes (CH3CHO)
- **Low reactivity**: Alkanes (CH4, C2H6), alcohols (CH3OH)

The mechanism captures the nonlinear relationship between VOC emissions, NOx concentrations, and ozone formation, enabling accurate simulation of ozone sensitivity regimes in different atmospheric conditions.

6 Special Features

6.1 Heterogeneous Chemistry

The mechanism includes several heterogeneous reactions that occur on aerosol surfaces:

- N2O5 hydrolysis: N2O5 → 2HNO3
- NO3 uptake: NO3 → HNO3
- HO2 uptake: HO2 → 0.5H2O2

These reactions use humidity and temperature-dependent rate coefficients.

6.2 Isoprene Chemistry

Detailed treatment of isoprene (C5H8) oxidation includes:

- OH-initiated oxidation forming ISOPO2
- Ozonolysis reactions
- Formation of methacrolein (MACR) and methyl vinyl ketone (MVK)
- Secondary oxidation products

6.3 Aromatic Chemistry

Simplified treatment of aromatic compounds:

- Toluene oxidation by OH
- Formation of cresol and peroxy radicals
- Fragmentation to smaller carbonyls

7 Implementation Notes

7.1 Fortran 90 Implementation

The mechanism is implemented with Fortran 90 functions for complex rate calculations. Custom functions handle:

- JPL Troe formalism for pressure dependence
- User-defined rate expressions
- Temperature and pressure scaling

7.2 Photolysis Rates

Photolysis rates are calculated externally and passed to the mechanism through the TUV (Tropospheric Ultraviolet-Visible) radiative transfer model. The mapping file `mozcart.tuv.jmap` connects KPP photolysis labels to TUV reaction numbers.

7.3 Integration with WRF-Chem

The mechanism is designed for use within the WRF-Chem modeling system with:

- Species mapping through `mozcart_wrfkpp.equiv`
- Consistent units and conventions
- Optimized for computational efficiency

8 Summary

The MOZCART chemical mechanism provides a comprehensive treatment of tropospheric gas-phase chemistry suitable for regional and global atmospheric modeling. With 83 species and 197 reactions, it captures the essential processes controlling:

- Ozone formation and destruction
- Radical cycling (HOx, NOx)
- Volatile organic compound oxidation
- Secondary organic aerosol precursors
- Sulfur chemistry

The mechanism balances chemical detail with computational efficiency, making it suitable for multi-dimensional atmospheric chemistry transport models.

9 References

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