Project Report

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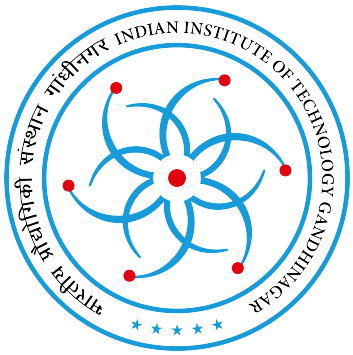

EH 611

Modelling of of Earth System and Sustainability
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Modelling of Photochemical Smog

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Abstract

Photochemical smog forms through complex interactions between nitrogen oxides (NO_x), volatile organic compounds (VOCs), and sunlight. In this project, I discuss two mathematical models of increasing complexity: Model 1 captures the basic NO-NO_2-O_3 photochemical cycle with 4 species and 5 reactions, while Model 2 extends to 11 species and 15 reactions, incorporating VOC oxidation and radical chemistry. Solving the equations numerically, it is demonstrates that Model 1 produces minimal ozone ($\sim 2 \times 10^{-3}$ ppb peak) due to rapid titration by NO, while Model 2 achieves realistic ozone levels (order of $\sim$0.1$\times$ ppm) through radical-mediated NO oxidation pathways. The enhancement factor highlights the critical role of VOCs and radicals in urban photochemical smog formation. Several studies from 80s have beautifully produced models for the same involving a large number of species [Bazzell and Peters(1981), McRae et al.(1982), Falls et al.(1979)]. The chapter *"Modelling of Photochemical Smog"* from the book "Environment Modelling and Pollution" [Duc et al.(2002)] aims to lump various species into a 7-reaction Generic Reaction Set (GRS); although their model is interpretable and easy to follow, I could not fetch parametric values for their system (this is briefly touched upon in the Appendix). Finally, I resorted to a detailed study by [Carrasco-Venegas et al.(2025)] that provided me with all the required reactions and parameters. Code is available at `https://github.com/guntas-13/modelling-photochemical-smog.git`.

Introduction

Photochemical smog, first documented in Los Angeles in the 1940s, remains a persistent urban air quality challenge. Unlike traditional industrial smog, photochemical smog arises from sunlight-driven reactions involving:

- **Primary pollutants:** NO_x (from combustion), VOCs (from vehicles, solvents)
- **Solar radiation:** Provides photochemical energy
- **Secondary pollutants:** Ozone (O_3), aldehydes, PAN

Ground-level ozone concentrations exceeding 0.07 ppm cause respiratory problems, crop damage, and ecosystem degradation.

Objectives

Develops two models, state the variables, describe chemical equations between them, using conservation of mass and rate law, formulate in ODE and solve numerically:

1. **Model 1:**
   (a) Simple 3-species photochemical cycle (NO, NO_2, O_3)
   (b) A bit refined 4-species photochemical cycle (NO, NO_2, O_3, O)
2. **Model 2:** Refined 11-species system with VOCs and radicals

Model 1: Basic Photochemical Cycle

3-species Model

Model 1 captures the fundamental NO-NO_2-O_3 photochemical cycle with three species and three reactions:

$$NO_2 + h\nu \xrightarrow{k_1} NO + O_3 \tag{1}$$

$$NO + O_3 \xrightarrow{k_3} NO_2 + O_2 \tag{2}$$

Reaction (1) is photochemical (requires sunlight with rate constant k_1), while reaction (2) occurs day and night (rate constant k_3). These reactions form a cycle that interconverts NO and NO_2 but *cannot produce net ozone*-a key limitation we'll address in Model 2.

Mathematical Formulation

General Mass Balance Equation

For a well-mixed box (closed system, uniform concentration):

$$\frac{dC_i}{dt} = r_i + E_i \tag{3}$$

The reaction rate r_i is the algebraic sum of production and consumption terms from all reactions involving species i:

$$r_i = \sum_{j=1}^{N_{\text{rxn}}} \nu_{ij} R_j \tag{4}$$

where:

- ν_{ij} = stoichiometric coefficient of species i in reaction j (positive for products, negative for reactants)
- R_j = rate of reaction j (ppm/h)
- N_{rxn} = total number of reactions

Applying mass conservation with emission sources:

$$\frac{d[\text{NO}]}{dt} = k_1[\text{NO}_2] - k_3[\text{NO}][\text{O}_3] + E_{\text{NO}} \tag{5}$$

$$\frac{d[\text{NO}_2]}{dt} = -k_1[\text{NO}_2] + k_3[\text{NO}][\text{O}_3] + E_{\text{NO}_2} \tag{6}$$

$$\frac{d[\text{O}_3]}{dt} = k_1[\text{NO}_2] - k_3[\text{NO}][\text{O}_3] \tag{7}$$

4-species Model

Reaction Mechanism

Model 1 captures the fundamental NO-NO_2-O_3 triad plus atomic oxygen:

$$\text{NO}_2 + h\nu \xrightarrow{k_1} \text{NO} + \text{O}(^3\text{P}) \tag{8}$$

$$\text{O}(^3\text{P}) + \text{O}_2 + M \xrightarrow{k_2} \text{O}_3 + M \tag{9}$$

$$\text{O}_3 + \text{NO} \xrightarrow{k_3} \text{NO}_2 + \text{O}_2 \tag{10}$$

$$\text{NO}_2 + \text{O}(^3\text{P}) \xrightarrow{k_4} \text{NO} + \text{O}_2 \tag{11}$$

$$\text{NO} + \text{O}(^3\text{P}) \xrightarrow{k_5} \text{NO}_2 \tag{12}$$

where M represents air as a third body in the termolecular reaction (9).

- Reaction (8): NO_2 photolysis produces atomic oxygen (photochemical, daytime only)
- Reaction (10): NO immediately reacts with O_3, **preventing accumulation**
- Reactions (11)-(12): Additional O-NO_x interactions

Mathematical Formulation

Applying species mass balance with emission sources:

$$\frac{d[\mathrm{NO}]}{dt} = R_1 - R_3 + R_4 - R_5 + E_{\mathrm{NO}} \tag{13}$$

$$\frac{d[\mathrm{NO_2}]}{dt} = -R_1 + R_3 - R_4 + R_5 + E_{\mathrm{NO_2}} \tag{14}$$

$$\frac{d[\mathrm{O_3}]}{dt} = R_2 - R_3 \tag{15}$$

$$\frac{d[\mathrm{O}]}{dt} = R_1 - R_2 - R_4 - R_5 \tag{16}$$

where reaction rates are:

$$R_1 = k_1(t)[\mathrm{NO_2}] \tag{17}$$

$$R_2 = k_2[\mathrm{O}][\mathrm{O_2}]M \tag{18}$$

$$R_3 = k_3[\mathrm{O_3}][\mathrm{NO}] \tag{19}$$

$$R_4 = k_4[\mathrm{NO_2}][\mathrm{O}] \tag{20}$$

$$R_5 = k_5[\mathrm{NO}][\mathrm{O}] \tag{21}$$

The photolysis rate $\mathrm{k_1(t)}$ varies diurnally:

$$k_1(t) = \begin{cases} k_{1,\max} \sin\left(\frac{\pi(t_{\mathrm{clock}}-6)}{12}\right) & \text{if } 6 \le t_{\mathrm{clock}} \le 18 \\ 0 & \text{otherwise} \end{cases} \tag{22}$$

Parameters and Initial Conditions

Table 1: Model 1 parameters at T = 288 K [Carrasco-Venegas et al.(2025)]

Parameter	Value	Units
$k_{1,\max}$	30.48	$\mathrm{h^{-1}}$
k_2	1.44×10^{-3}	$\mathrm{ppm^{-2}\ h^{-1}}$
k_3	1.20×10^{5}	$\mathrm{ppm^{-1}\ h^{-1}}$
k_4	8.04×10^{5}	$\mathrm{ppm^{-1}\ h^{-1}}$
k_5	1.99×10^{5}	$\mathrm{ppm^{-1}\ h^{-1}}$
$[\mathrm{O_2}]$ M	210,000	ppm
E_{NO}	0.02	$\mathrm{ppm\ h^{-1}}$
$E_{\mathrm{NO_2}}$	0.01	$\mathrm{ppm\ h^{-1}}$

Table 2: Model 1 initial conditions (5:00 AM)

Species	Initial Concentration (ppm)
NO	0.100
$\mathrm{NO_2}$	0.050
$\mathrm{O_3}$	0.0
O	0.0

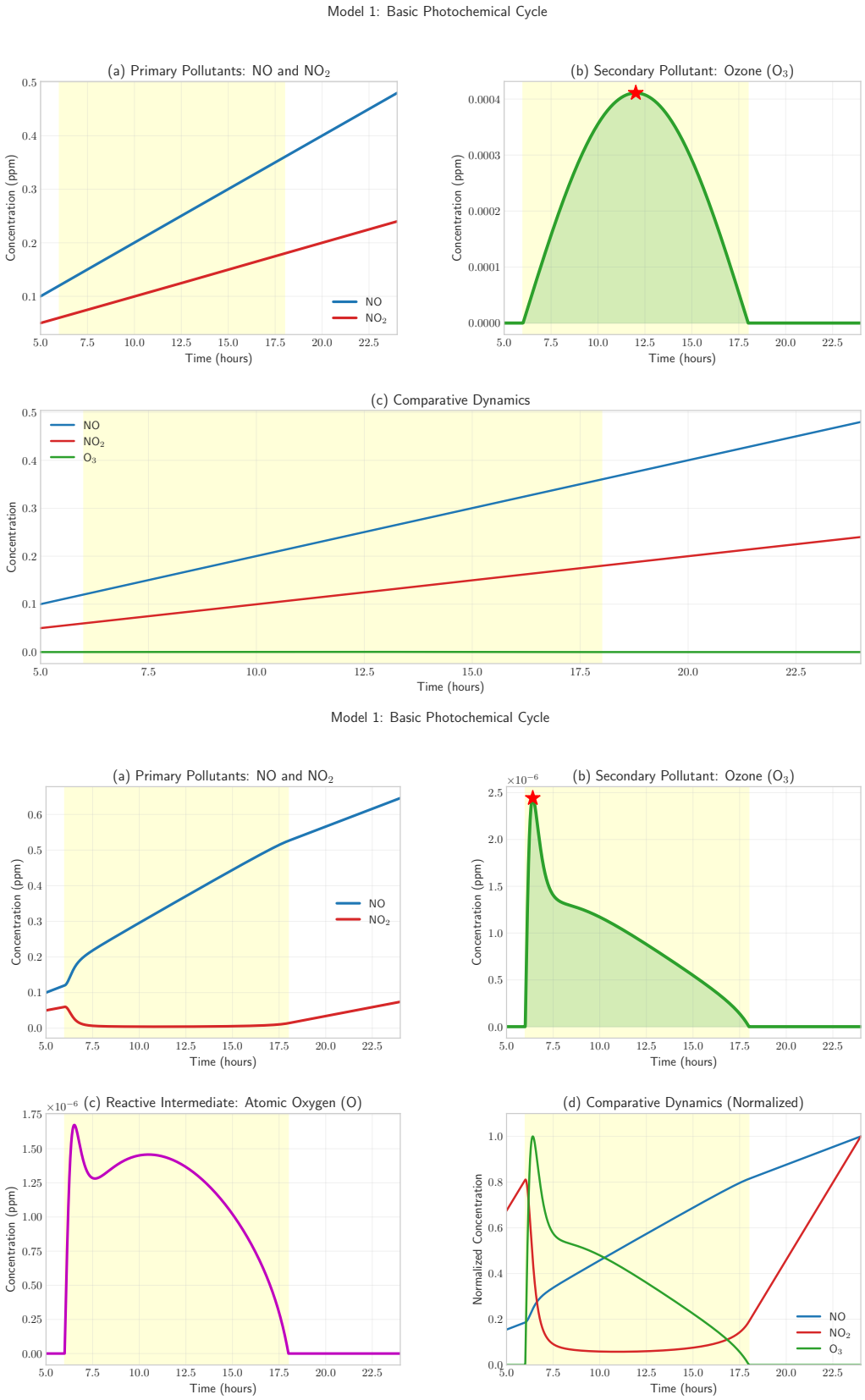

Figure 1: Model 1 (a) 3-species and (b) 4-species concentration profiles from 5:00 AM to midnight. (Top left) NO and NO_2 concentrations. (Top right) Ozone formation with (a) peak ($\sim$ 0.0004 ppm)(b) very low peak ($\sim$0.006 ppb). (b) (Bottom left) Atomic oxygen (scaled) tracking photolysis. (Bottom right) Normalized comparison showing relative dynamics. Yellow shading indicates daylight hours (6:00-18:00).

Key Observations

1. **Minimal ozone production:** Peak O_3 reaches only $\sim$0.003 ppb at 8:00, far below ambient air quality standards (0.07 ppm)
2. **NO-NO_2 concentration:** Unable to show increase-decrease pattern in either - indicating some key species missing in our model.
3. **Atomic oxygen:** Very low steady-state concentration ($\sim 10^{-6}$ ppm) due to fast reaction with O_2 (R_2)

Limitations

- **Unrealistic ozone:** Cannot explain observed urban smog episodes ($O_3 > 0.07$ ppm)
- **Missing VOC chemistry:** No role for hydrocarbons in oxidation
- **No radical pathways:** Lacks OH, HO_2, RO_2 that drive real atmospheric chemistry

The fundamental problem: *there is no mechanism to convert NO to NO_2 without consuming O_3*. This motivates Model 2.

Model 2: Refined System with VOCs

System Extension

Model 2 adds 7 new species to capture VOC oxidation and radical chemistry:

- **CO:** Carbon monoxide (primary pollutant, radical precursor)
- **HCHO:** Formaldehyde (VOC oxidation product, radical source)
- **ALK:** Lumped alkanes (saturated hydrocarbons)
- **OLE:** Lumped olefins (unsaturated hydrocarbons)
- **OH:** Hydroxyl radical (primary atmospheric oxidant)
- **HO_2:** Hydroperoxyl radical
- **RO_2:** Organic peroxy radicals

Total species: 11 (NO, NO_2, O_3, O, CO, HCHO, ALK, OLE, OH, HO_2, RO_2)

Extended Reaction Mechanism

Building on Model 1's 5 reactions, we add 10 more:

$$O_3 + h\nu \xrightarrow{k_4} O(^1D) + O_2 \tag{23}$$

$$O(^1D) + H_2O \xrightarrow{k_5} 2OH \tag{24}$$

$$CO + OH \xrightarrow{k_6} HO_2 + CO_2 \tag{25}$$

$$HCHO + h\nu \xrightarrow{k_7} 2HO_2 + CO \tag{26}$$

$$HCHO + OH \xrightarrow{k_8} HO_2 + CO + H_2O \tag{27}$$

$$ALK + OH \xrightarrow{k_9} RO_2 \tag{28}$$

$$OLE + OH \xrightarrow{k_{10}} RO_2 \tag{29}$$

$$OLE + O_3 \xrightarrow{k_{11}} 0.5HCHO + \text{products} \tag{30}$$

$$HO_2 + NO \xrightarrow{k_{12}} NO_2 + OH \quad \textbf{(Key!)} \tag{31}$$

$$RO_2 + NO \xrightarrow{k_{13}} NO_2 + HO_2 \quad \textbf{(Key!)} \tag{32}$$

$$HO_2 + HO_2 \xrightarrow{k_{14}} H_2O_2 + O_2 \tag{33}$$

$$OH + NO_2 \xrightarrow{k_{15}} HNO_3 \tag{34}$$

Critical breakthrough: Reactions (31) and (32) convert NO to NO_2 *without consuming* O_3! This enables net ozone accumulation.

Parameters

Table 3: Additional rate constants for Model 2 (T = 288 K) [Carrasco-Venegas et al.(2025)]

Reaction	Rate Constant	Units
k_4 (O_3 photolysis)	1.968	h^{-1}
k_5 ($O(^1D) + H_2O$)	6.0×10^6	$ppm^{-1}\ h^{-1}$
k_6 ($CO + OH$)	2.64×10^4	$ppm^{-1}\ h^{-1}$
k_7 (HCHO photolysis)	0.170	h^{-1}
k_8 ($HCHO + OH$)	1.152×10^6	$ppm^{-1}\ h^{-1}$
k_9 ($ALK + OH$)	2.82×10^5	$ppm^{-1}\ h^{-1}$
k_{10} ($OLE + OH$)	5.349×10^6	$ppm^{-1}\ h^{-1}$
k_{11} ($OLE + O_3$)	8.16	$ppm^{-1}\ h^{-1}$
k_{12} ($HO_2 + NO$)	7.2×10^5	$ppm^{-1}\ h^{-1}$
k_{13} ($RO_2 + NO$)	7.2×10^5	$ppm^{-1}\ h^{-1}$
k_{14} ($HO_2 + HO_2$)	2.22×10^5	$ppm^{-1}\ h^{-1}$
k_{15} ($OH + NO_2$)	Complex T-dep.	$ppm^{-1}\ h^{-1}$

Table 4: Model 2 initial conditions and emissions

Species	Initial (ppm)	Emission (ppm h^{-1})
NO	0.100	0.02
NO_2	0.050	0.01
CO	0.100	0.02
HCHO	0.010	0.03
ALK	1.000	0.10
OLE	0.200	0.0
OH	0	0
HO_2	0	0
RO_2	0	0

Results

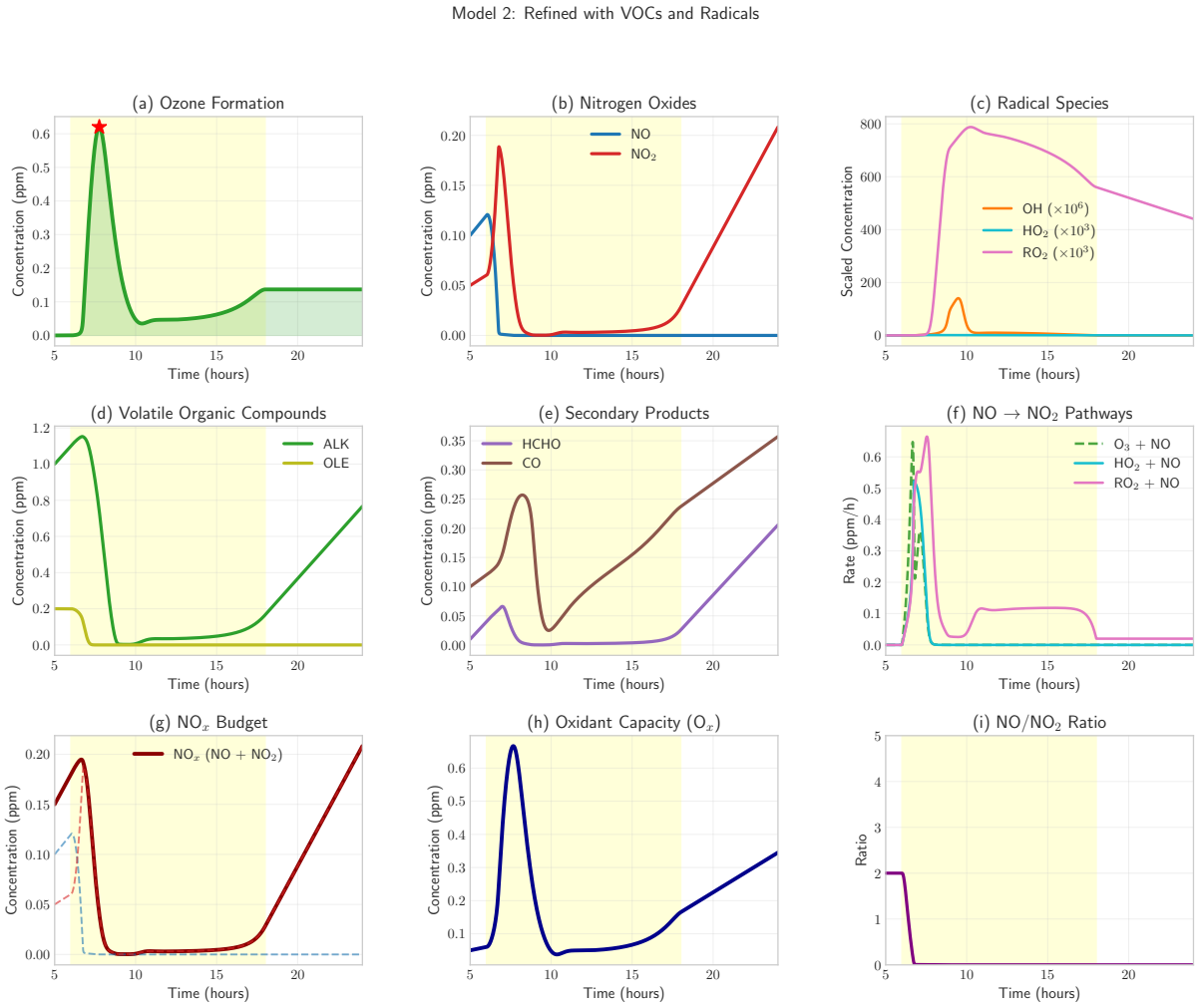

Figure 2: Model 2 comprehensive results. (Top row) Ozone reaches realistic levels (∼0.08 ppm), NO-NO_2 dynamics, and radical species tracking solar radiation. (Middle row) VOC depletion, secondary products (HCHO, CO), and NO→NO_2 conversion pathways. (Bottom row) NO_x budget, oxidant capacity, and NO/NO_2 ratio evolution. Model successfully produces net ozone through radical chemistry.

Key Observations

1. **Realistic ozone:** Peak $O_3 = 0.619979$ ppm at 7:30.
2. **Radical dynamics:** OH, HO_2, RO_2 peak at early hours ($\sim 10^{-6}$ to 10^{-3} ppm), drop to zero at night
3. **VOC consumption:** ALK decreases 23%, OLE decreases 100% (fully depleted), demonstrating active oxidation
4. **Pathway dominance:** At peak O_3, NO→NO_2 conversion is dominated by RO_2 + NO (94.5%), with only HO_2 + NO (2.9%) and 2.6% via O_3 titration
5. **Radical catalysis:** Despite trace OH ($\sim 10^{-6}$ ppm), substantial ozone forms.
6. **NO_x budget:** Total NO_x decreases from 0.15 to 0.08 ppm due to HNO_3 formation (R_{15})
7. **Oxidant capacity:** O_x (O_3 + NO_2) steadily increases, indicating net oxidation

Comparison with Model 1

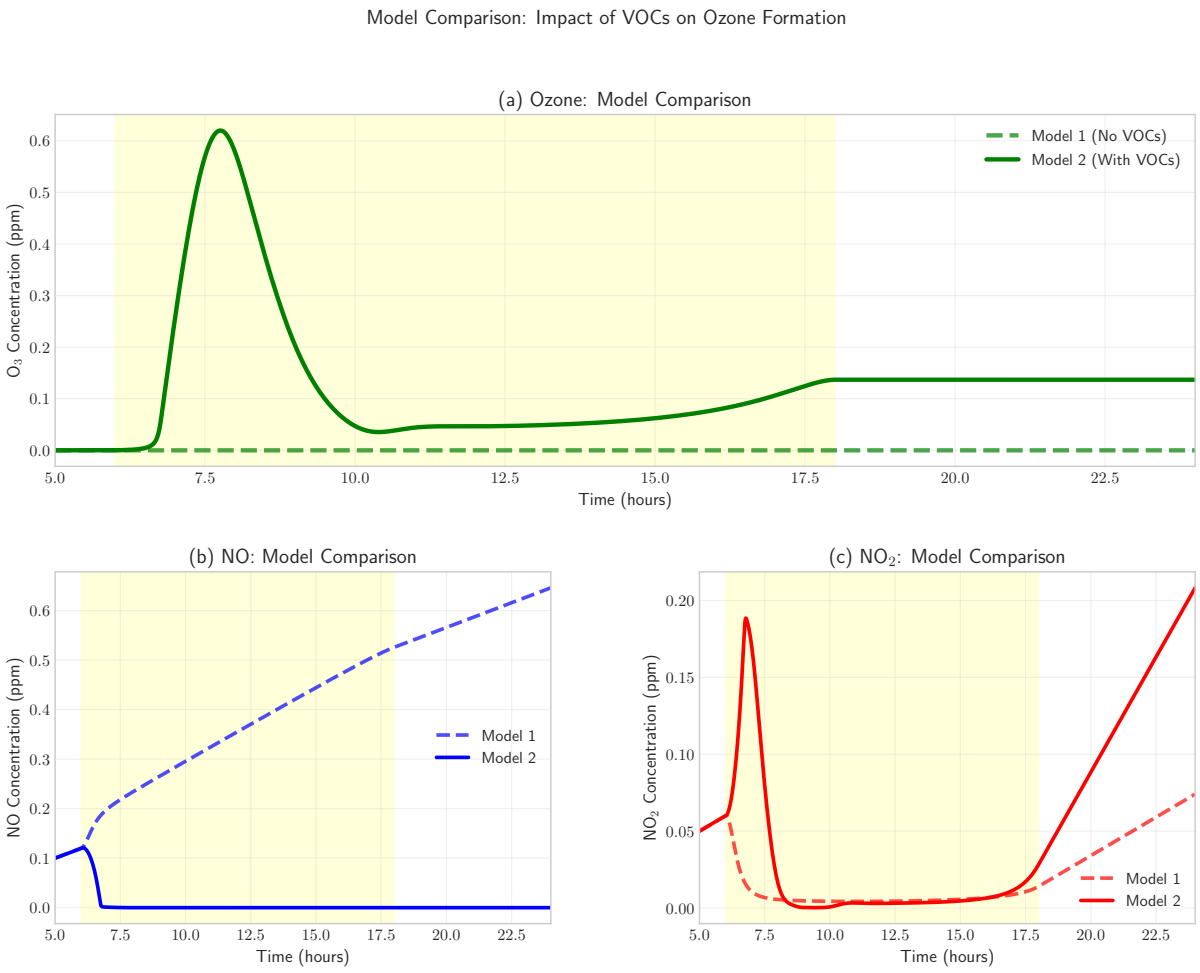

Figure 3: Direct comparison between models. (Top left) Ozone enhancement: Model 2 produces 27Œ more O_3 than Model 1. (Top right) NO depletion is faster in Model 2 due to additional radical pathways. (Bottom left) NO_2 shows more complex dynamics. (Bottom right) O_3 enhancement factor peaks in afternoon when radical chemistry is most active.

Appendix: Mathematical Formulation, GRS ODEs, parameter table

Model 2: Complete Differential Equations

Species Conservation Equations

For Model 2 with 11 species and 15 reactions:

1. **Nitric Oxide (NO):**

$$\begin{aligned}\frac{d[\mathrm{NO}]}{dt} &= R_1 - R_3 - R_{12} - R_{13} + E_{\mathrm{NO}} \\ &= k_1[\mathrm{NO_2}] - k_3[\mathrm{O_3}][\mathrm{NO}] - k_{12}[\mathrm{HO_2}][\mathrm{NO}] \\ &\quad - k_{13}[\mathrm{RO_2}][\mathrm{NO}] + E_{\mathrm{NO}}\end{aligned} \tag{35}$$

2. **Nitrogen Dioxide ($\mathrm{NO_2}$):**

$$\begin{aligned}\frac{d[\mathrm{NO_2}]}{dt} &= -R_1 + R_3 + R_{12} + R_{13} - R_{15} + E_{\mathrm{NO_2}} \\ &= -k_1[\mathrm{NO_2}] + k_3[\mathrm{O_3}][\mathrm{NO}] + k_{12}[\mathrm{HO_2}][\mathrm{NO}] \\ &\quad + k_{13}[\mathrm{RO_2}][\mathrm{NO}] - k_{15}[\mathrm{OH}][\mathrm{NO_2}] + E_{\mathrm{NO_2}}\end{aligned} \tag{36}$$

3. **Ozone ($\mathrm{O_3}$):**

$$\begin{aligned}\frac{d[\mathrm{O_3}]}{dt} &= R_2 - R_3 - R_4 - R_{11} \\ &= k_2[\mathrm{O}][\mathrm{O_2}] - k_3[\mathrm{O_3}][\mathrm{NO}] - k_4[\mathrm{O_3}] - k_{11}[\mathrm{OLE}][\mathrm{O_3}]\end{aligned} \tag{37}$$

4. **Atomic Oxygen (O):**

$$\begin{aligned}\frac{d[\mathrm{O}]}{dt} &= R_1 - R_2 \\ &= k_1[\mathrm{NO_2}] - k_2[\mathrm{O}][\mathrm{O_2}]\end{aligned} \tag{38}$$

5. **Carbon Monoxide (CO):**

$$\begin{aligned}\frac{d[\mathrm{CO}]}{dt} &= -R_6 + R_7 + R_8 + E_{\mathrm{CO}} \\ &= -k_6[\mathrm{CO}][\mathrm{OH}] + k_7[\mathrm{HCHO}] + k_8[\mathrm{HCHO}][\mathrm{OH}] + E_{\mathrm{CO}}\end{aligned} \tag{39}$$

6. **Formaldehyde (HCHO):**

$$\begin{aligned}\frac{d[\mathrm{HCHO}]}{dt} &= 0.5R_{11} - R_7 - R_8 + E_{\mathrm{HCHO}} \\ &= 0.5k_{11}[\mathrm{OLE}][\mathrm{O_3}] - k_7[\mathrm{HCHO}] - k_8[\mathrm{HCHO}][\mathrm{OH}] \\ &\quad + E_{\mathrm{HCHO}}\end{aligned} \tag{40}$$

7. **Alkanes (ALK):**

$$\begin{aligned}\frac{d[\mathrm{ALK}]}{dt} &= -R_9 + E_{\mathrm{ALK}} \\ &= -k_9[\mathrm{ALK}][\mathrm{OH}] + E_{\mathrm{ALK}}\end{aligned} \tag{41}$$

8. Olefins (OLE):

$$\begin{aligned}\frac{d[\text{OLE}]}{dt} &= -R_{10} - R_{11} + E_{\text{OLE}} \\ &= -k_{10}[\text{OLE}][\text{OH}] - k_{11}[\text{OLE}][\text{O}_3] + E_{\text{OLE}}\end{aligned} \tag{42}$$

9. Hydroxyl Radical (OH):

$$\begin{aligned}\frac{d[\text{OH}]}{dt} &= 2R_5 - R_6 - R_8 - R_9 - R_{10} - R_{15} + R_{12} \\ &= 2k_5[\text{O}(^1\text{D})][\text{H}_2\text{O}] - k_6[\text{CO}][\text{OH}] - k_8[\text{HCHO}][\text{OH}] \\ &\quad - k_9[\text{ALK}][\text{OH}] - k_{10}[\text{OLE}][\text{OH}] - k_{15}[\text{OH}][\text{NO}_2] \\ &\quad + k_{12}[\text{HO}_2][\text{NO}]\end{aligned} \tag{43}$$

10. Hydroperoxyl Radical (HO_2):

$$\begin{aligned}\frac{d[\text{HO}_2]}{dt} &= R_6 + 2R_7 + R_8 + 0.5R_{11} + R_{13} - R_{12} - 2R_{14} \\ &= k_6[\text{CO}][\text{OH}] + 2k_7[\text{HCHO}] + k_8[\text{HCHO}][\text{OH}] \\ &\quad + 0.5k_{11}[\text{OLE}][\text{O}_3] + k_{13}[\text{RO}_2][\text{NO}] \\ &\quad - k_{12}[\text{HO}_2][\text{NO}] - 2k_{14}[\text{HO}_2]^2\end{aligned} \tag{44}$$

11. Organic Peroxy Radical (RO_2):

$$\begin{aligned}\frac{d[\text{RO}_2]}{dt} &= R_9 + R_{10} + 0.5R_{11} - R_{13} \\ &= k_9[\text{ALK}][\text{OH}] + k_{10}[\text{OLE}][\text{OH}] + 0.5k_{11}[\text{OLE}][\text{O}_3] \\ &\quad - k_{13}[\text{RO}_2][\text{NO}]\end{aligned} \tag{45}$$

Reaction Rates

The individual reaction rates for Model 2 are:

$$R_1 = k_1(t)[\text{NO}_2] \quad (\text{NO}_2 \text{ photolysis}) \tag{46}$$
$$R_2 = k_2[\text{O}][\text{O}_2] \quad (\text{O}_3 \text{ formation}) \tag{47}$$
$$R_3 = k_3[\text{O}_3][\text{NO}] \quad (\text{NO oxidation by O}_3) \tag{48}$$
$$R_4 = k_4(t)[\text{O}_3] \quad (\text{O}_3 \text{ photolysis}) \tag{49}$$
$$R_5 = k_5[\text{O}(^1\text{D})][\text{H}_2\text{O}] \quad (\text{OH formation}) \tag{50}$$
$$R_6 = k_6[\text{CO}][\text{OH}] \quad (\text{CO oxidation}) \tag{51}$$
$$R_7 = k_7(t)[\text{HCHO}] \quad (\text{HCHO photolysis}) \tag{52}$$
$$R_8 = k_8[\text{HCHO}][\text{OH}] \quad (\text{HCHO oxidation}) \tag{53}$$
$$R_9 = k_9[\text{ALK}][\text{OH}] \quad (\text{Alkane oxidation}) \tag{54}$$
$$R_{10} = k_{10}[\text{OLE}][\text{OH}] \quad (\text{Olefin oxidation by OH}) \tag{55}$$
$$R_{11} = k_{11}[\text{OLE}][\text{O}_3] \quad (\text{Olefin ozonolysis}) \tag{56}$$
$$R_{12} = k_{12}[\text{HO}_2][\text{NO}] \quad \textbf{(Key: NO}\rightarrow\textbf{NO}_2 \textbf{ via HO}_2\textbf{)} \tag{57}$$
$$R_{13} = k_{13}[\text{RO}_2][\text{NO}] \quad \textbf{(Key: NO}\rightarrow\textbf{NO}_2 \textbf{ via RO}_2\textbf{)} \tag{58}$$
$$R_{14} = k_{14}[\text{HO}_2]^2 \quad (\text{HO}_2 \text{ termination}) \tag{59}$$
$$R_{15} = k_{15}[\text{OH}][\text{NO}_2] \quad (\text{HNO}_3 \text{ formation}) \tag{60}$$

Excited State Oxygen (Quasi-Steady-State)

For $O(^1D)$ (excited singlet oxygen), we apply the quasi-steady-state approximation:

$$\frac{d[O(^1D)]}{dt} \approx 0 \tag{61}$$

Production equals consumption:

$$k_4[O_3] = k_5[O(^1D)][H_2O] \tag{62}$$

Solving for $[O(^1D)]$:

$$[O(^1D)] = \frac{k_4[O_3]}{k_5[H_2O]} \tag{63}$$

This concentration is substituted directly into Equation 43.

GRS reaction list (symbolic)

The Generic Reaction Set (GRS) used in [Duc et al.(2002)] (will discuss this during presentation):

$$\begin{aligned}
&(R1) \quad ROC + h\nu \longrightarrow RP + ROC \\
&(R2) \quad RP + NO \longrightarrow NO_2 \\
&(R3) \quad NO_2 + h\nu \longrightarrow NO + O \\
&(R4) \quad NO + O_3 \longrightarrow NO_2 + O_2 \\
&(R5) \quad RP + RP \longrightarrow \text{termination products} \\
&(R6) \quad RP + NO_2 \longrightarrow SGN \\
&(R7) \quad RP + NO_2 \longrightarrow SNGN
\end{aligned}$$

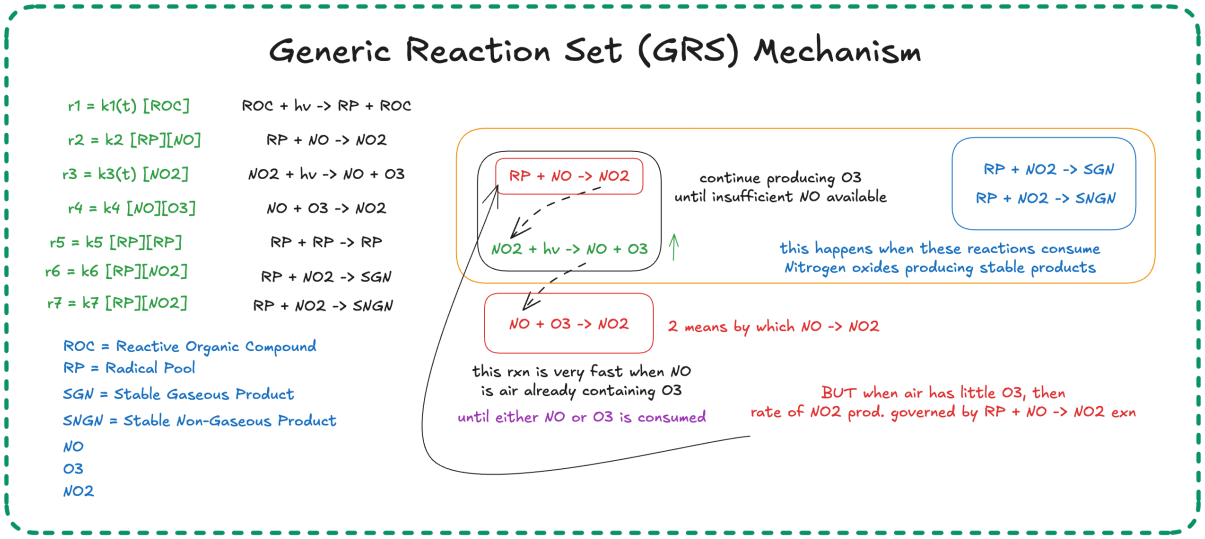

Figure 4: Brief discussion on a generic reaction set as described by [Duc et al.(2002)]

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