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Numerical modeling of tropospheric chemistry in an Earth System Model

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Abstract.

This work presents the incorporation of a tropospheric isoprene oxidation scheme into an Earth System Model to enhance the simulation of tropospheric ozone levels. Numerical experiments were performed using two distinct model setups: one accounting for isoprene oxidation and another in which this chemical pathway was not considered.

A | RELEVANCE AND RESEARCH OBJECTIVE

Tropospheric chemistry affects both climate and air quality:

- Non-methane volatile organic compounds (NMVOCs), methane (CH_4), and carbon monoxide (CO) regulate the formation of ozone (O_3) and hydroxyl radicals (OH)
- In industrial regions, the contribution of NMVOCs is particularly significant, including isoprene
- Due to their relatively slow removal, these substances influence the atmosphere on a global scale and, through exchange with the stratosphere, can even affect its chemical composition

Objective:

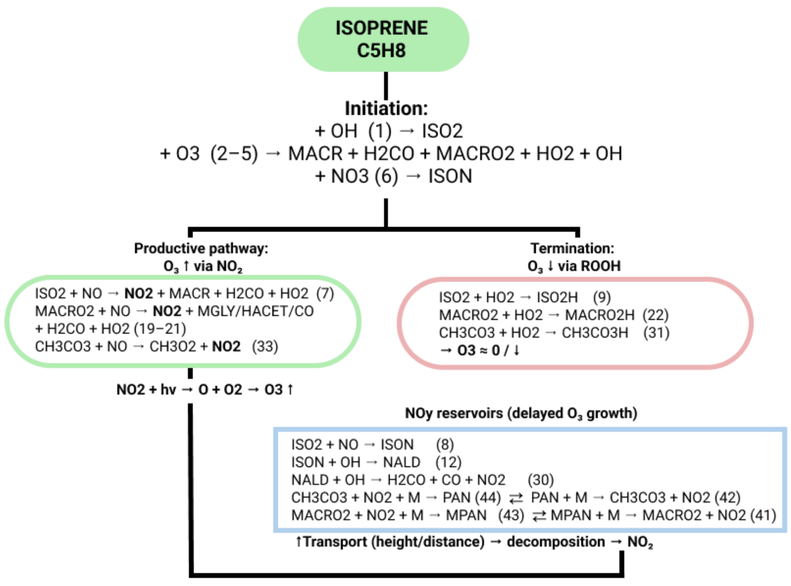
The aim of this study is to further develop the INM RAS–RSHU chemical–climate model [Volodin E. M. et al.,2017], a component of the Earth System Model (ESM), with a focus on a more accurate representation of tropospheric chemical processes.

B | COMPARISON OF CHEMICAL MECHANISMS

Why MIM1?
- Accuracy–efficiency balance (global modeling)
- Key tropospheric processes
- Proven for climate studies

Mechanism	Species	Reactions	Photolysis Reactions	Reference
CBM-Z	55	156	~20	Gregory Zaveri & Robert Peters, 1999
CB05 / CB6	51–80	156–220	~25	Greg Yarwood et al., 2005; Emery et al., 2015
MIM1	**16**	**44**	**10**	**Ulrich Pöschl et al., 2000; Geiger et al., 2003**
MIM2	68–69	~178–199	~30–44	Domenico Taraborrelli et al., 2009
RACM	77	214	23	William Stockwell et al., 1997
MOZART-4	85	196	39	Louisa Emmons et al., 2010
MOZART-T1	151	287	65	Emmons et al., 2020
MOZART-TS1\TS2	229–280	418–580	~125	Emmons et al., 2020

C | MIM1 REACTION SCHEME



D | MODEL DESCRIPTION

INM-CM6.0 Earth System Model (INM RAS)

Includes coupled atmosphere, ocean, sea ice, and land components

Horizontal resolution:

2° × 1.5° (longitude × latitude)

Vertical structure:

73 σ-levels from ~60 km (σ ≈ 0.0001) to ~7 m (σ = 0.993)

With MIM1:

78 chemical species
171 chemical reactions

E | NUMERICAL EXPERIMENTS

Parameter	CTRL (Control)	MIM1 (with Isoprene)
Chemical mechanism	Base scheme (CH_4-CO-HO_x-NO_x)	Base scheme + MIM1 (44 reactions, 16 species)
Isoprene emissions	Disabled	ACCMIP, ~503 Tg C yr^{-1}
C_5H_8 and product concentrations	Forced to zero	Prognostic
Simulation period	2008–2019 (12 years)	
Spin-up	2008–2009 (2 years)	
Analysis period	2010–2019 (10 years)	

*The chemistry is implemented in a one-way coupling framework, i.e., without accounting for the feedback of atmospheric composition on dynamics and radiative processes.

F | RESULTS

Relative changes in ozone (O_3), carbon monoxide (CO), nitrogen dioxide (NO_2), and hydroxyl radical (OH) concentrations after implementation of the MIM1 isoprene oxidation mechanism are shown. The strongest impact is observed in the tropics and mid-latitudes, where biogenic isoprene emissions are highest

Tropical lower troposphere (0–5 km):
- O_3 decreases by 10–15%
- OH decreases by 15–30%
- CO increases by 30–60%

→ Due to OH consumption and radical chain termination (RO_2 + HO_2 reactions)

Mid-troposphere (8–12 km):

O_3 increases by 10–20%, especially in the subtropics

NO_2 increases due to decomposition of PAN and MPAN

→ Released NO_2 enhances photochemical ozone production

CO shows the largest relative changes (up to 40–60%) in the middle and upper troposphere due to transport and low background concentrations

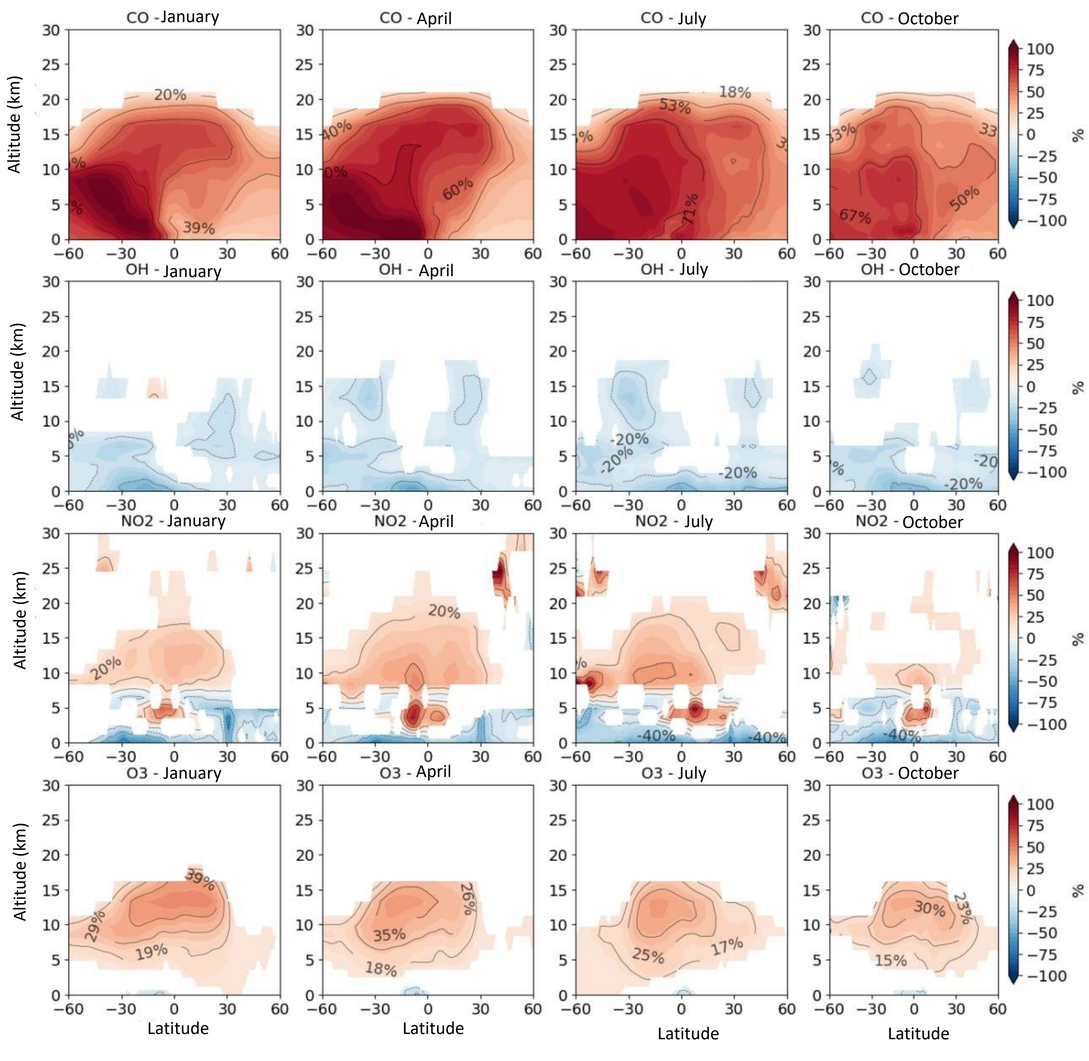


Fig.1 - Relative changes in zonally averaged concentrations of carbon monoxide CO, hydroxyl radical OH,NO2, ozone O_3 upon inclusion of isoprene chemistry via the MIM1 mechanism for January, April, July, and October. Changes shown as percentages: Δ = (MIM1 − CTRL)/CTRL × 100%

G | CONCLUSION

Accounting for tropospheric chemistry is essential for consistent and realistic modeling of atmospheric composition. Even the use of a relatively compact chemical mechanism (MIM1) leads to significant changes in ozone distribution, highlighting the importance of representing the oxidation of biogenic volatile organic compounds.

Key results:

- Decrease of ozone by **10–15%** in the tropical lower troposphere (0–5 km) due to radical chain termination under low NO_x conditions
- Increase of ozone by **10–20%** in the mid-troposphere (8–12 km) driven by thermal decomposition of transported PAN-type species
- One-way coupling mainly affects tropospheric composition, while two-way chemistry–dynamics interactions may also impact the stratosphere
- The results provide a basis for improving atmospheric composition forecasts and understanding chemistry–climate interactions

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