# Global intercomparison of tropospheric oxidant chemistry in a common Earth system model environment using GEOS-Chem (v14.1.1) and CAM-chem chemistry within the Community Earth System Model version 2 (CESM2)

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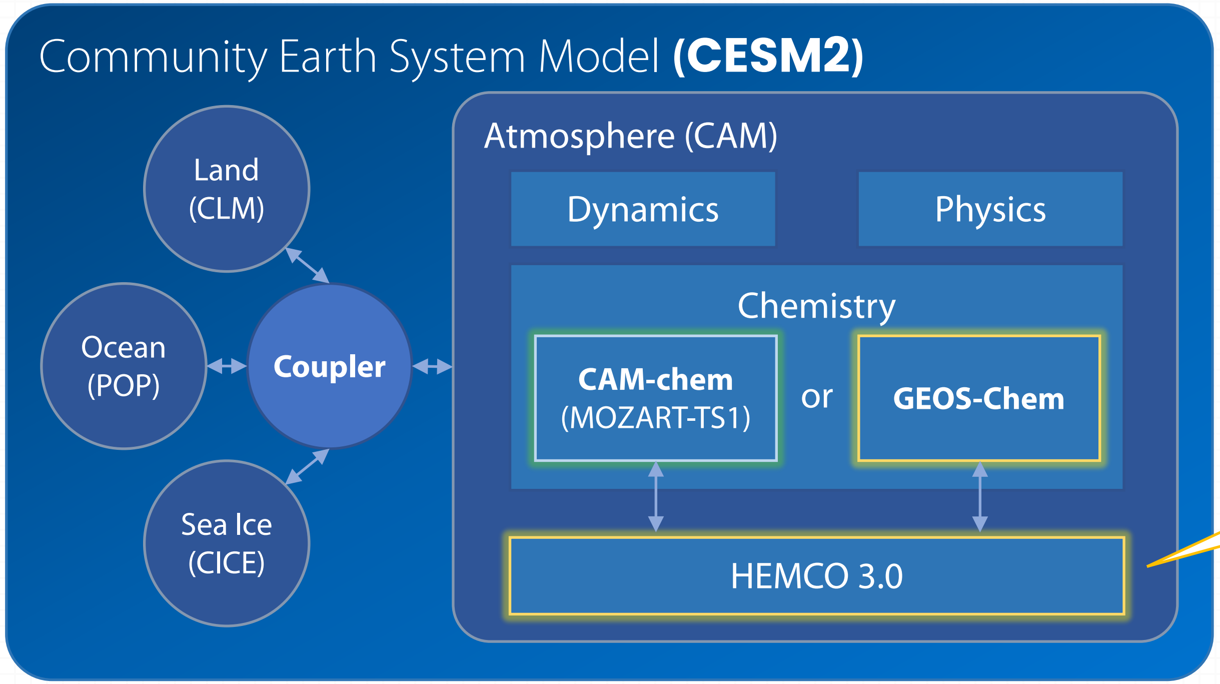
# GEOS-Chem has been implemented in CESM2 as **an alternative chemistry option to CAM-chem**, allowing for side-by-side comparisons

**GEOS-Chem**

- Best known as a chemical transport model (CTM) using archived met fields (MERRA2)
- Different development heritage from CAM-chem

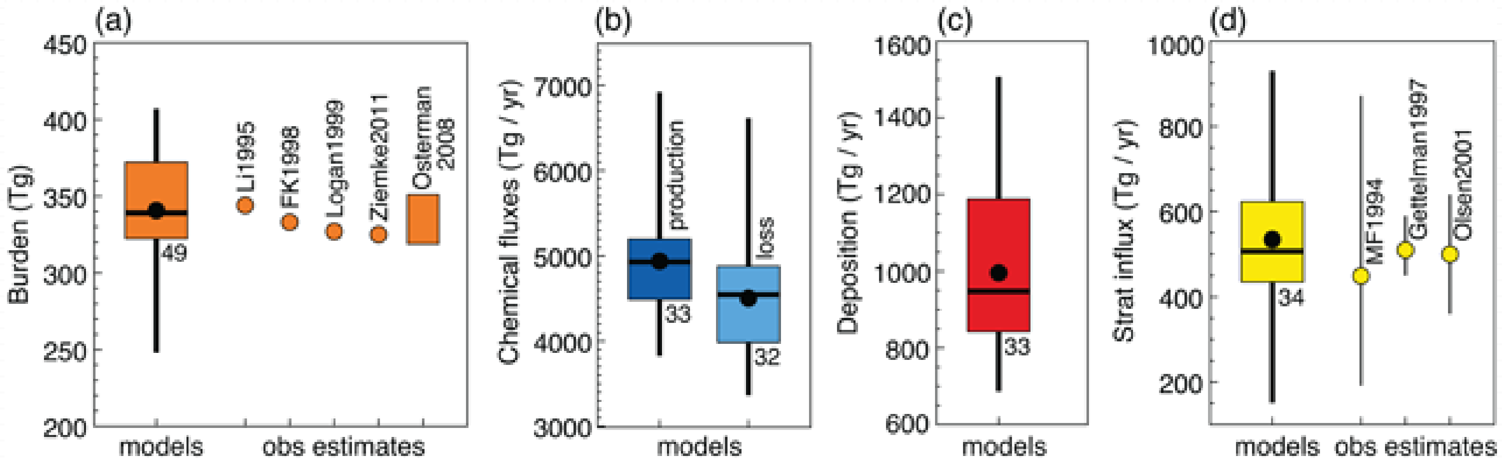



Previous work: implementing the **HEMCO emissions component** from GEOS-Chem into CAM-chem/CESM2

**Previous model intercomparisons generally compared entire modeling systems.**
**Implementation of GEOS-Chem within CESM2 allows for detailed, process-based comparison to CAM-chem**

***GEOS-Chem within CESM:*** *Fritz et al., 2022*
***HEMCO 3.0:*** *Lin et al., 2021*

# Ozone is a central species in tropospheric chemistry and an important indicator of model skill, but current models show large differences in individual processes controlling it




***TOAR:** Young et al., 2018*

**Large differences in process magnitudes imply large differences in sensitivity to perturbations, which pose difficulty for chemistry-climate models aiming to quantify chemical feedbacks to climate change**

# Our work identifies and evaluates major differences between GEOS-Chem and CAM-chem chemistry and their effect on reproducing features in observations

| | Chemistry Mechanism | Aerosol composition/ Microphysics | Photolysis scheme |
|---|---|---|---|
| GEOS Chem | **GEOS-Chem v14.1.1**<br>286 species, 914 reactions<br>$O_x$-$NO_x$-VOC-**halogen**-aerosol<br>• Aerosol nitrate photolysis<br>• $N_2O_5$ uptake in clouds | Bulk aerosols mapped to MAM4 modes for ARI/ACI effects<br>• Explicitly represents nitrate aerosol | Fast-JX<br>• Aerosol extinction effects |
| **CAM-chem** (within CESM®) | **MOZART-TS1**<br>229 species, 541 reactions<br>$O_x$-$NO_x$-VOC-aerosol | MAM4 modal aerosols | TUV lookup table |

**Both models use meteorology from CESM2.3** (`cam6_3_095`) **nudged to MERRA2** (`FCnudged 0.9x1.25`) **and emissions from HEMCO (CEDSv2+KORUSv5)**

# Both models show **similar global burden** of tropospheric ozone and OH **but large differences in budget terms**

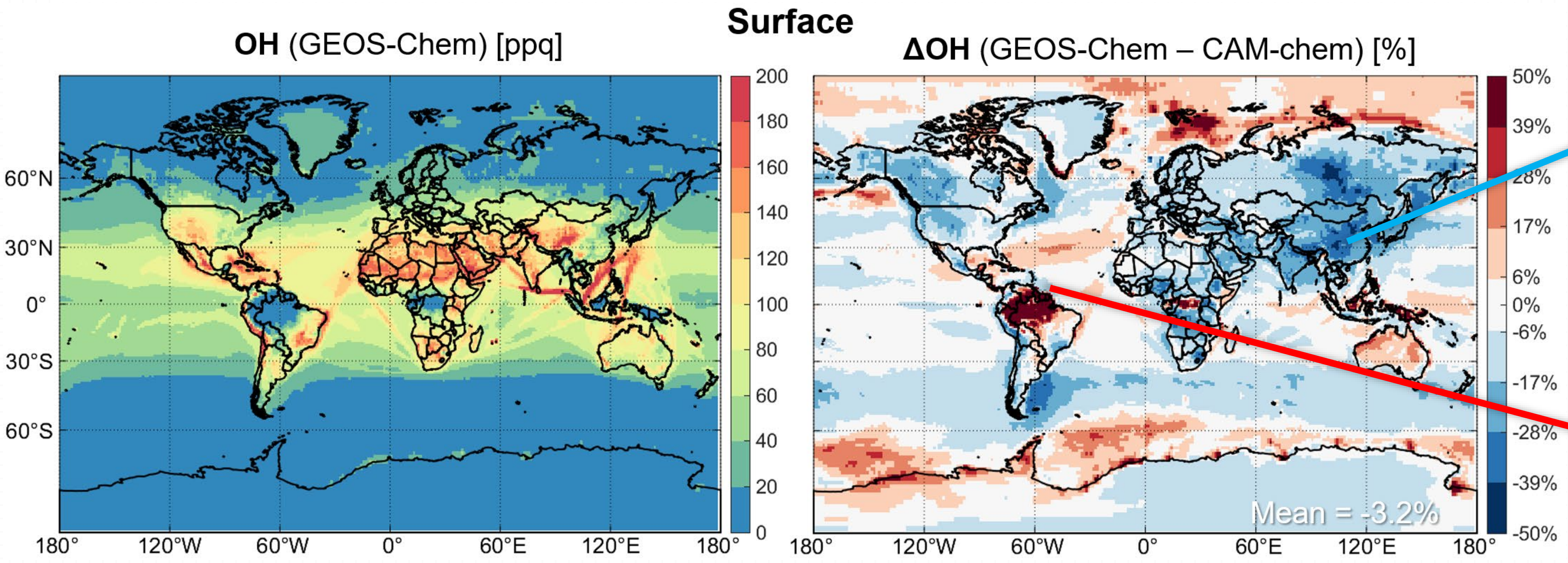
| **Budget terms** | **GEOS-Chem** | **CAM-chem** | **Model ranges from literature** (Young et al., 2018, Naik et al., 2013) |
|---|---|---|---|
| **Tropospheric** ozone **burden** (Tg) | 350 | 342 | 340 (250-410) |
| $O_x$ chemical **production** (Tg $a^{-1}$) | 5395 | 5052 | 4900 (3800-6900) |
| $O_x$ chemical **loss** (Tg $a^{-1}$) | 4813 | 4465 | 4600 (3300-6600) |
| $O_x$ **deposition** (Tg $a^{-1}$) | 878 | 967 | |
| Ozone **dry deposition** (Tg $a^{-1}$) | 749 | 826 | 1000 (700-1500) |
| $O_x$ **STE** (Tg $a^{-1}$) | 341 | 380 | 500 (180-920) |
| $O_x$ **Lifetime** (days) | 23.0 | 23.7 | 22.3 (19.9-25.5) |
| Global **OH** ($10^6$ molecule $cm^{-3}$) | 1.21 | 1.22 | 1.11 ± 0.16 |
| **Stratospheric** ozone **burden** (Tg) | 2743.7 | 2744.4 | |

**Driven by:**
Aerosol nitrate photolysis
& Halogen chemistry

Slower deposition velocities over the ocean from **GEOS-Chem**
(~20 days)

# Both models show similar global burden of tropospheric ozone and **OH but large regional differences**

**2016 annual mean surface OH from GEOS-Chem and differences with CAM-chem**




**GEOS-Chem has**

**Lower OH over polluted regions**

- Lower $J(O^1D)$ from Fast-JX vs TUV
- Higher OH reactivity

**Higher OH over Amazon/Congo basin**

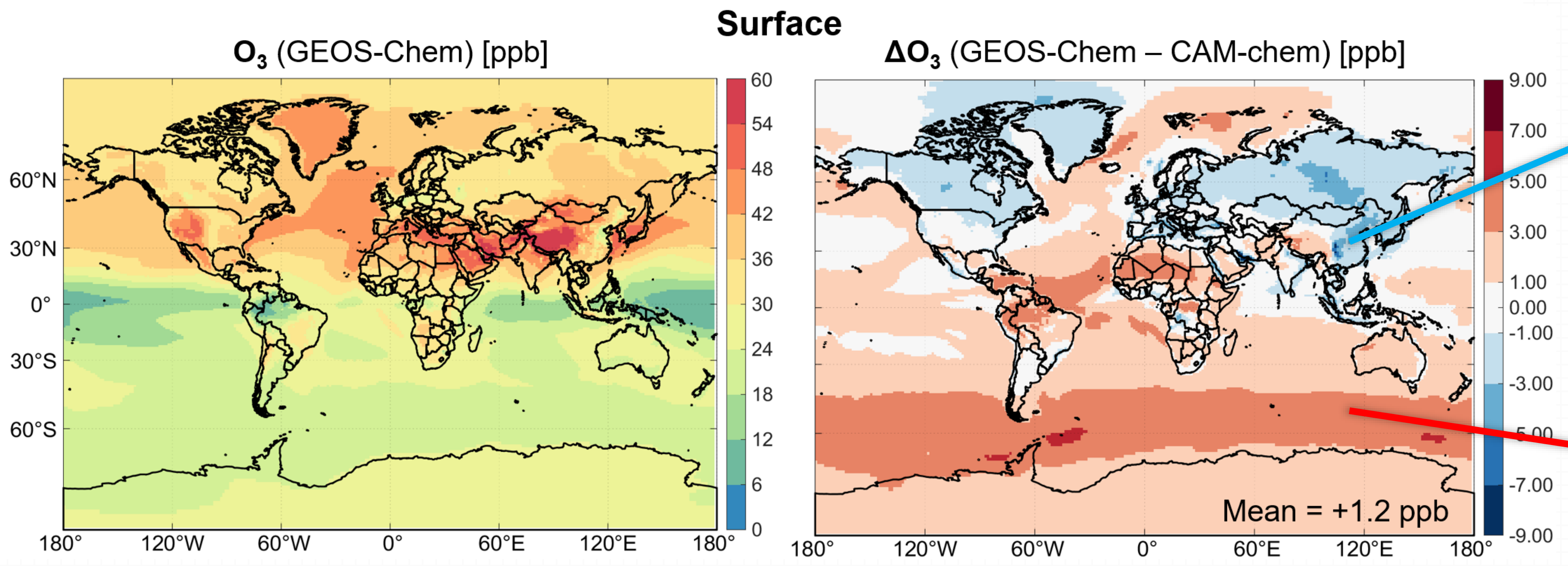
- Updated isoprene chemistry recycling OH in low-$NO_x$ conditions

*(Bates & Jacob, 2019)*

Leads to lower CO in CAM-chem

# Both models show similar global burden of tropospheric **ozone** and OH **but large regional differences**

**2016 annual mean surface ozone from GEOS-Chem and differences with CAM-chem**




**GEOS-Chem has**

**Lower ozone in the NH**

- Loss to halogen chemistry and cloud $N_2O_5$ uptake *(Wang et al., 2021; Holmes et al., 2019)*

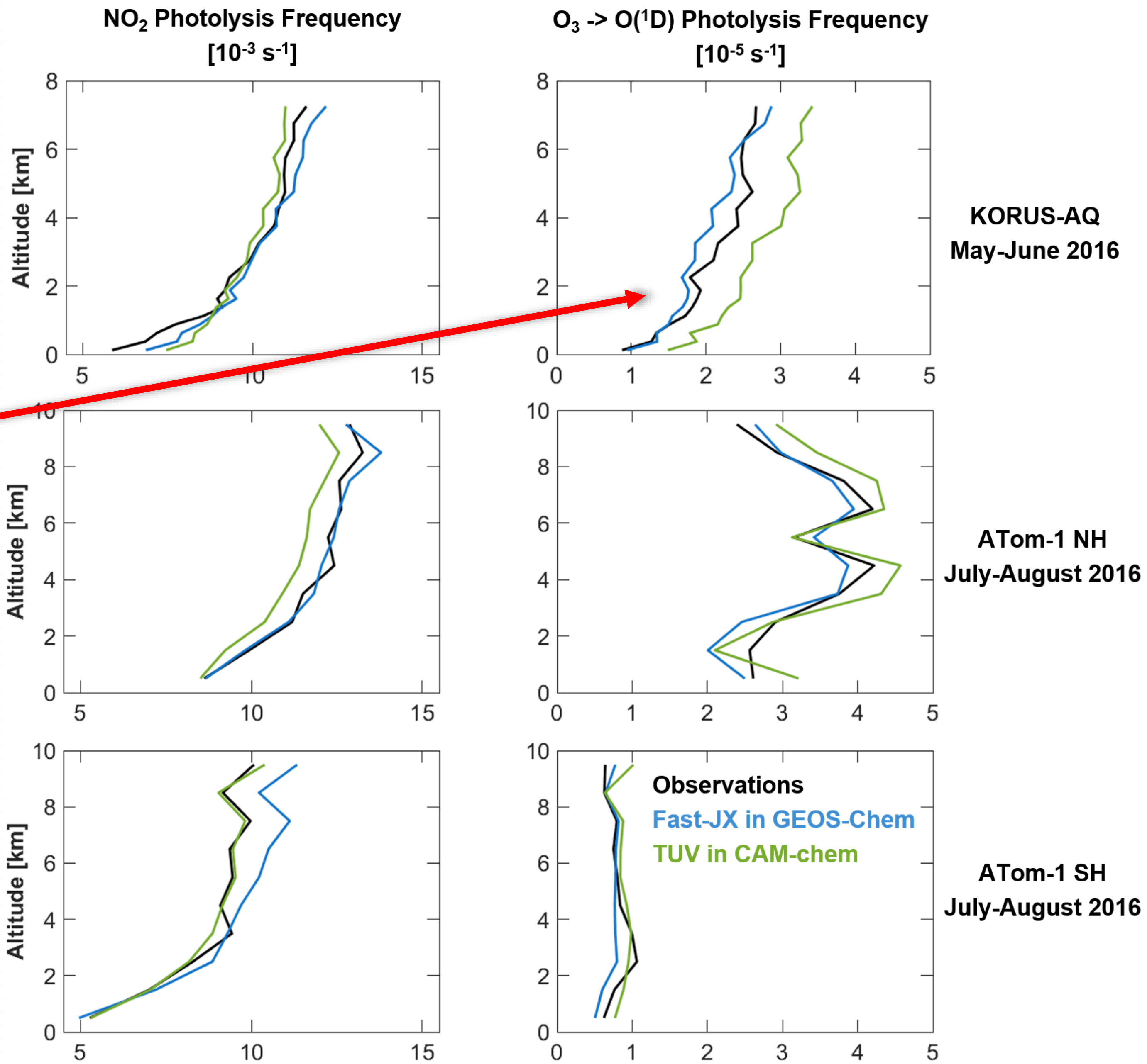
**Higher ozone in the oceans and SH**

- Slower ozone deposition over ocean due to using GEOS-Chem velocities *(Pound et al., 2020)*

Fast-JX (in GEOS-Chem) and TUV (in CAM-chem) photolysis schemes generally agree on $J(NO_2)$ but **differ in $J(O^1D)$ over polluted regions**

***J*(O¹D) is overestimated by TUV (CAM-chem)**

- *Not* aerosol extinction (or clouds), as difference persists in clear-sky *J*-values
- *Not* overhead ozone column
- **Difference disappears by using Fast-JX in CAM-chem**
- Most noticeable over polluted regions. Why?

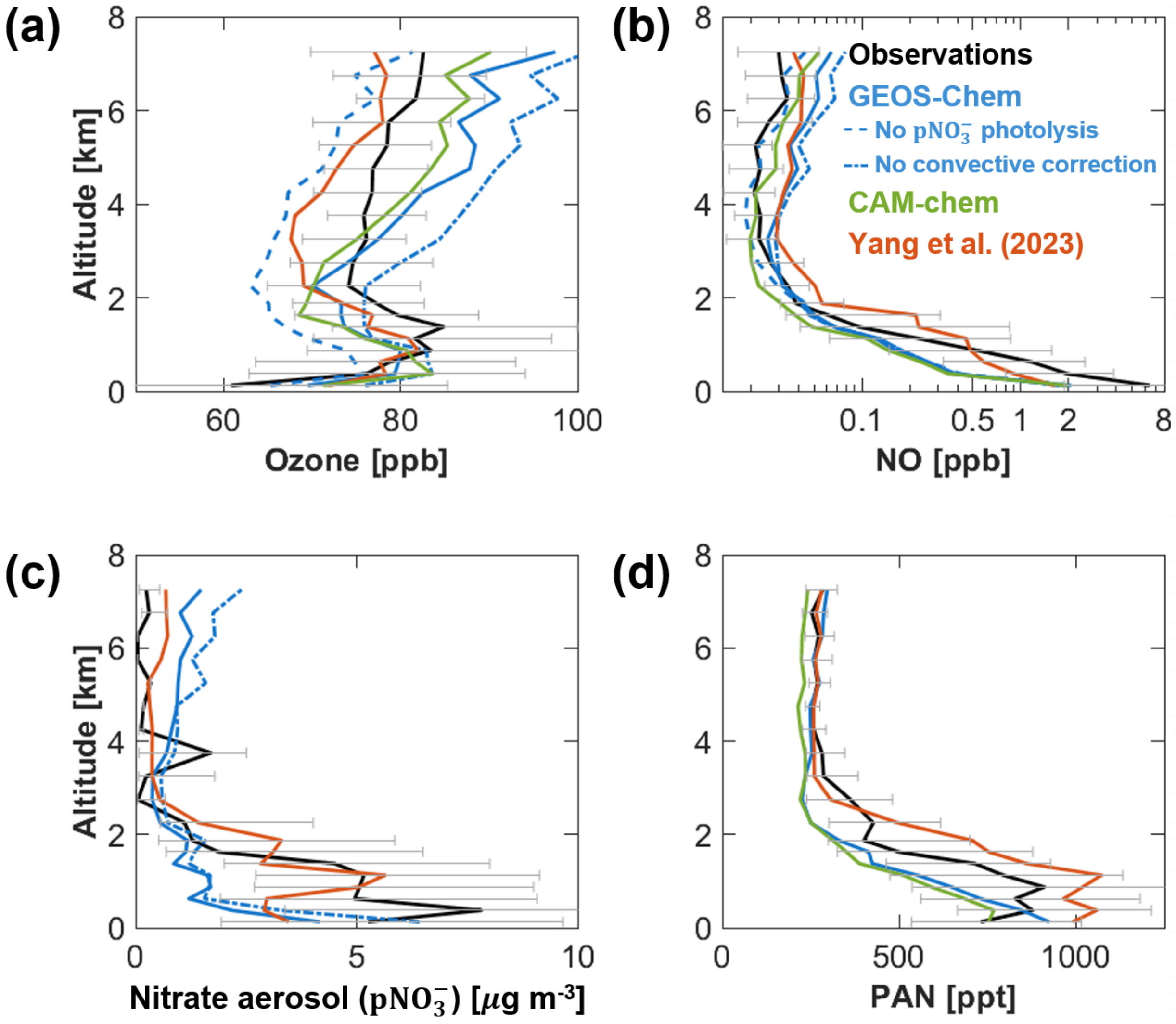



**Future versions with TUV-X & Cloud-J will allow for further diagnosis of these differences**

# We can attribute particular features of GEOS-Chem chemistry to differences against CAM-chem in the comparison to KORUS-AQ

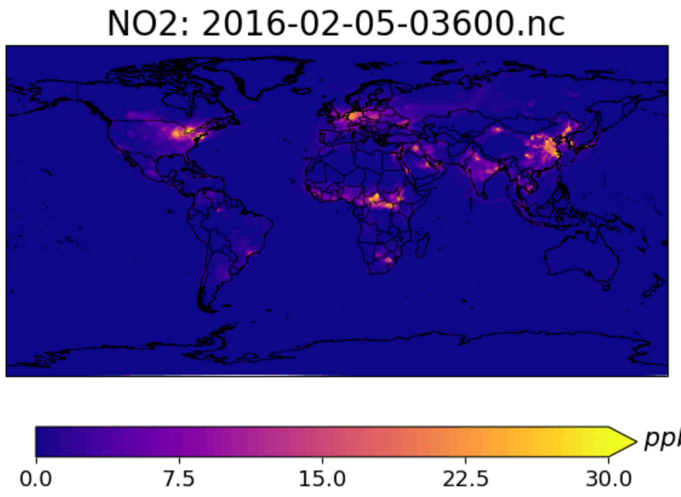
- **CAM-chem** simulates ozone well but **GEOS-Chem** can only do so with aerosol nitrate ($pNO_3^-$) photolysis
- Effect of $pNO_3^-$ photolysis in GEOS-Chem has a strong dependence on $pNO_3^-$ which is **not wet scavenged in convective updrafts** in the CESM2 environment
- **GEOS-Chem (offline)** can simulate $pNO_3^-$ well below 2km but not **GEOS-Chem (CESM).** This may be due to boundary layer dynamics in CESM cf. GEOS-Chem (offline)

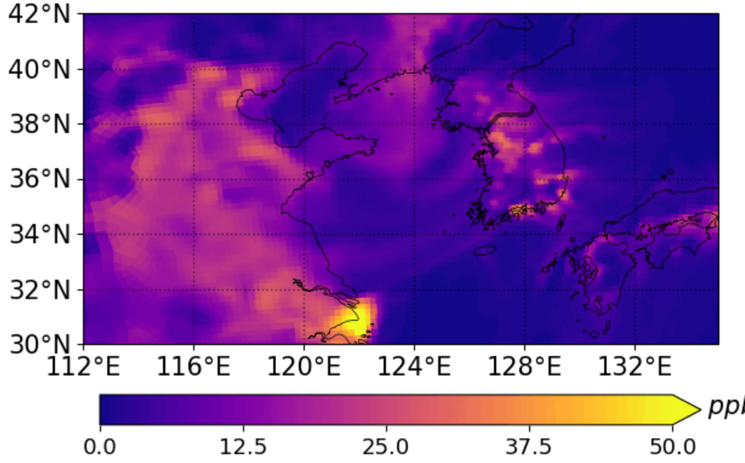
**Tropospheric vertical profiles, KORUS-AQ (May-June 2016)**
**Over the Seoul Metropolitan Area (SMA)**



# Take home messages

- **GEOS-Chem** as an **alternative chemistry option to CAM-chem** in CESM2 provides a **high-quality simulation of tropospheric oxidant chemistry**, as well as **enabling side-by-side intercomparison with CAM-chem**
- Major differences between GEOS-Chem and CAM-chem are driven by: (1) the photolysis scheme, (2) aerosol nitrate photolysis, (3) $N_2O_5$ uptake in clouds, (4) tropospheric halogen chemistry, and (5) ozone deposition to oceans.
- While GEOS-Chem and CAM-chem have similar ozone and OH budgets, **there are important differences in the underlying processes** and **major regional differences**, which imply differences in sensitivity to perturbations.




GEOS-Chem in MUSICA KORUS grid. For demo only.
KORUS refined grid via *Jo et al., 2023*

**GEOS-Chem within CESM2 is available for testing and available in beta versions of CESM (cam6_3_147+)** 🎉

HEMCO emissions for CAM-chem are available in beta versions of CESM (cam6_3_118+)