Benchmarking of chemical mechanisms

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Rationale for benchmarking

- Three main chemical mechanisms (list of reactions and rates) are available: full, intermediate and fast. They differ in their decreasing representation of hydrocarbon chemistry and therefore their decreasing computational cost

Gas-phase tropospheric chemistry only

- Full mechanism: 79 species
- Intermediate mechanism: 39 species
- Fast mechanism: 28 species

Purpose of interactive chemistry

- Provides distribution of radiatively-active greenhouse gases (troposphere and stratosphere)
- Provides distribution of oxidants for aerosol production (both online and offline)
- Provides distribution of secondary-organic aerosols
- Provides distribution of air quality
- Provides interaction with biogeochemistry: nitrogen deposition, ozone damage

Approach for benchmarking

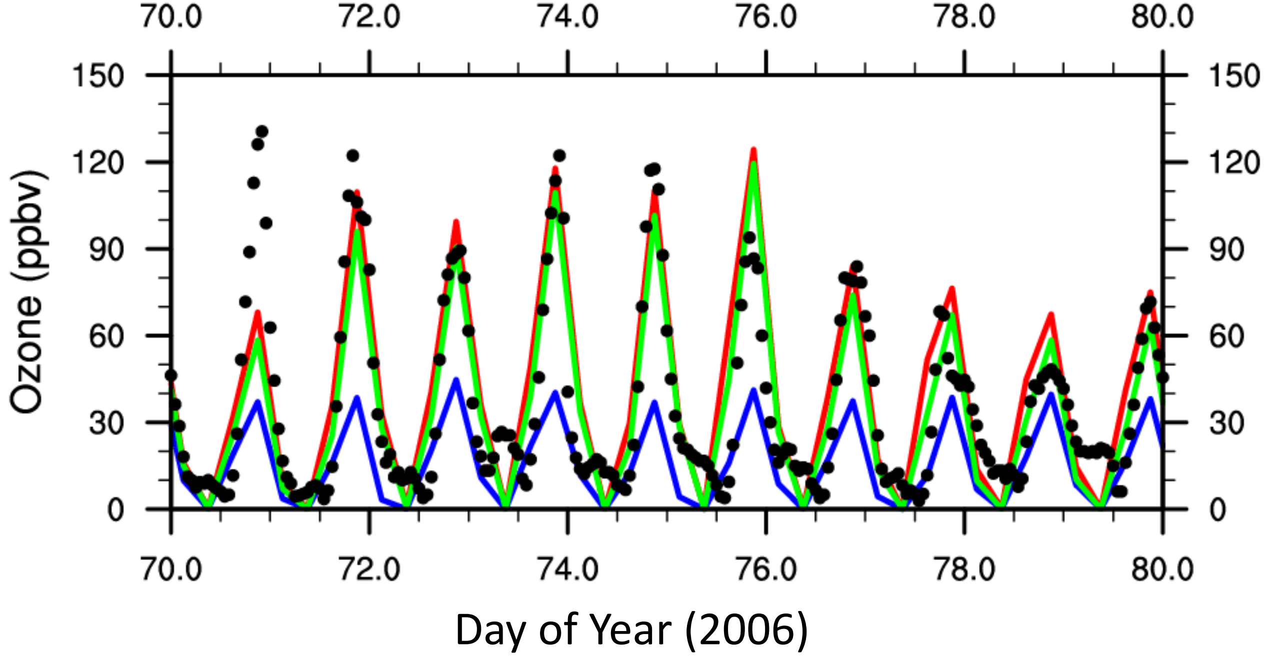
- Simulation with relevance to air quality

    1. High-resolution simulation (0.47°x0.63°)
    2. Driven by observed meteorology
    3. Compared with MIRAGE campaign observations (Mexico City pollution)

- Simulation with relevance to climate

    1. Medium-resolution simulation (1.9°x2.5°)
    2. Driven by observed meteorology
    3. Two sets of emissions: base case and perturbed (30% reduction of Southeast Asia industrial sector, based on CCSP simulations) to study the response to a change in emissions
    4. Use full mechanism as "Truth"

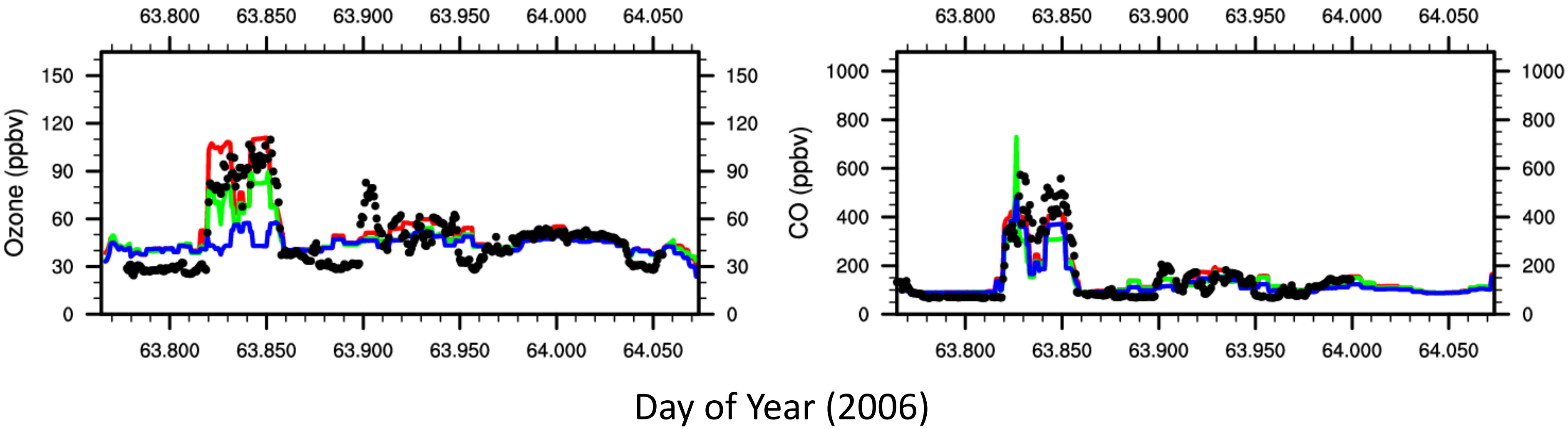
Air quality: Comparison with Mexico City surface observations



Red: Full mechanism
Green: Intermediate mechanism
Blue: Fast mechanism
Dots: observations

On most days, full and intermediate capture well the diurnal cycle and amplitude; the fast mechanism is much lower

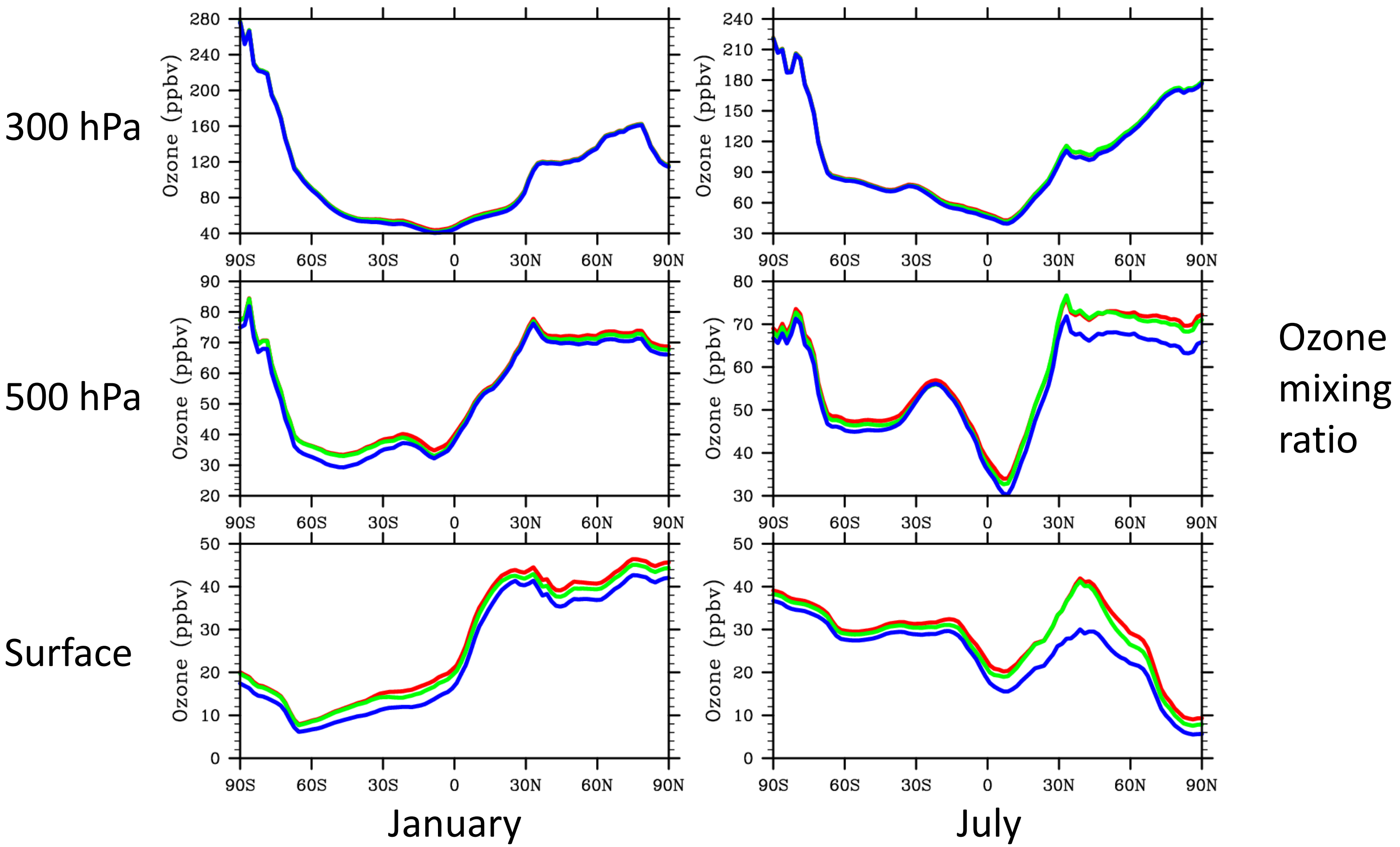
Air quality: Comparison with aircraft observations



Red: Full mechanism
Green: Intermediate mechanism
Blue: Fast mechanism
Dots: observations

1. On most days, full and intermediate capture well the background and plume ozone; the fast mechanism captures well the background.
2. CO is will captured by all.

Climate: base emissions



Red: Full mechanism

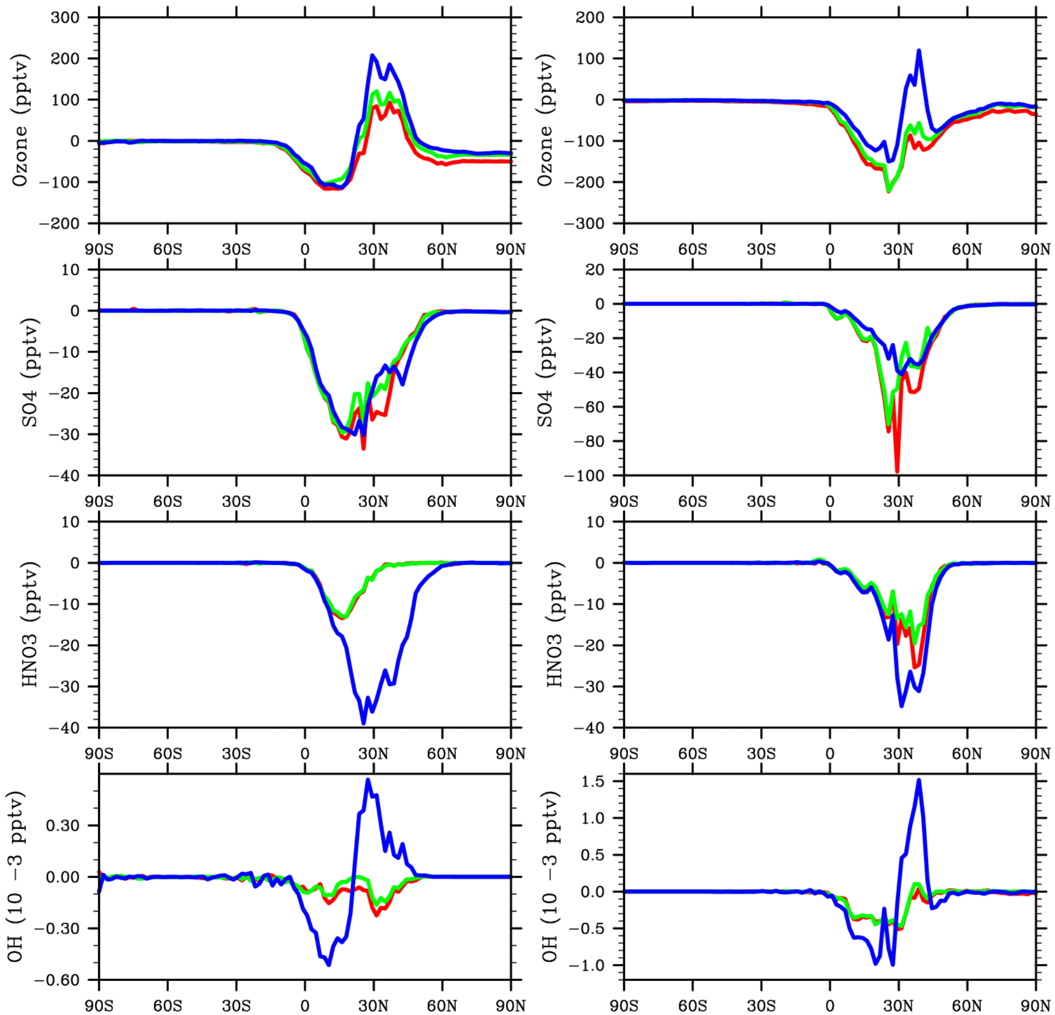
Green: Intermediate mechanism

Blue: Fast mechanism

Very good agreement amongst methods in radiatively important upper-troposphere ozone (but fixed stratosphere!); larger bias for the fast mechanism at lower altitudes

Climate: change in emissions

Change in surface mixing ratio



January

July

Sulfate: important for indirect effect

Nitric acid: important for nitrogen deposition

OH: important for methane lifetime

Red: Full mechanism

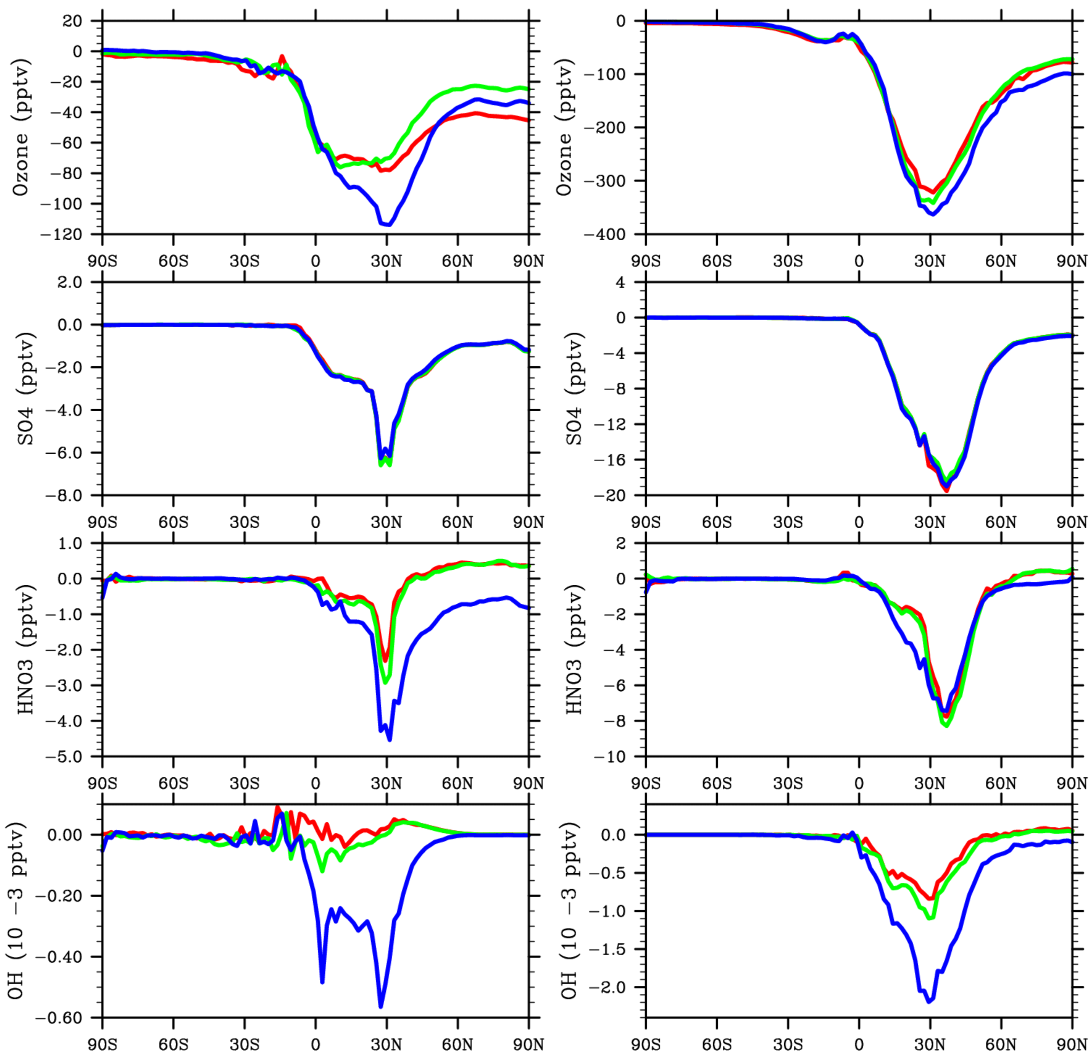
Green: Intermediate mechanism

Blue: Fast mechanism

Response in surface ozone and sulfate well captured; stronger biases for the fast mechanism for HNO_3 and OH

Climate: change in emissions

Change in 500 hPa mixing ratio



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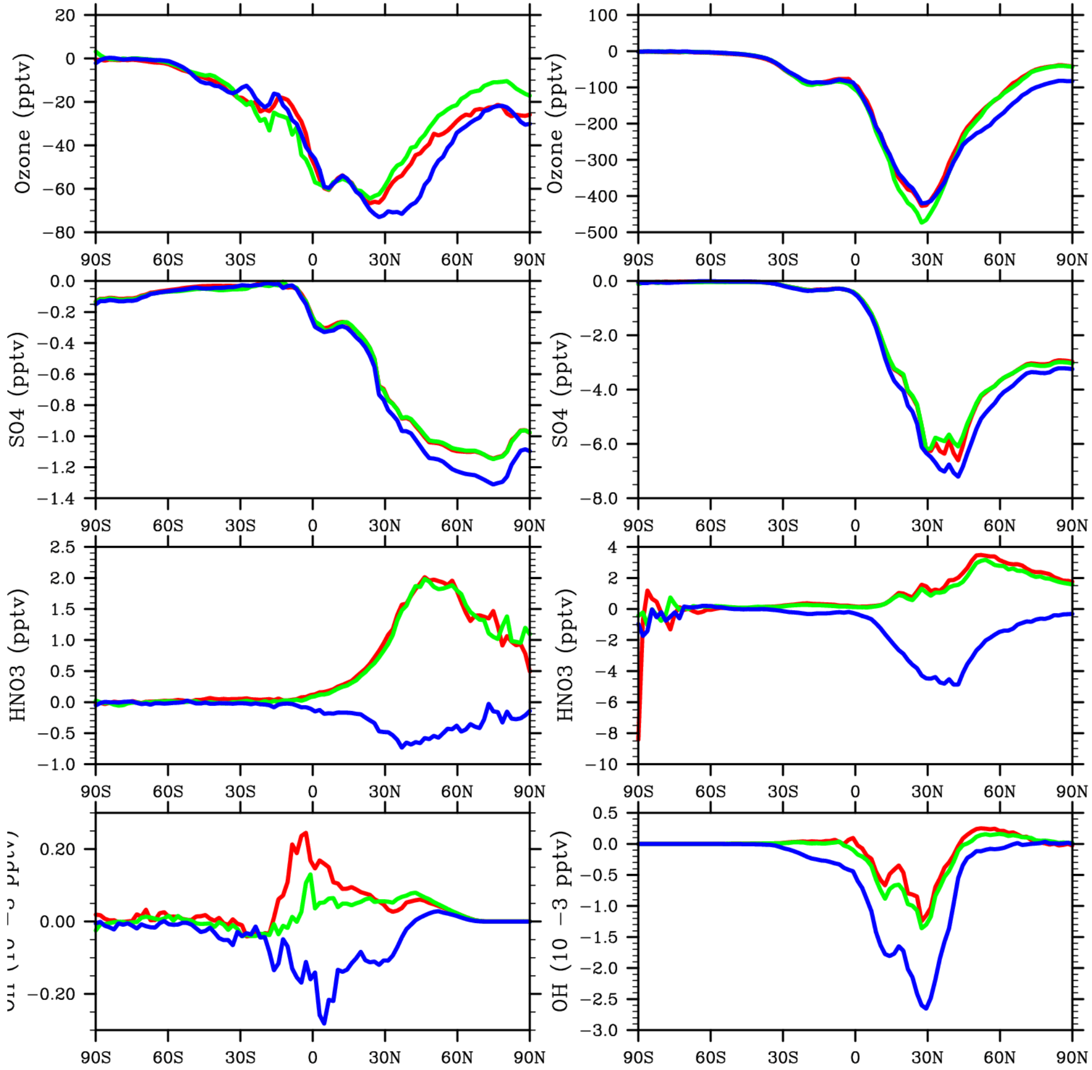
Blue: Fast mechanism

Climate: change in emissions

Change in 250 hPa mixing ratio



Red: Full mechanism

Green: Intermediate mechanism

Blue: Fast mechanism

Conclusions

- Background ozone is well represented by all chemical mechanisms
- Response in ozone and sulfate to changes in emissions is similar in all three mechanisms
- For the diagnostics selected, the intermediate mechanism is closer to the full mechanism and to observations than the fast mechanism, especially in strongly polluted regions
- Computational cost:
  - Full = 5x CAM (3 tracers)
  - Intermediate = 1/2 of full
  - Fast = 1/3 of full, and could be reduced further for troposphere-only applications)