

Fast Chemistry Mechanisms for Climate Applications

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Interactive chemistry brings many benefits to climate simulations.



1. Provides consistent distribution of greenhouse gases (troposphere and stratosphere), including the effects of:
 - i. Changes in stratosphere-troposphere exchange (STE),
 - ii. Feedback on climate through the GHGs and aerosols.
2. Provides consistent distribution of oxidants for:
 - i. Aerosol production, including sulfate & secondary-organic aerosols,
 - ii. Lifetimes of many species of interest, including methane.
3. Provides distribution of air quality (background).
4. Provides interaction with biogeochemistry: nitrogen deposition, ozone damage, dimethyl sulfide (CLAW).

Interactive chemistry brings many benefits to climate simulations.



5. Provides statistics from IPCC simulations on:
 - i. O₃ columns,
 - ii. tropospheric O₃ (radiative forcing),
 - iii. tropospheric OH (CH₄ & HCFC lifetimes).

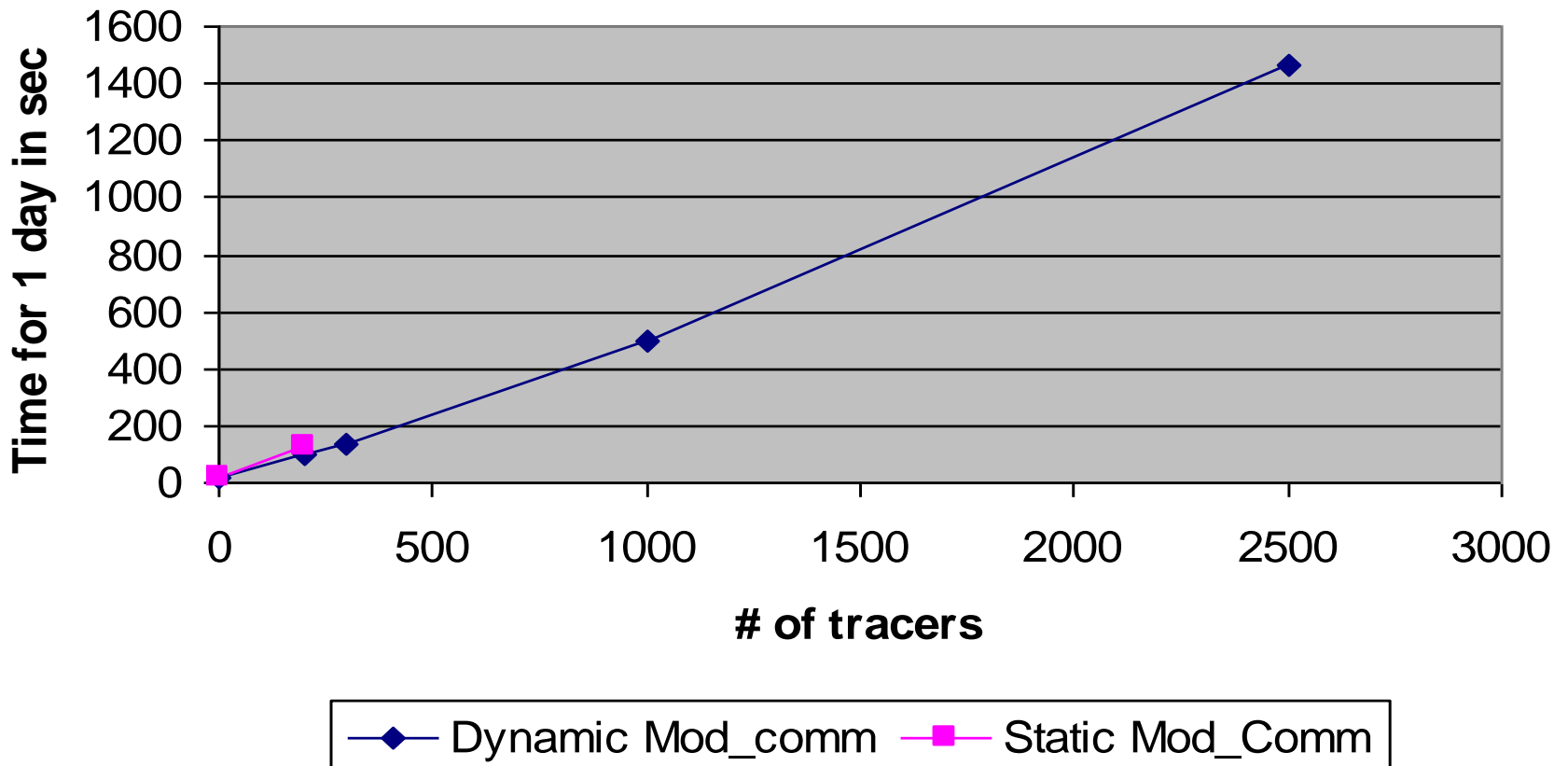
6. Tracers good for diagnosing and validating GCM:
 - i. Interhemispheric mixing time,
 - ii. Stratospheric lifetime,
 - iii. Convective massfluxes.

7. Offline chemical fields take human & computer time too.

Half of chem time is advection. Tracers scale as 2-3% of CAM/tracer



Tracer scaling on Thunder (Linux cluster)



Our fast & super-fast mechanisms increase GCM computational cost by 100% and 40%.



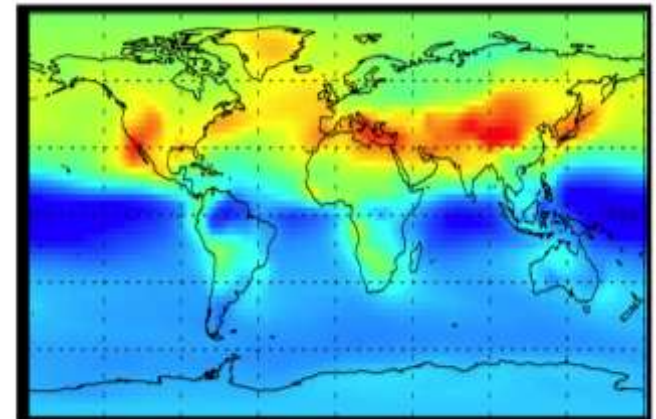
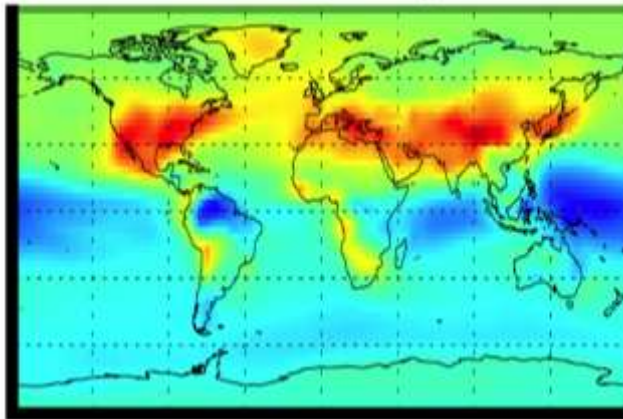
- | | |
|-------------------------------------|--|
| (1) O ₃ | (15) HO ₂ NO ₂ |
| (2) O | (16) CO |
| (3) O(¹ D) | (17) CH ₄ |
| (4) OH | (18) CH ₂ O |
| (5) HO ₂ | (19) HCOOH |
| (6) H ₂ O ₂ | (20) CH ₃ O ₂ |
| (7) N | (21) CH ₃ O ₃ |
| (8) N ₂ O | (22) CH ₃ OOH |
| (9) NO | (23) CH ₃ O ₂ NO ₂ |
| (10) NO ₂ | (24) DMS |
| (11) NO ₃ | (25) H ₂ S |
| (12) N ₂ O ₅ | (26) MSA |
| (13) HONO | (27) SO ₂ |
| (14) HNO ₃ | (28) SO ₄ |

Super-fast captures 70-80% of O₃ & OH large-scale amplitude AND variability.

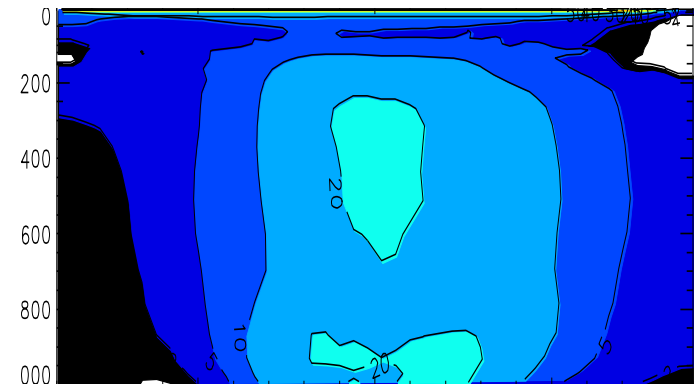
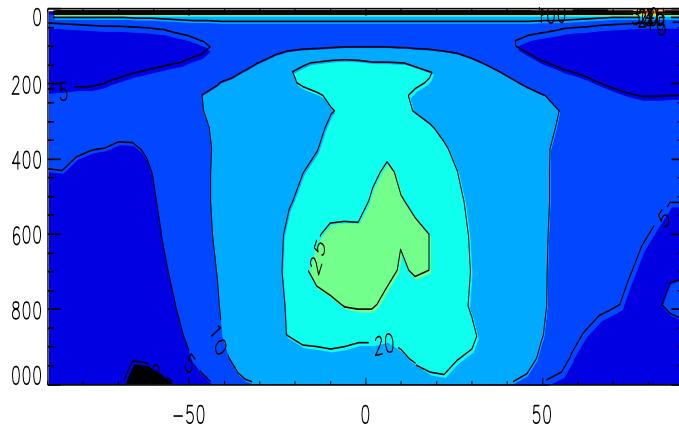
Full Chemistry

Super-fast Chemistry

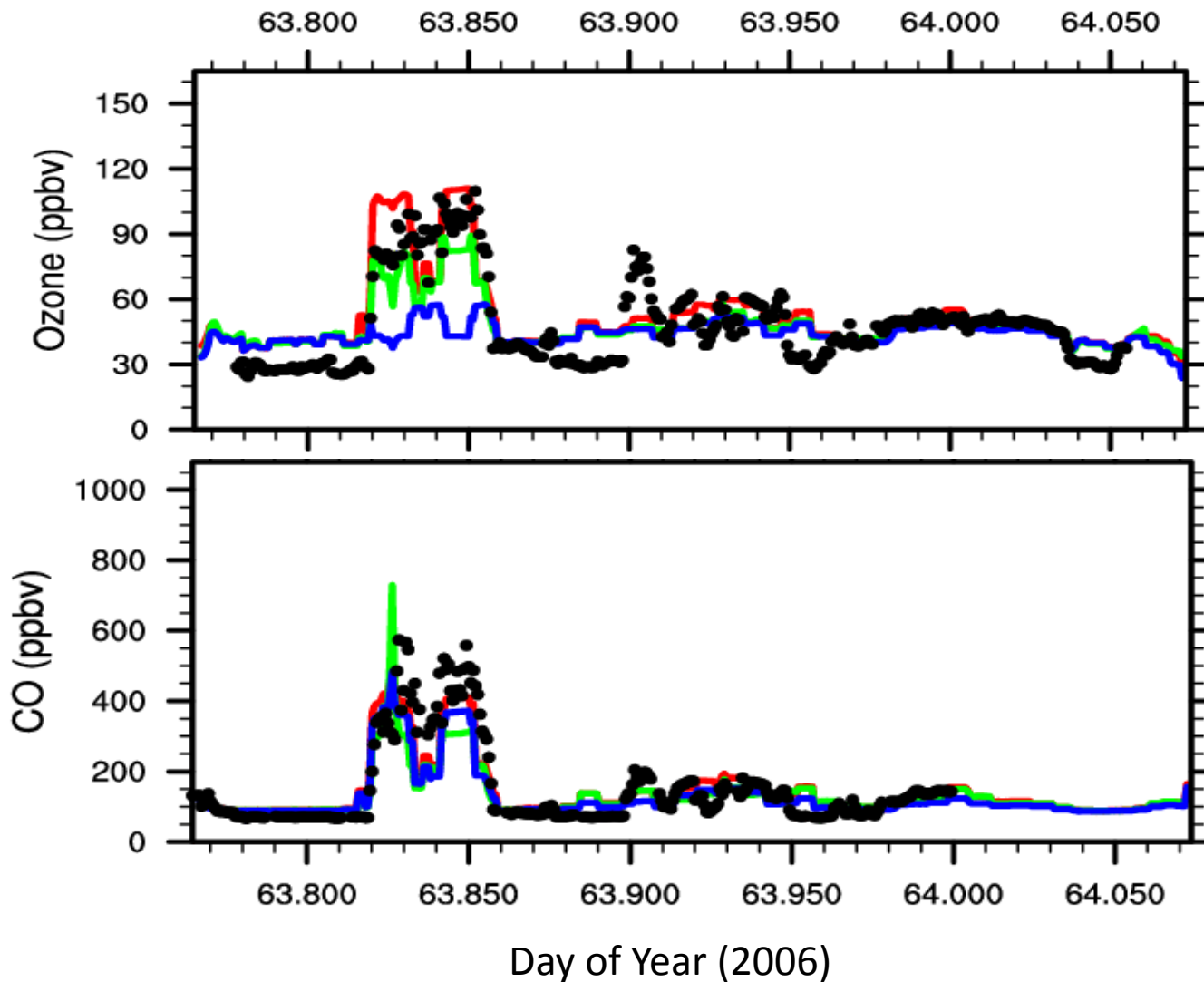
Surface
[O₃]
ppb



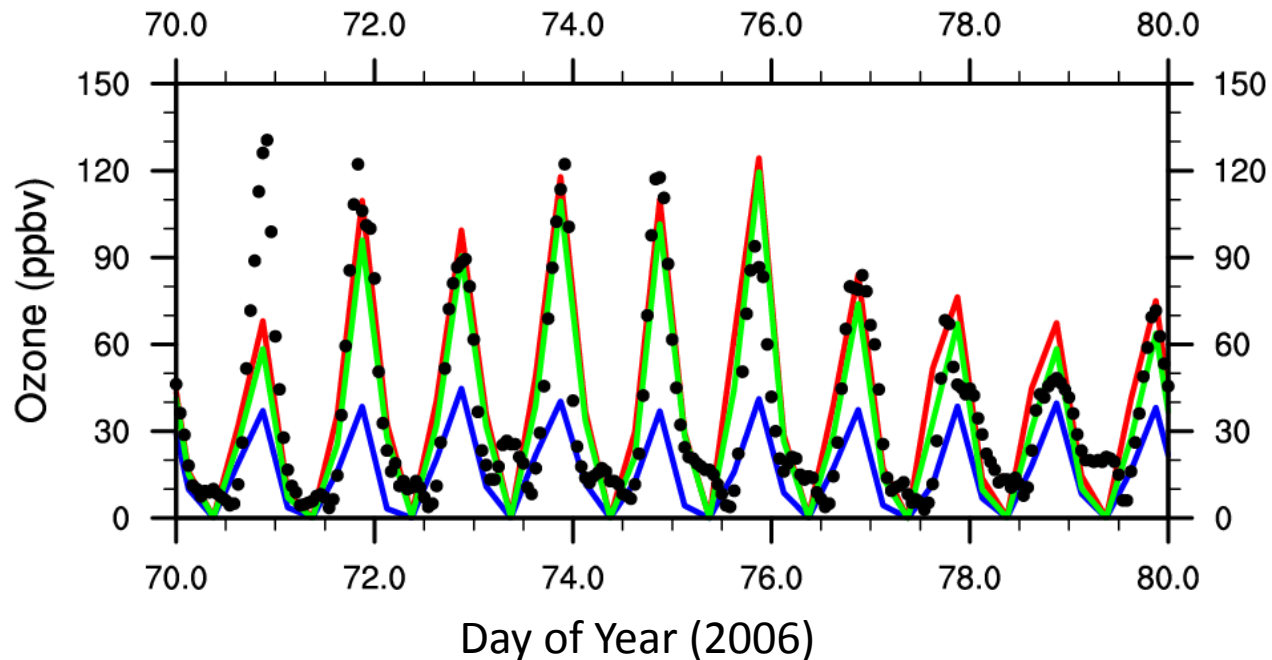
Zonal mean
[OH]
10⁵mol/cm³



Mexico City aircraft obs. confirm good background, but weak pollution plumes.



Mexico City surface observations confirm weak response to urban diurnal cycle.



Red: Full mechanism

Green: Intermediate mechanism

Blue: Fast mechanism

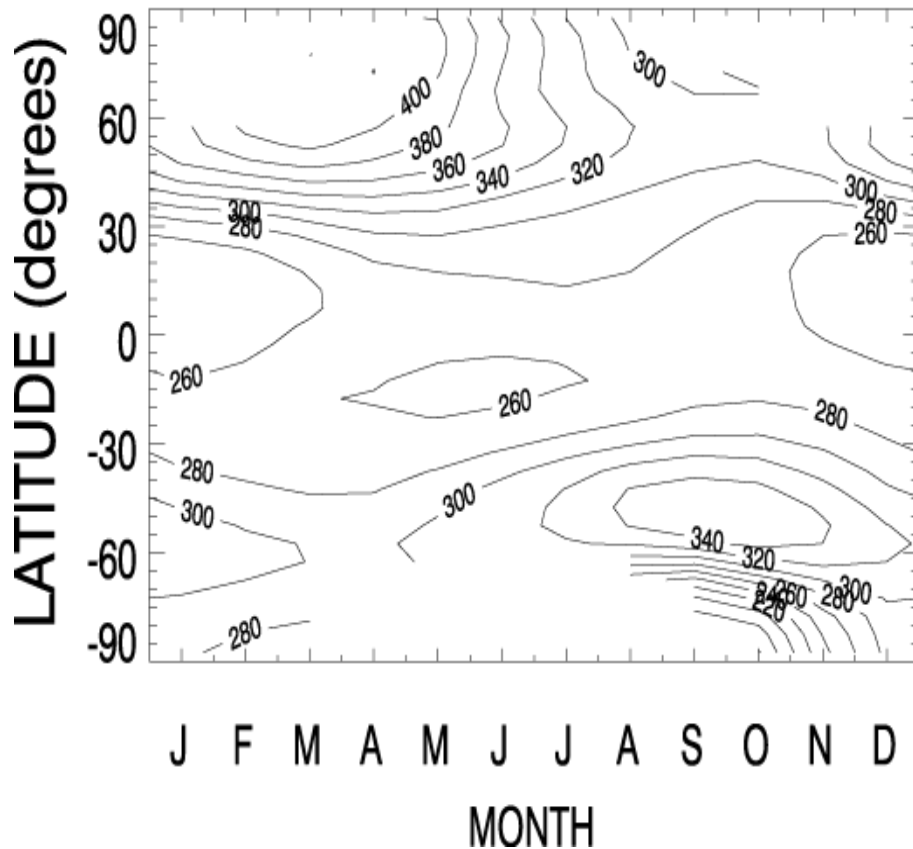
Dots: observations

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

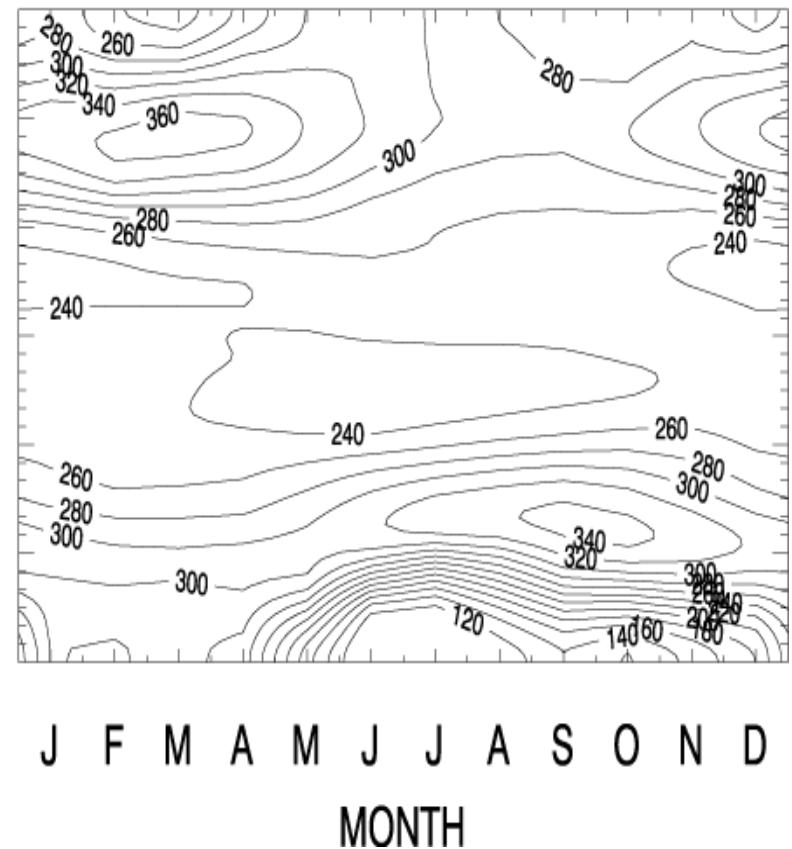
Linoz only needs 1 tracer. Its stratospheric columns compare well with observations.



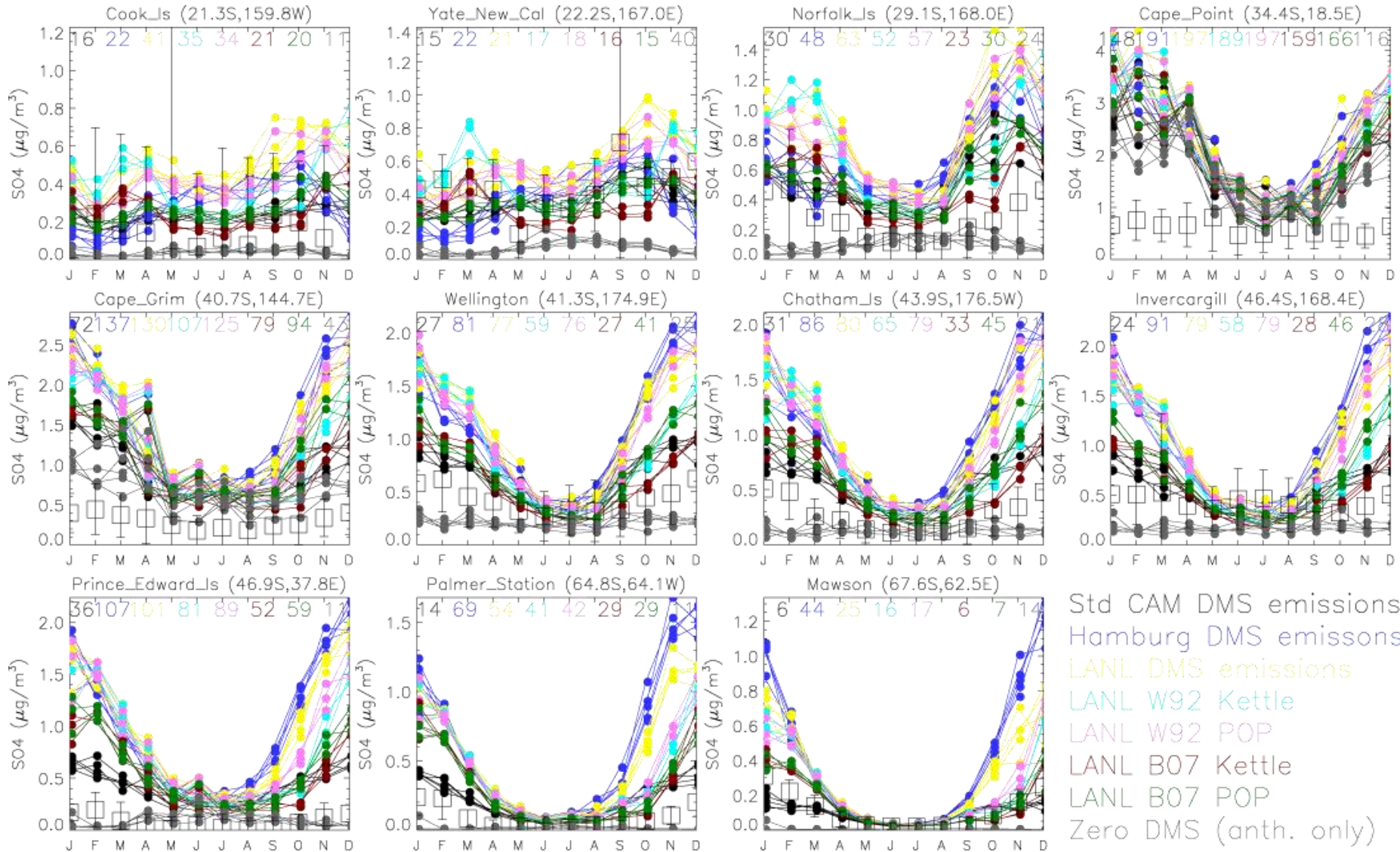
TOMS climatology (1996-2003)



Super-fast chemistry with Linoz



Sulfate aerosols validate well against surface observations.



Fast mechanisms maintain sensitivity of methane lifetime to perturbations.

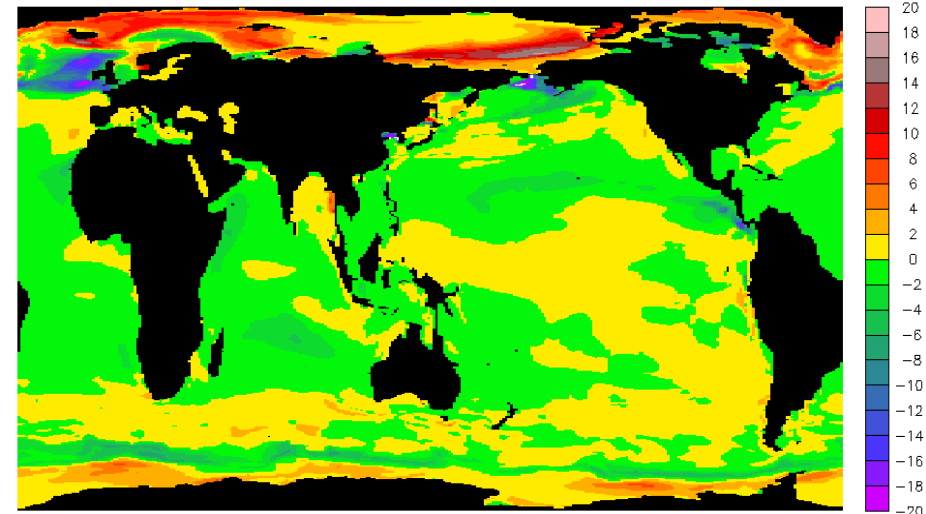
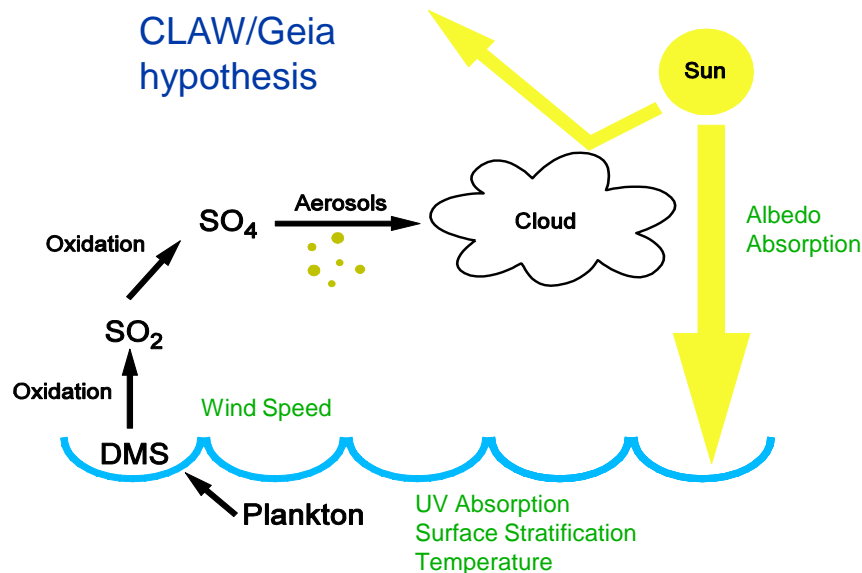


	Full mechanism	Fast	Super-fast
Control	7.03	7.16	8.45
Increase NO_x 10%	6.83 (-0.199 = -2.83%)	6.96 (-0.205 = -2.87%)	8.24 (-0.211 = -2.50%)
Increase CO 10%	7.11 (+0.086 = +1.22%)	7.26 (+0.100 = +1.40%)	8.56 (+0.110 = +1.30%)
Increase CH₄ 10%	7.26 (+0.231 = +3.29%)	7.43 (+0.267 = +3.73%)	8.72 (+0.264 = +3.12%)

Methane lifetime in years. In parentheses, the change in lifetime due to the change in emission relative to the control.

Our fast mechanisms make Earth System Model simulations feasible (eg, CLAW/Gaia).

- Atmos. chem. and biosphere interact to affect climate.
- We have integrated our atmospheric chemistry with the ocean sulfur cycle from Los Alamos National Lab.
- We are now testing the CLAW/Gaia climate stabilization hypothesis.

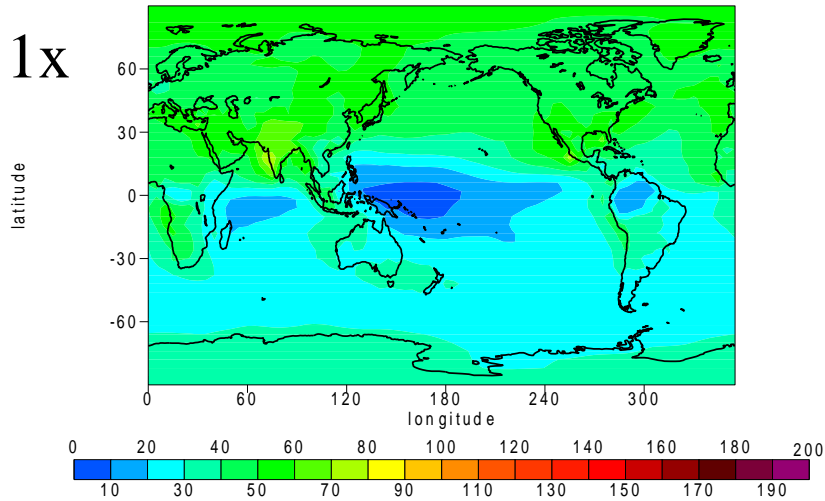


DMS emission change over 21st century
Philip Cameron-Smith, LLNL, LLNL-PRES-411136

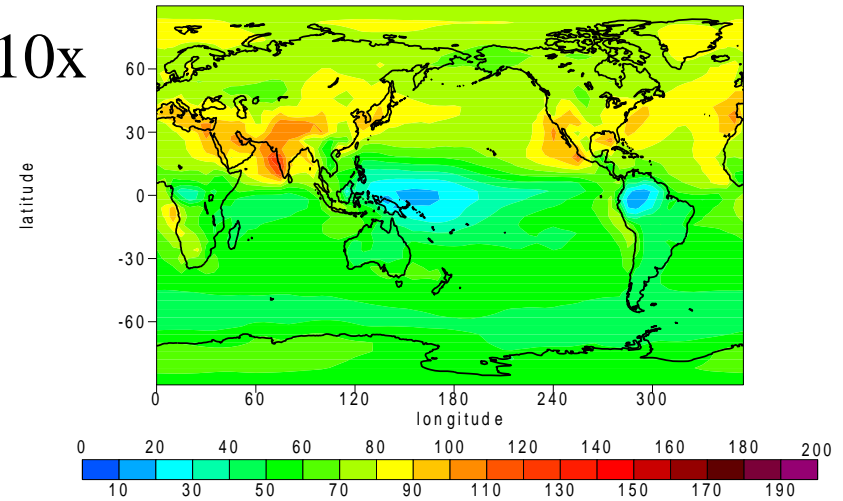
Extreme methane emissions affect ozone

10x

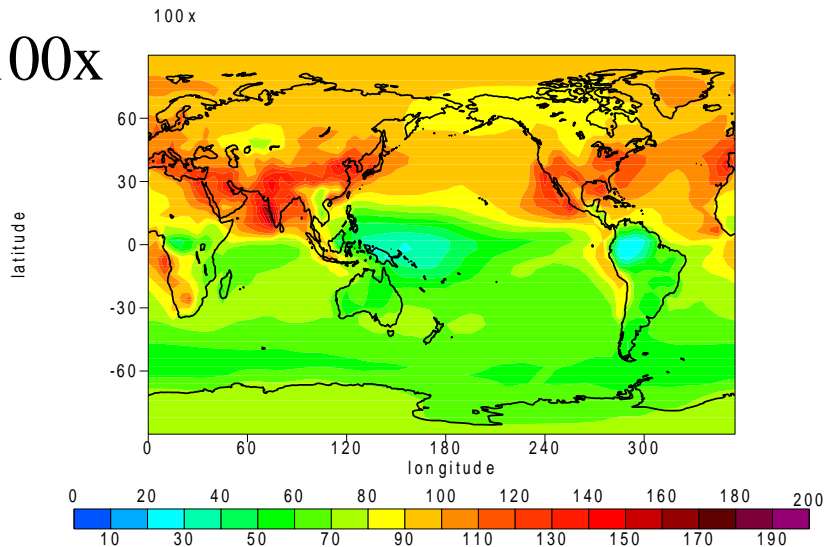
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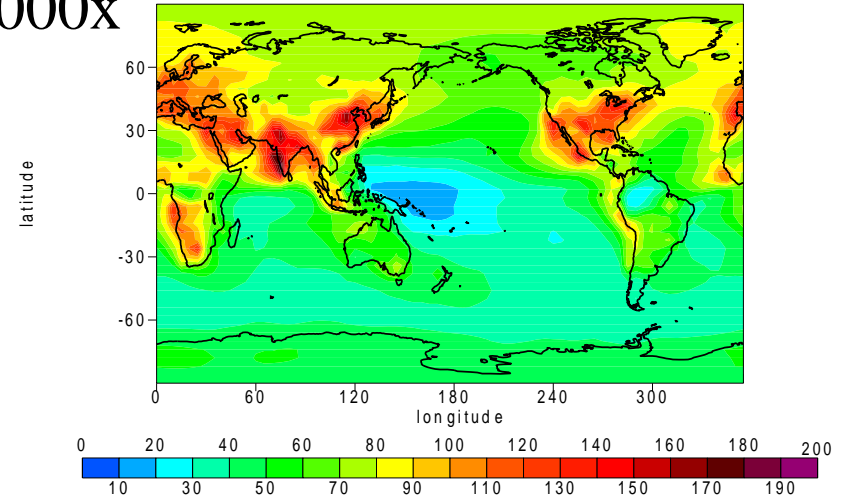
10x



100x

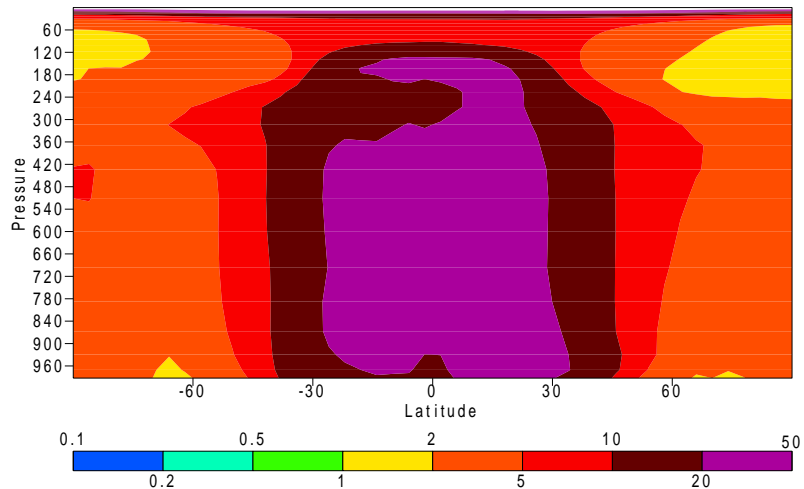


1000x

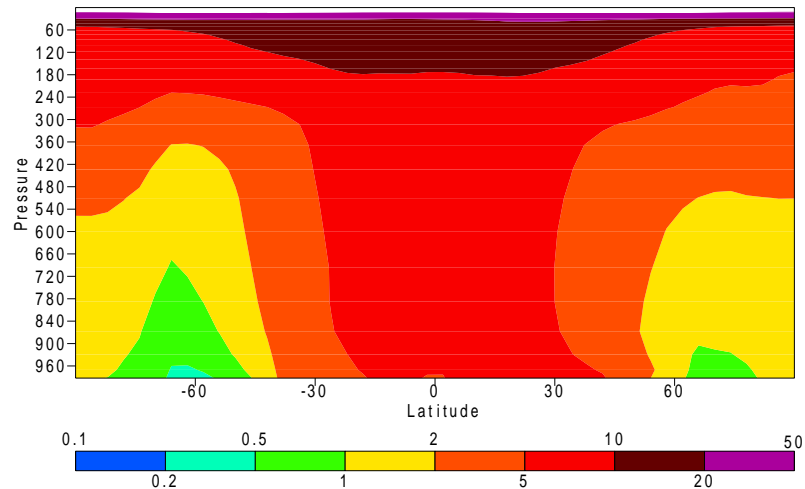


Extreme methane emissions affect OH

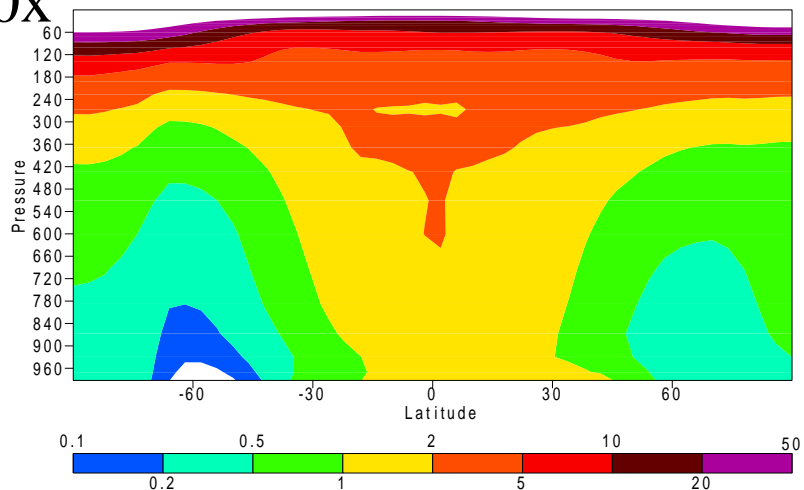
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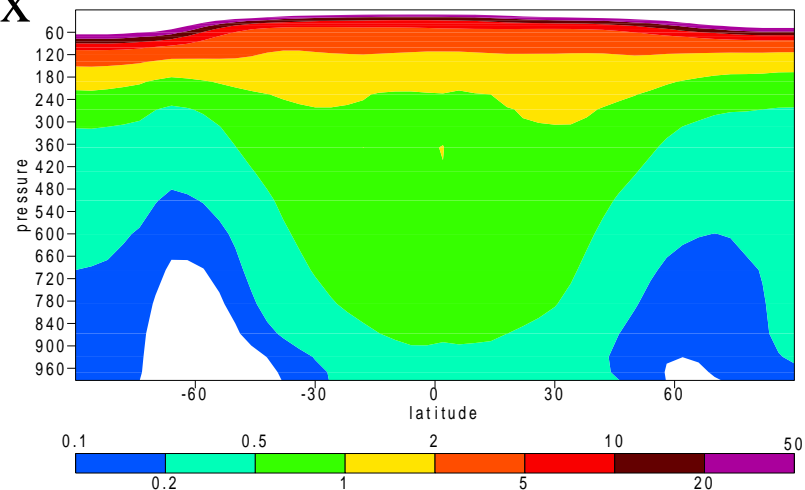
10x



100x



1000x



Conclusions

- Our fast mechanisms validate well for present day.
- Chemical *sensitivities* of fast mechanisms compare well to full mechanism.
- Fast mechanisms provide:
 - Consistent greenhouse gas and aerosol fields,
 - Climate feedbacks,
 - Interaction with biogeochemistry,
 - Only background air-quality calculated.
- These mechanisms are fast enough (1.4x) for inclusion in main IPCC simulations:
 - Provides statistics on these effects from main IPCC simulations.
- ESM simulations for CLAW hypothesis are underway.
- Studying risk of methane clathrates.