

Chemistry and Organics Working Groups

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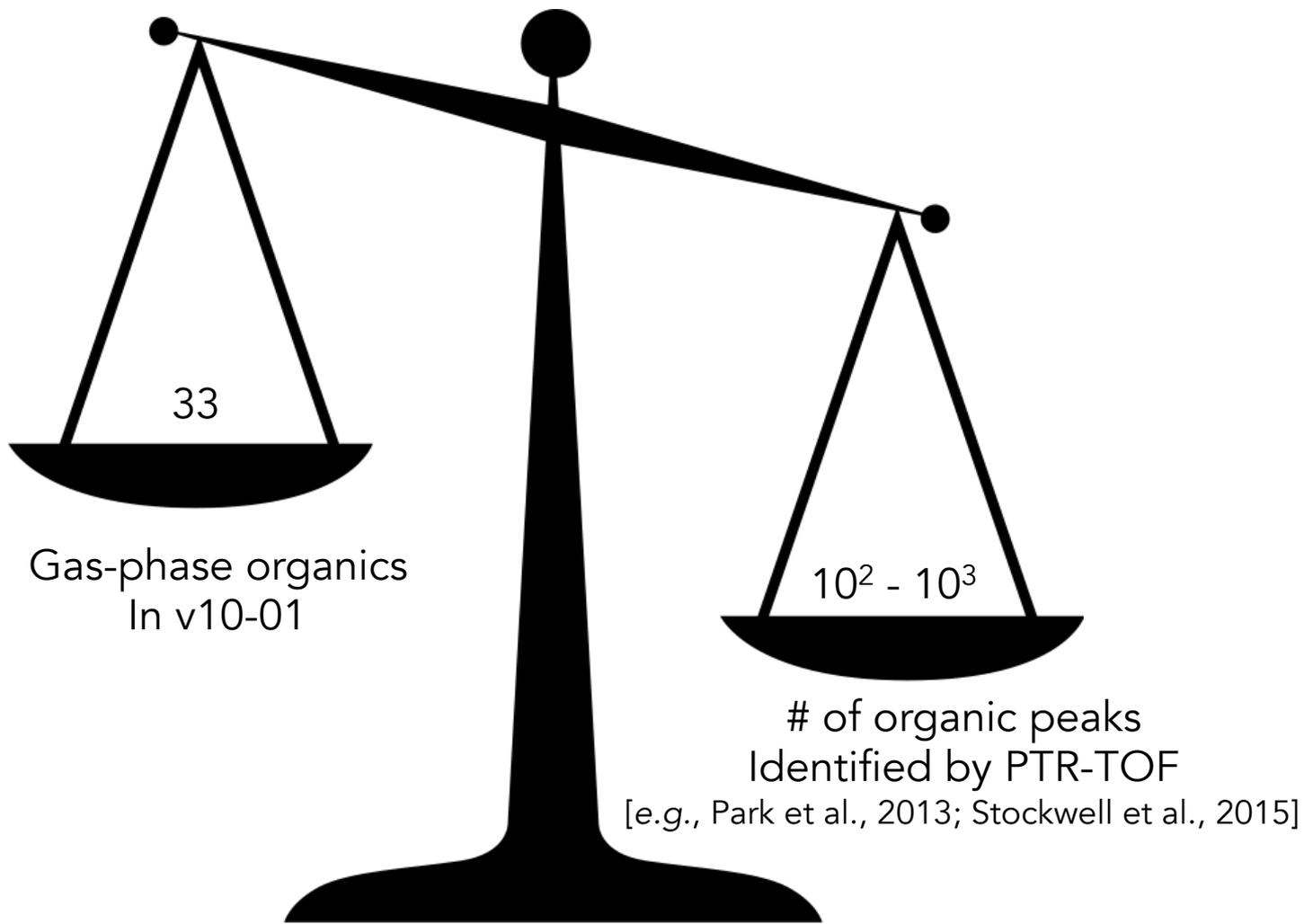


Working Group Meetings:

Emissions and Deposition: Wednesday 3:00 – 4:15, Room MD119

Chemistry: Thursday 9:00 – 10:15, Room G115

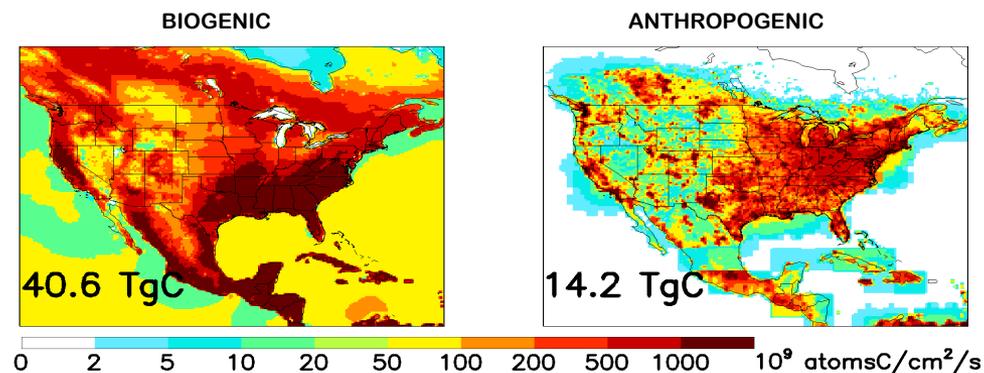
GEOS-Chem may be a bit light on gas phase tracers, but we can't add them all. What/where are the priorities?



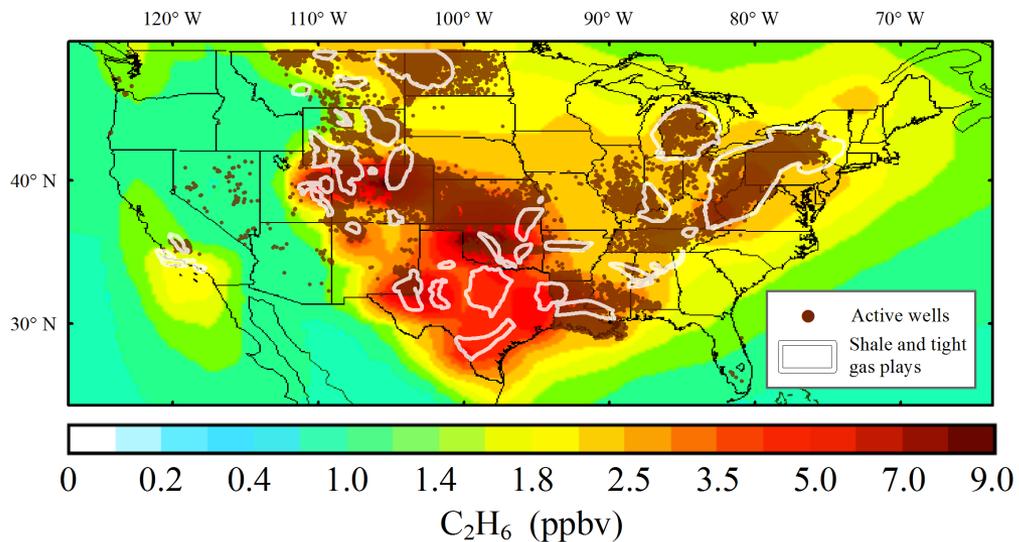
Theoretically, the problem could be much worse.
To fully describe oxidation: $10^4 - 10^{10}$

One common research theme across these WGs is constraining emissions.

Over North America...



See Poster A.8 (Xin Chen, U. Minnesota)

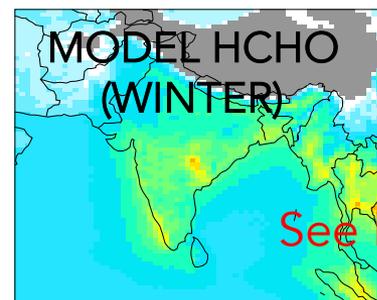
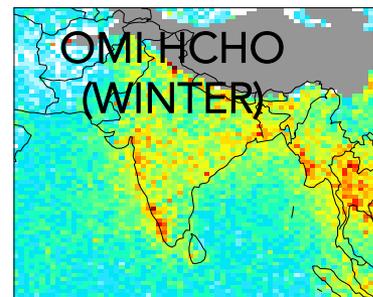
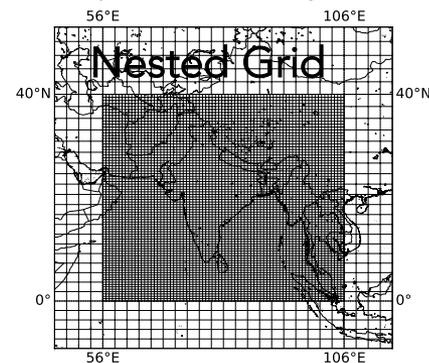


See Poster B.23 (Zitely Tzompa, CSU)

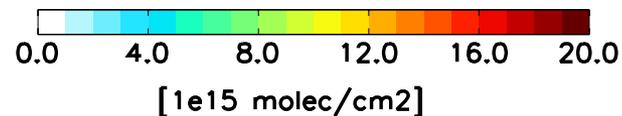
New NEI implementation

And India...

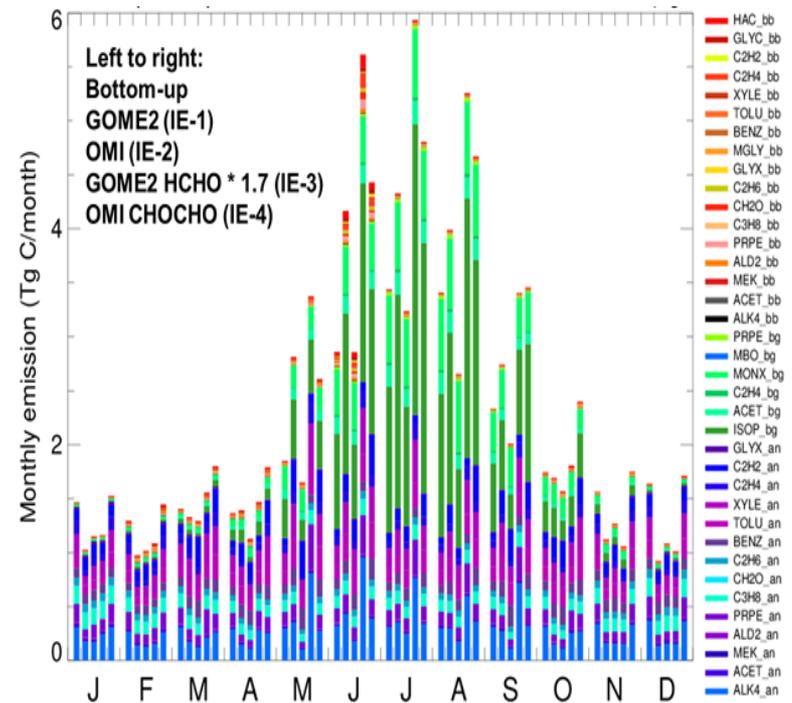
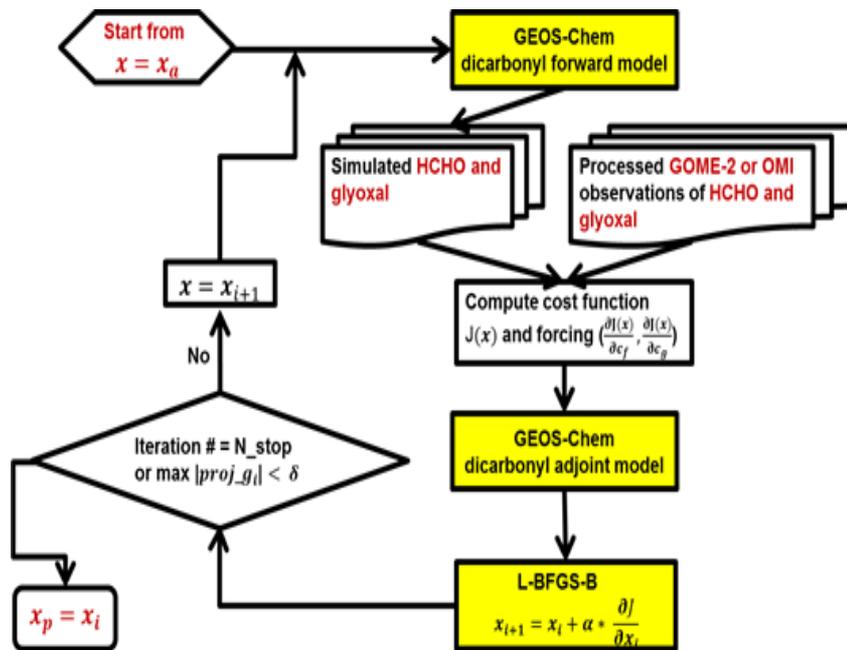
(Sreelekha Chaliyakunnel, U. Minnesota)



See Poster A.6

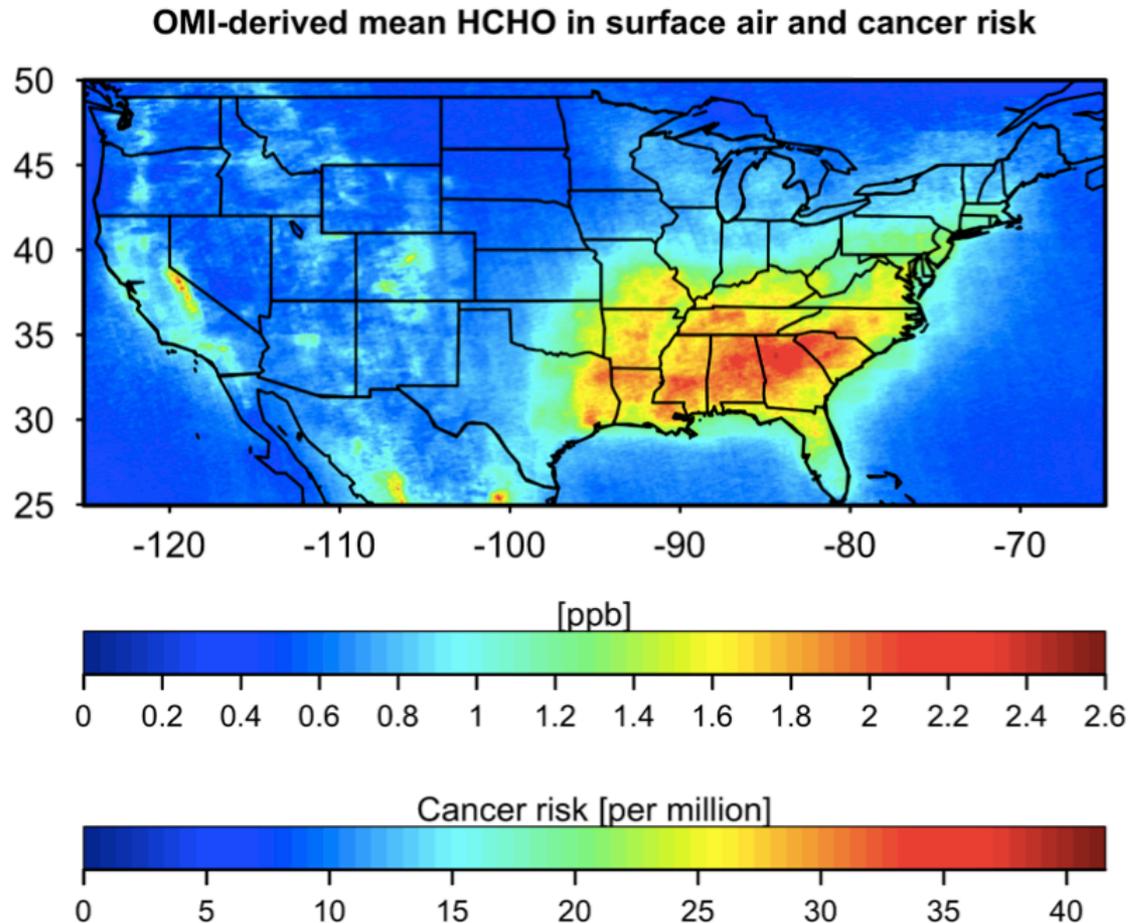


There is a dicarbonyl simulation and adjoint, and its been used in a full adjoint inversion for Chinese and global VOC emissions.



See Poster A.7

The model has also been used to derive surface HCHO mixing ratios, and quantify implications for health.

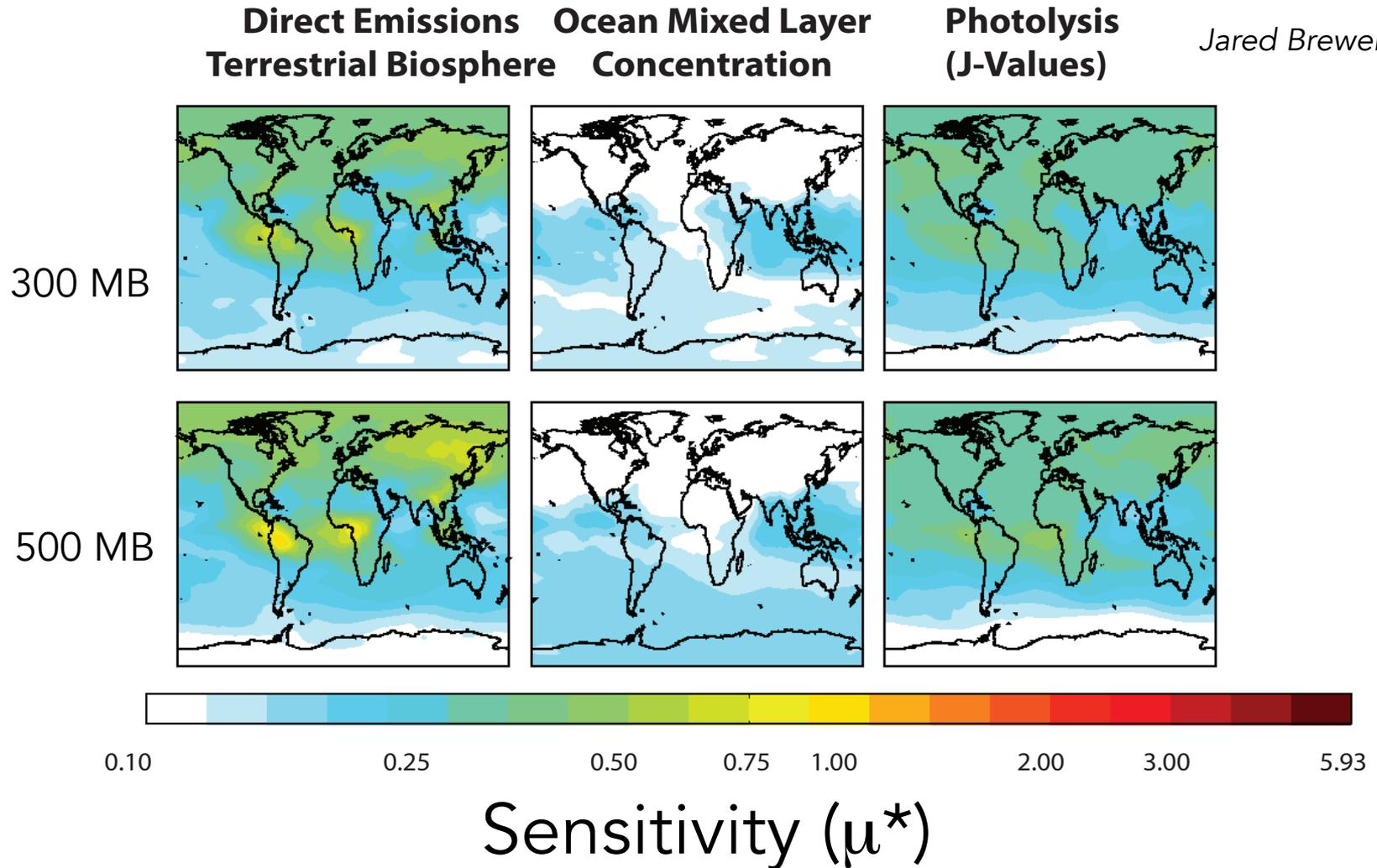


6600–13200 people in the US will develop cancer over their lifetimes by exposure to outdoor HCHO.

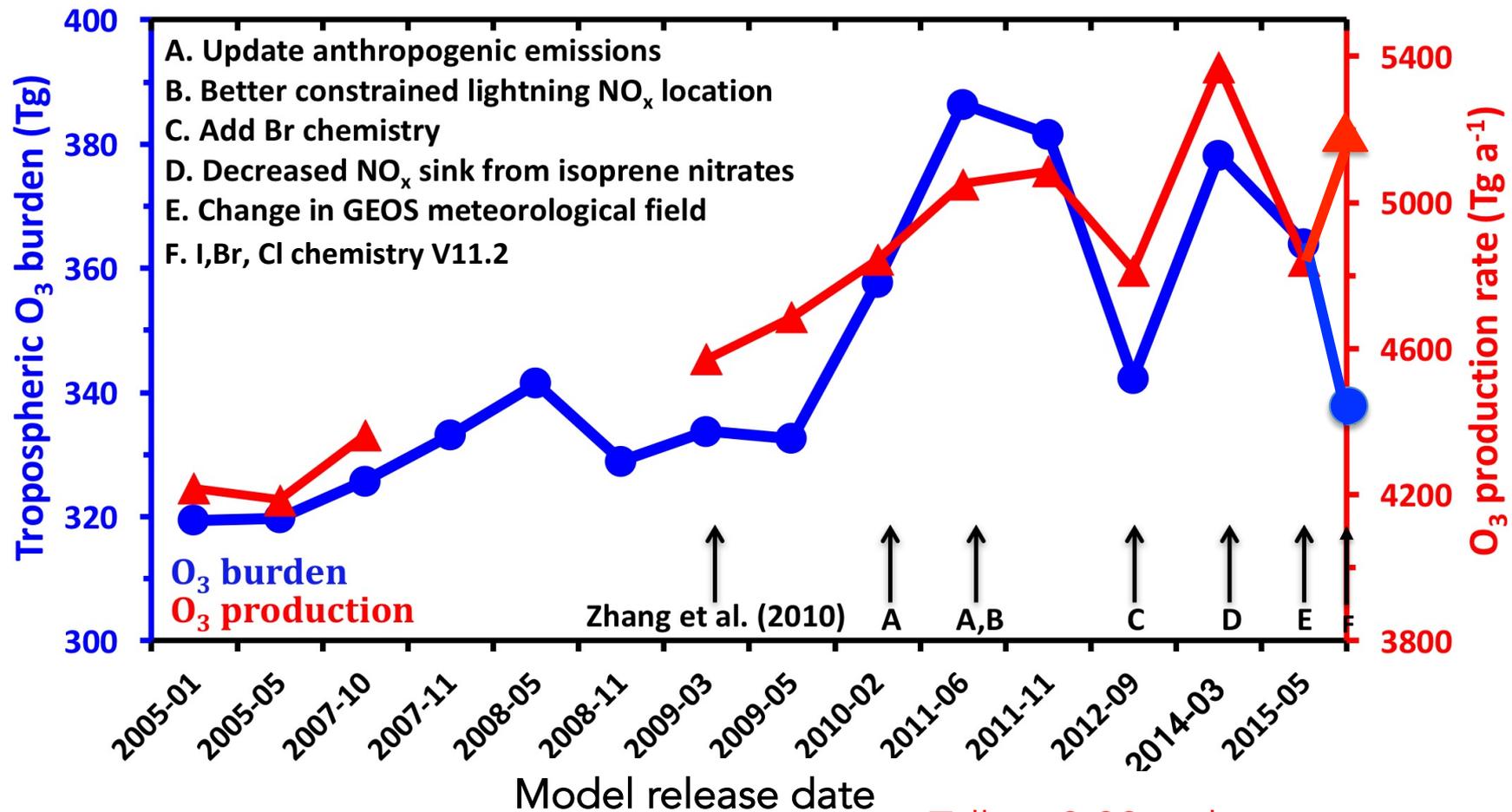
We have new strategies for setting research priorities, e.g. Morris Method. What uncertainties matter for which questions?

Talk at 4:30 today

Jared Brewer, CSU.



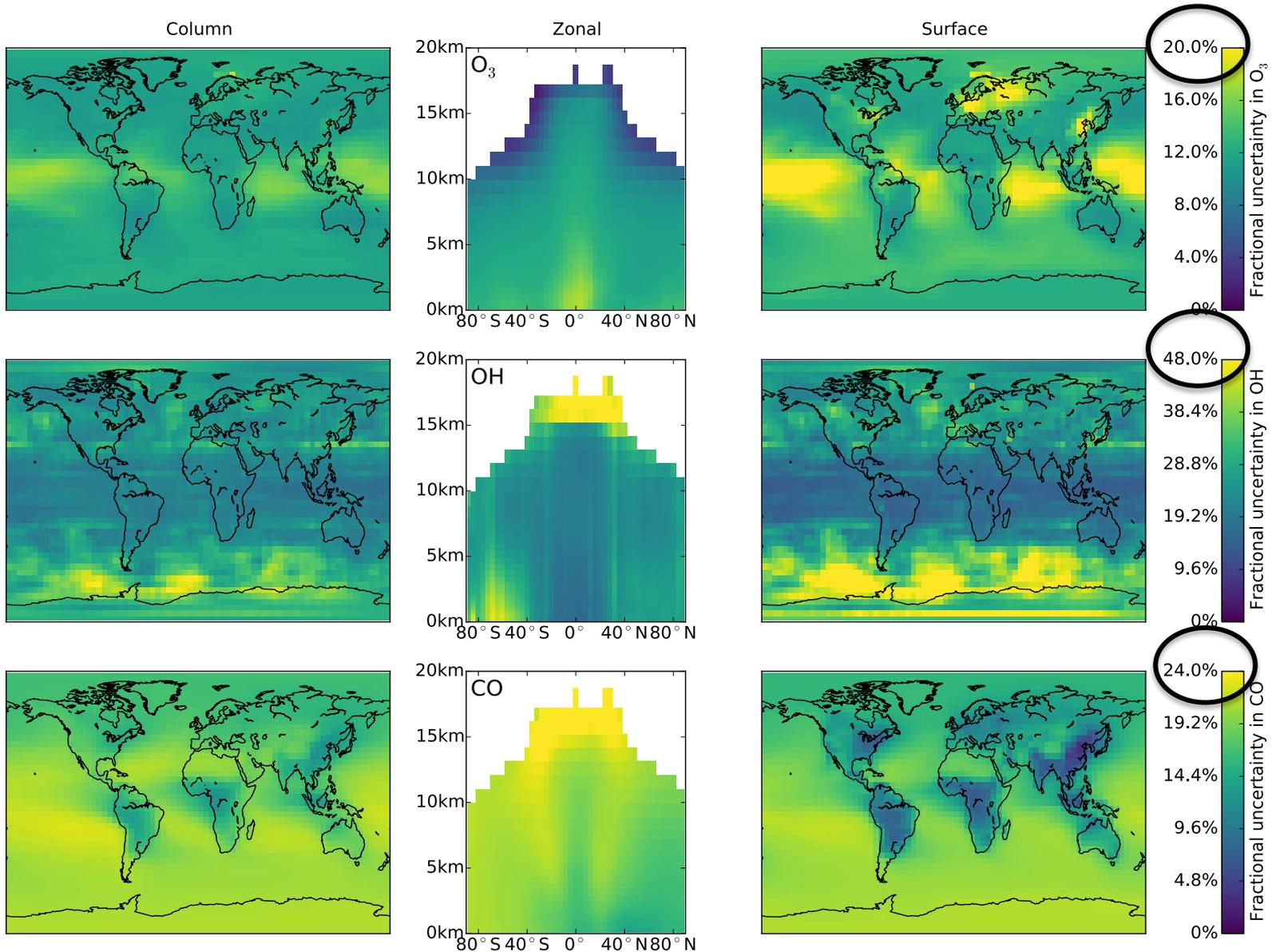
Updates have led to more active tropospheric ozone chemistry, and the best simulations yet.



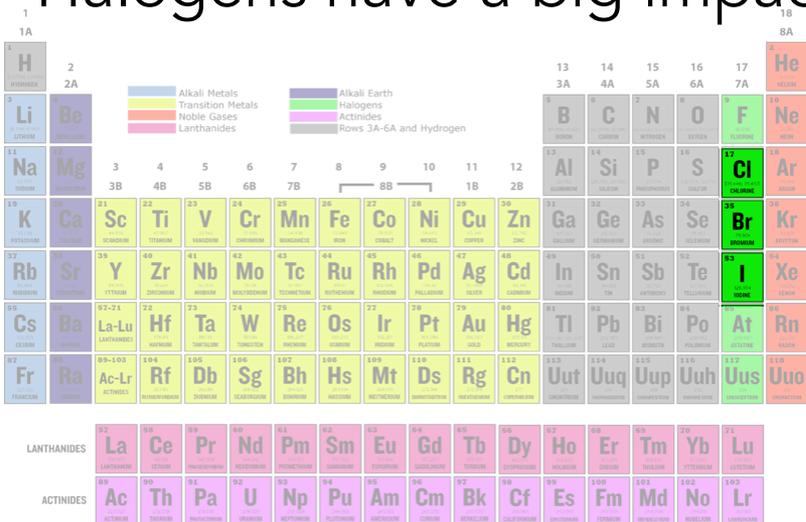
Talk at 3:00 today

Hu et al. Atmos. Environ. In review

But, a Monte Carlo ensemble on inorganic rate constants shows that chemical uncertainties on what we know best are still large.



Halogens have a big impact on troposphere.



Br: Parrella et al., 2012 V9

Br+Cl: Schmidt et al., 2016

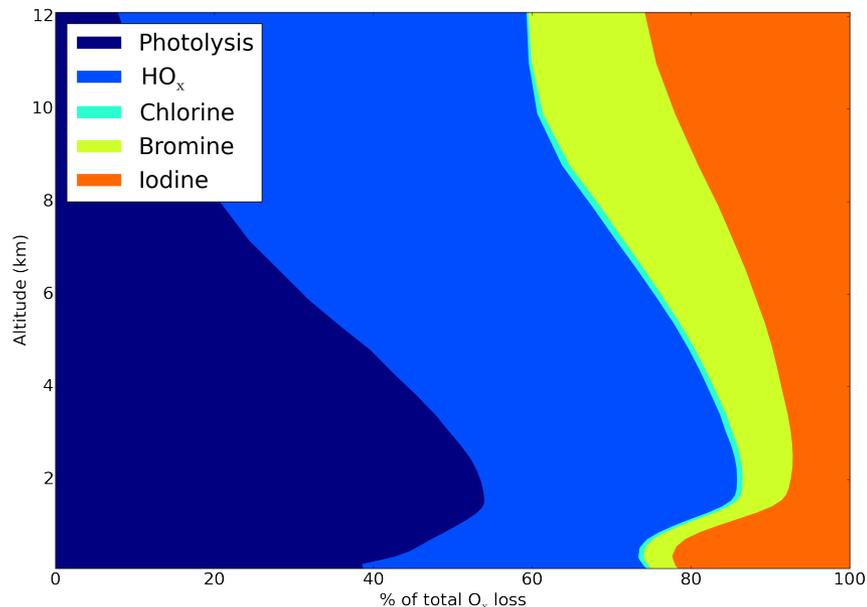
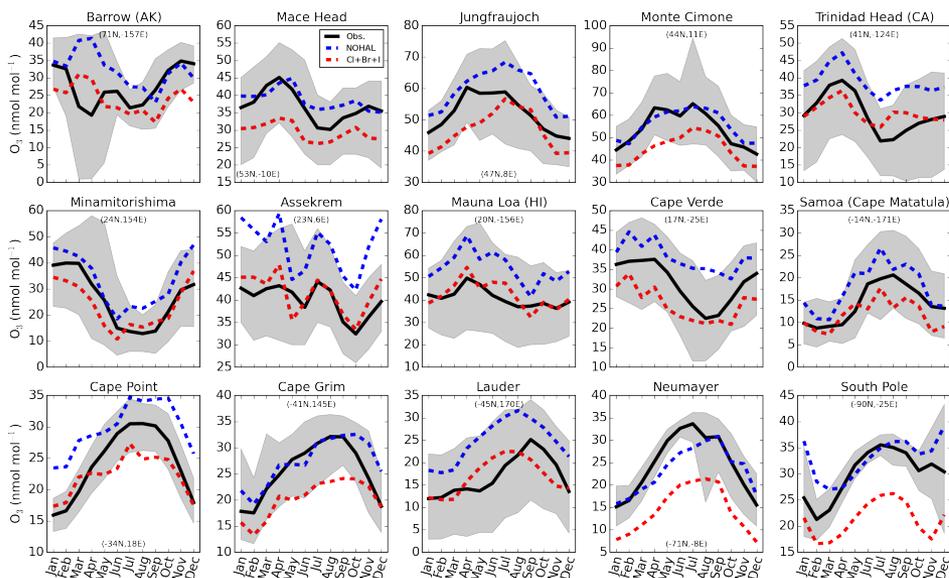
I: Sherwen et al., 2016a

I+Br+Cl: Sherwen et al., 2016b

Trying to include I+Br+Cl in V11.2

Talk from Mat Evans 2:30.

Sherwen et al., ACP, 2016



FLEXChem arrived in V11. This is a BIG change to the representation of the chemistry.

- From GEOS-Chem V1 we used globchem.dat and SMVGear to describe the chemistry.
- From V8 we had KPP and SMVGear running simultaneously. This was rather inelegant.
- For V11 we have a clean implementation of KPP within the model thanks to Mike Long and the support team.
- Need to have all diagnostics – concentrations, fluxes, rate constants working and efficient.

There are many recent updates that overlap the Chemistry and Organics working groups.

v11.1 Error Corrections / Updates

PMN + O ₃ – Update products	Dylan Millet
MOBA + OH → MOBAOO	Will Porter
ISNOAA + NO ₂ → PMN	Mike Long
Fix molecular weight of N ₂ O ₅	Chi Li

v11.1 New Science

Criegee intermediates	Dylan Millet
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v11.1 New Engineering

FlexChem	Mike Long
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v11.2 Error Corrections / Updates

JPL 15 Barron Henderson / Thomas Sherwen	
ALK4 lumping	Barron Henderson
Monthly mean NEI2011	GCST / Katie Travis

v11.2 New Science

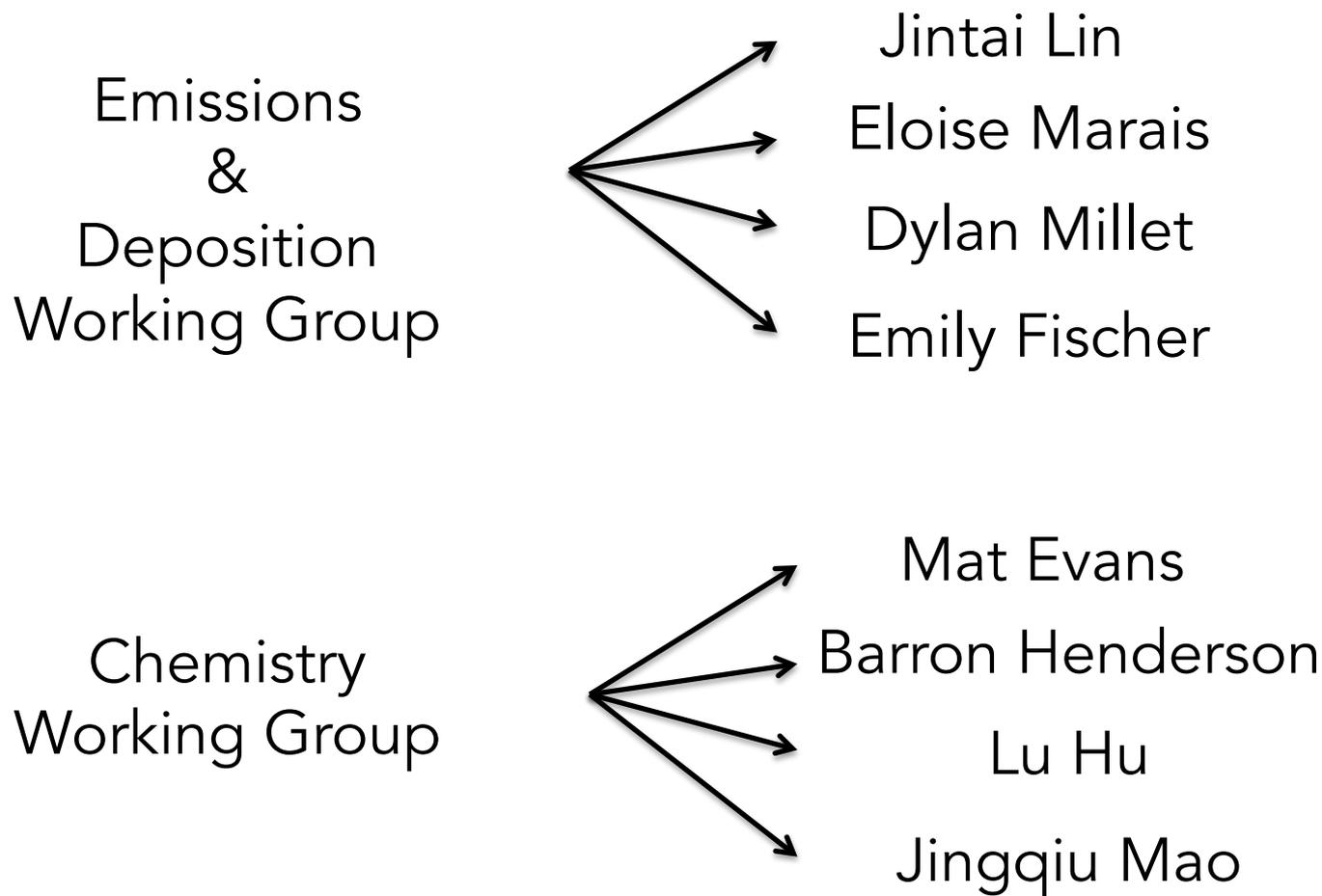
PAN Updates	Emily Fischer
Isoprene nitrates updates	Jenny Fisher / Eloise Marais / Kelvin Bates / Katie Travis
I, Br, Cl Trop Chemistry	Tomas Sherwen

These are the updates relevant to Emissions & Deposition that are also slated for v11.2.

v11.2 Error Corrections / Updates

EDGAR v4.3 emissions	Chi Li
EPA BC/OA emissions over the U.S.	David Ridley
Historical CAC emissions	Chi Li
Default US emissions to NEI after 2011	Dalhousie group
Arctic seabird NH ₃ emissions	Betty Croft
Ocean NH ₃ emissions	Fabien Paulot
NO _x from snowpack	Maria Zatko, Becky Alexander
Non-agricultural NH ₃	Amos Tai

This is the new working group structure, and your chairs.



We have much to discuss during the breakout sessions.
Emissions and Deposition Topics:

- Should bi-directional fluxes be prioritized?
- Are parameterizations of fire plume injection heights ready for global application?
- What are emerging issues for prioritization? Which emerging issues are your highest priorities? Which will provide the most benefit to the broader community?
- Other questions/challenges?

Emissions and Deposition:
Wednesday 3:00 – 4:15, Room MD119

Among others, the Chemistry WG is planning on discussing these questions?

- As we extend the hydrocarbons (i.e. terpenes, aromatics, larger VOCs), how should we handle speciation?
- Should we be moving all chemistry to KPP (e.g., lumped monoterpenes)?
- What are emerging issues for prioritization? Which emerging issues are your highest priorities? Which will provide the most benefit to the broader community?
- Other questions/challenges?

Chemistry:
Thursday 9:00 – 10:15, Room G115