New chemistry and diagnostics for the MOZART chemistry suite in WRF-Chem

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T1-MOZCART Chemistry Option

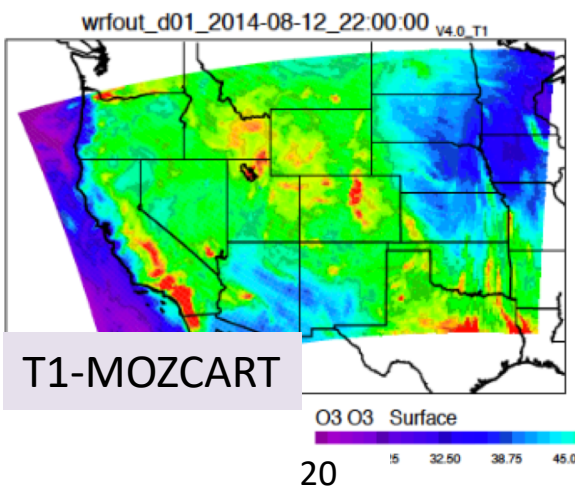
- Gas chemistry is updated from MOZART v4 (Emmons et al., 2010)
- Isoprene chemistry expanded
- Lumped aromatics and terpenes split into individual species
  - Toluene → benzene, toluene, xylenes
  - Monoterpenes → a-pinene, b-pinene, limonene
  - Detailed representation of organic nitrates
- Heterogeneous reactions (13 reactions between trace gas and aerosol)
  - HO_2 → 0.5 H_2O_2
  - N_2O_5 → 2 HNO_3
  - NO_2 → 0.5 OH+0.5 NO+0.5 HNO_3
  - NO_3 → HNO_3
  - hydroxy nitrates → HNO_3
  - GLYOXAL → CO_2

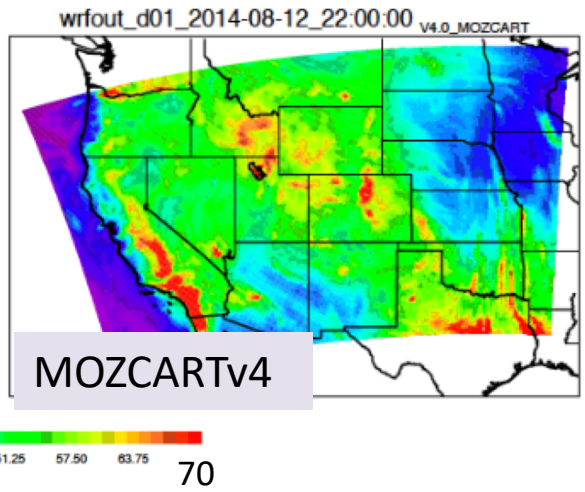
New chemistry allows researcher to analyze boundary layer chemistry in more (better) detail

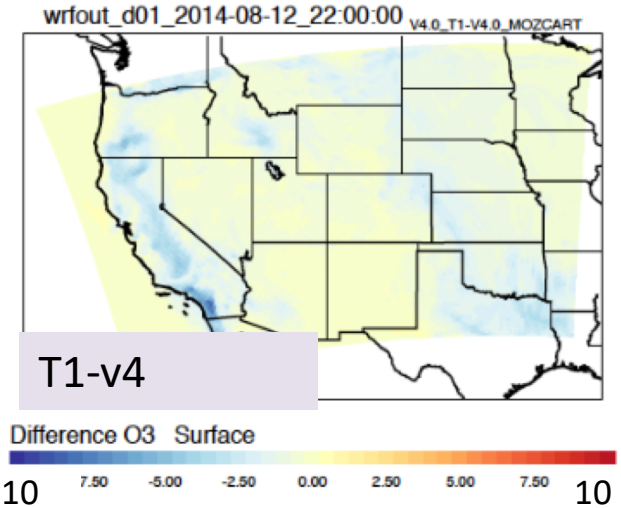
Example: August 12, 2014 FRAPPE/DISCOVER-AQ simulation

- 10-13 August 2014 simulation time with analysis nudging
- 12-km grid spacing with 51 vertical levels to 50 hPa
- Adjusted NEI2011v2 anthropogenic emissions, MEGAN biogenic emissions, FINN fire emissions

Surface Ozone: ± 2 ppbv differences





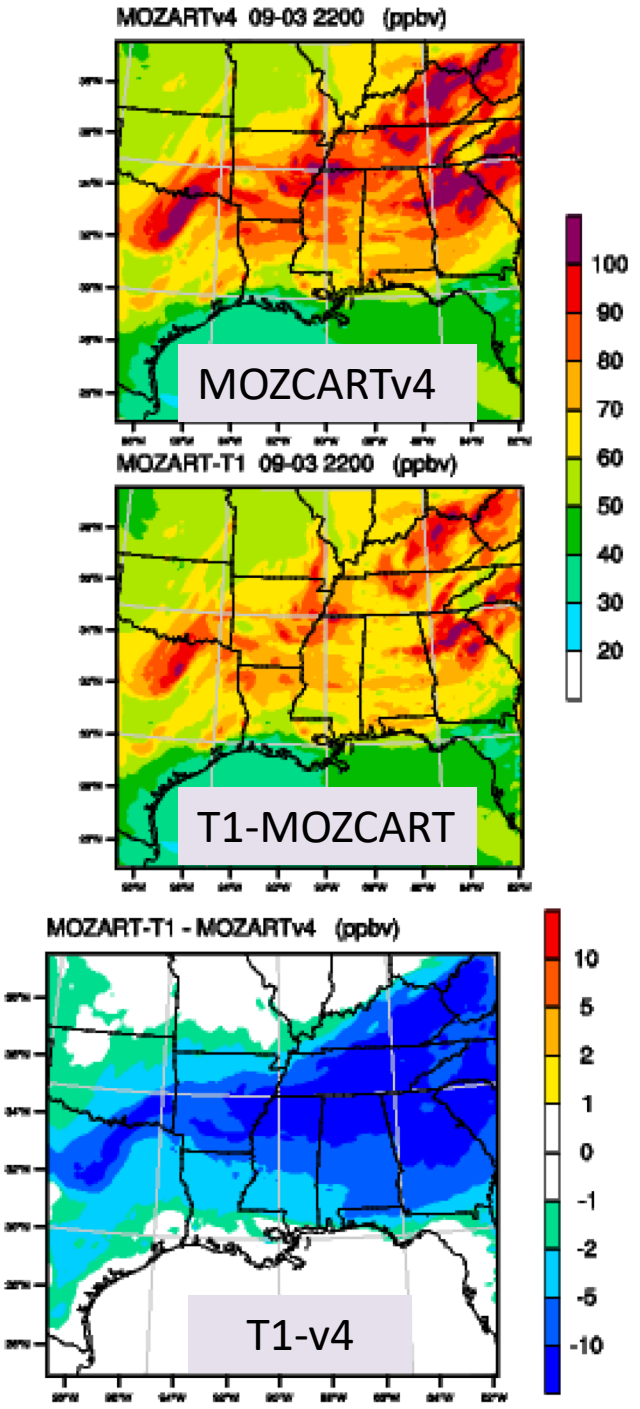


Example: September 2, 2013 SEAC4RS simulation

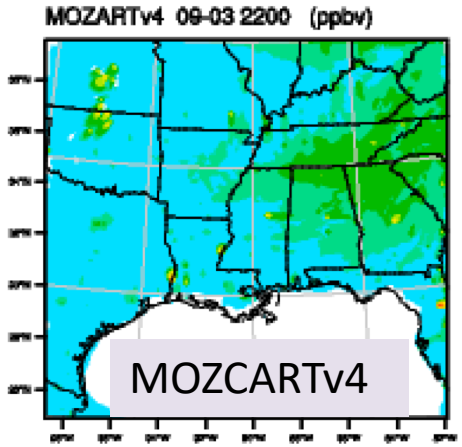
- 1-2 September 2013 simulation time
- 12-km grid spacing with 74 vertical levels to 50 hPa
- NEI2011v2 anthropogenic emissions, MEGAN biogenic emissions, FINN fire emissions

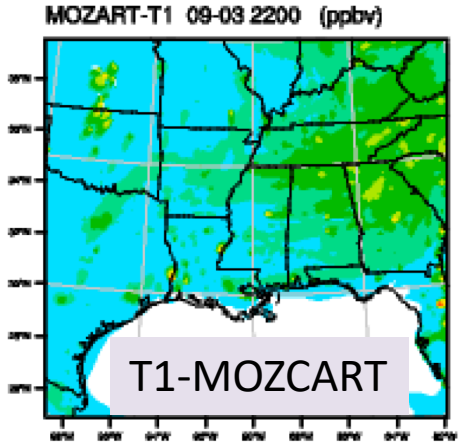
- **Preliminary results** – just beginning to evaluate with obs

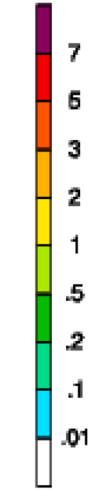
Surface Ozone: -10 ppbv differences



Effect of Unlumping Aromatic Alkenes

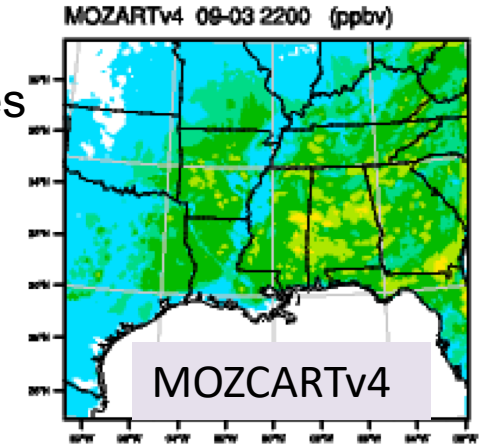


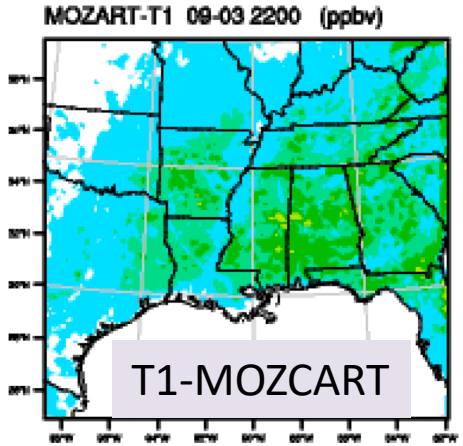




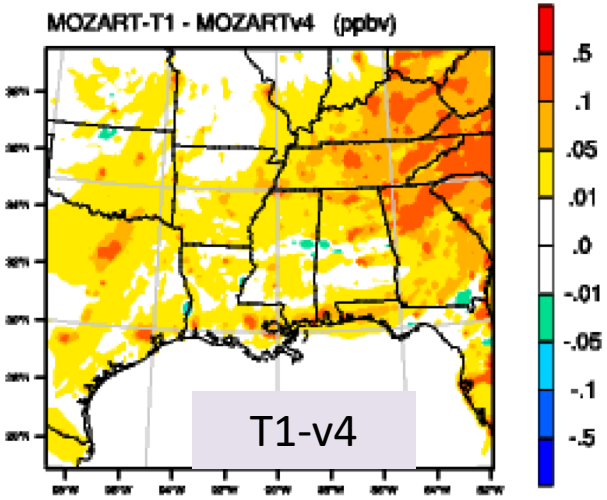
← Toluene

Monoterpenes →

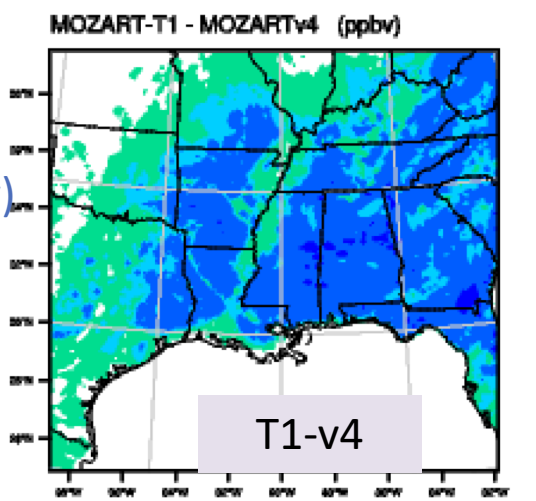


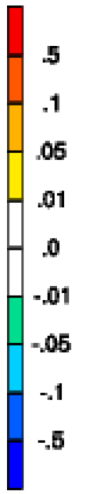


Surface Toluene vs SUM(TOL,BENZ,XYL) causes ~2x more (250 pptv to 500 pptv) of these alkenes over anthropogenic regions in T1-MOZCART



Surface monoterpenes are up to ~2x less (1 ppbv to 0.5 ppbv) of these alkenes over forest regions in T1-MOZCART





T1-MOZCART Chemistry Option

- T1-MOZART description paper to be submitted to JAMES (Emmons et al.)
- T1-MOZART (chem_opt = 114) has 142 compounds
- MOZART v4 (chem_opt = 112) has 84 compounds
- → Increase in computational costs and memory
- 48-hour simulation with 144 processors on Cheyenne
  - 215 CPU hours (1 hr 34 min wall clock time) and 62 Gb memory for MOZART v4
  - 406 CPU hours (2 hr 53 min wall clock time) and 76 Gb memory for T1-MOZCART

New compounds → updating compounds for wet deposition and dry deposition

Key update is the Henry's Law (solubility) coefficients

New chemistry allows researcher to analyze boundary layer chemistry in more (better) detail

Updated Henry's Law Coefficients

- Input table of Henry's Law and Dissociation Constants based on JPL (2015) and Sander (2015)
- Accessed by wet deposition, dry deposition, convective-parameterized wet deposition
- Consistent values used throughout model
- Only available for MOZART suite of chemistry options (chem_opt = 111, 112, 114, 201, 202)
- module_dep_simple needs to be cleaned up

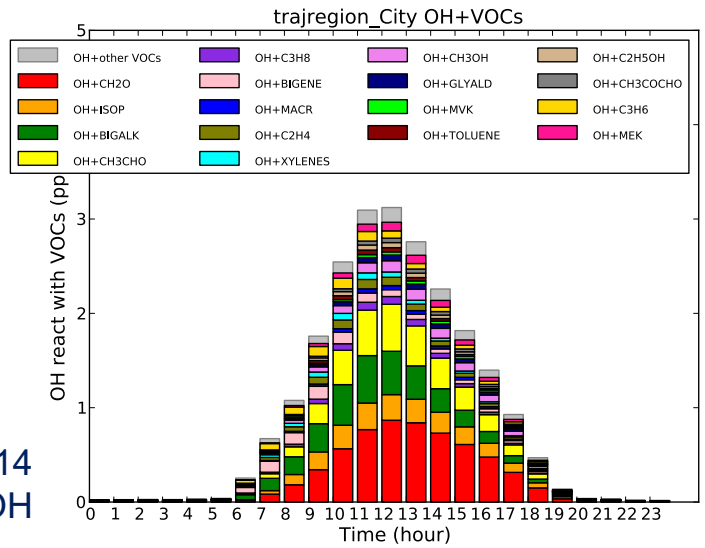
HLC.TBL contains:

Species	Eqn Type	MW	KH(298)	-ΔH/R	K1(298)	-ΔE/R	K2(298)	-ΔE/R
H2O2	0	34.0136	87000	7320	2.20E-12	-3730	0	0
HCHO	0	30.0252	3230	7100	0	0	0	0
CH3OOH	0	48.0394	300	5280	0	0	0	0
O3	0	47.9982	0.0103	2830	0	0	0	0
SO2	0	64.0648	1.36	3100	0.013	1960	6.60E-08	1500
NH3	1	17.0289	60.2	4160	1.70E-05	-4325	1.00E-14	-6716

Integrated Reaction Rates (IRR) Output

collaboration with Will Vizuete (UNC), Chi-Tsan Wang (UNC)

- IRR = summation of a reaction rate from a start time to an output time (e.g. from start of simulation to each output time)
- Can specify which domain, how often the output occurs, which reaction rates are printed out (including all reactions)
- Output can be analyzed to determine chemical evolution, OH cycling, NOx budget, and chemical production and loss terms

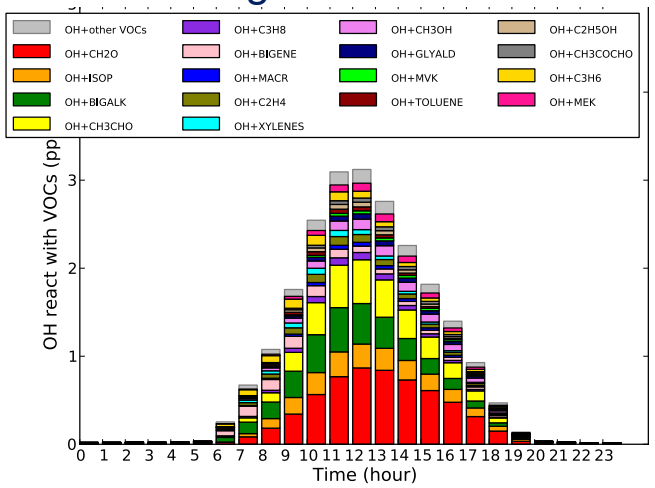


IRR analysis for Denver Metro Area during FRAPPÉ 2014
→ VOC + OH reactions dominated by CH_2O+OH

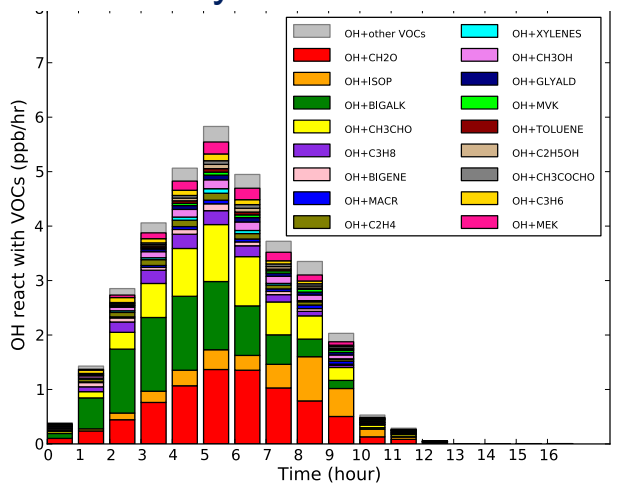
Integrated Reaction Rates (IRR) Output

- Analysis can be done over regions of interest (e.g. urban plume) or along trajectories
- See P17, Pfister et al. poster for more information

OH reactivity for Denver Metro Area during FRAPPÉ 2014

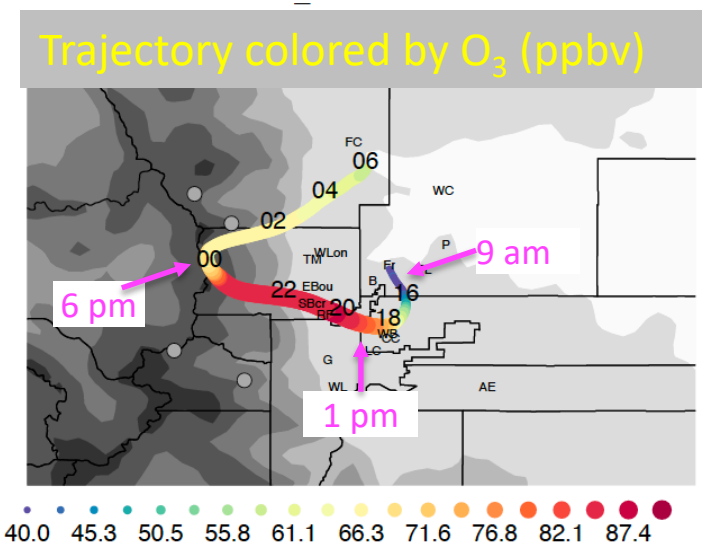


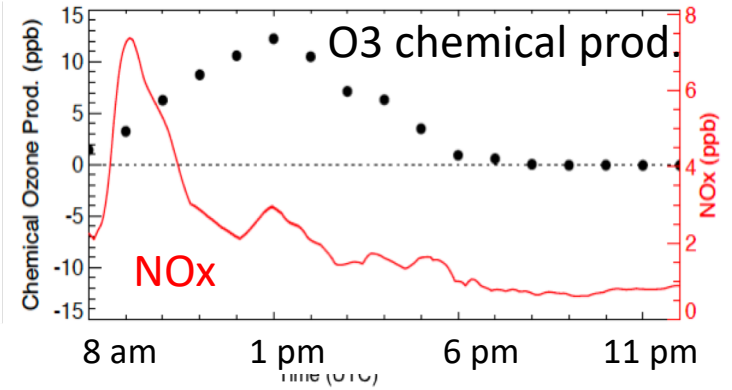
OH reactivity along a trajectory from SW Weld Cty to Denver to ~RMNP

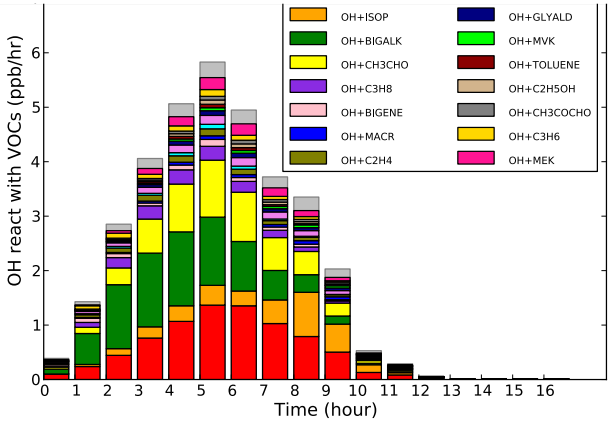


Integrated Reaction Rates (IRR) Output

- IRR output complements the tendency terms in the chem_diag option: advz_tend, advh_tend, conv_tend, vmix_tend, chem_tend
- See P17, Pfister et al. poster for more information



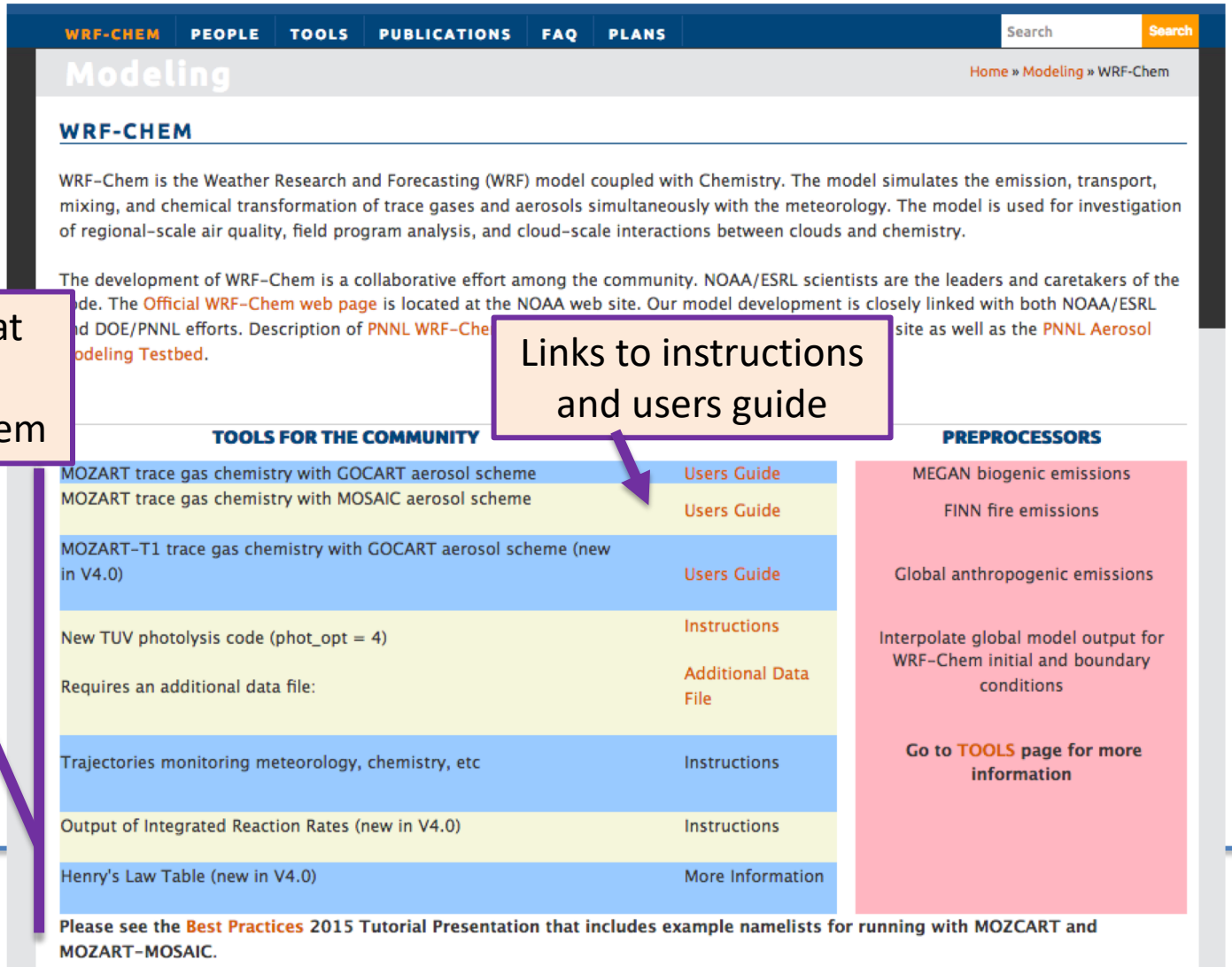




OH reactivity along a trajectory from SW Weld Cty to Denver to ~RMNP

NCAR/ACOM WRF-Chem Web Page

https://www2.acom.ucar.edu/wrf-chem



Developments that NCAR/ACOM has added in WRF-Chem

Links to instructions and users guide

NCAR/ACOM WRF-Chem Discussion Forum

https://www2.acom.ucar.edu/wrf-chem/discussion-forum

DISCUSSION FORUM

Note: The Discussion Forum is open for viewing but to participate, you must have or create a Google account.
Please note that we can only provide help with the MOZART chemistry packages and the from us developed processing tools.

WRF-Chem general discussion. Subscribe

These are **only** for NCAR/ACOM tools and developments

WRF-Chem anthro_emiss: Anthropogenic emissions. Subscribe

WRF-Chem bio_emiss: Biogenic emissions. Subscribe

WRF-Chem fire_emiss: Fire emissions. Subscribe

WRF-Chem lightning: Lightning and Lightning NOx. Subscribe

WRF-Chem mozbc: Boundary conditions using MOZART global model output. Subscribe

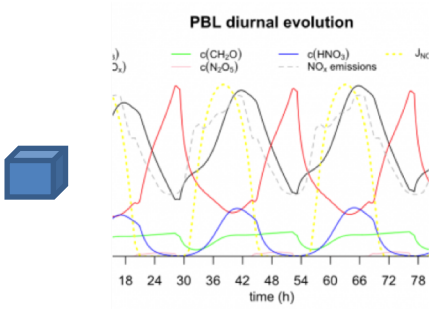
WRF-Chem Run: Running WRF-chem for MOZCART and MOZART-MOSAIC. Subscribe

Future Model Development: Currently we have 3 scales of models

Understanding the Chemistry in Detail

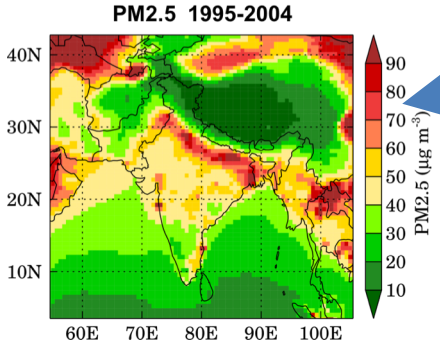
Generator of Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A)

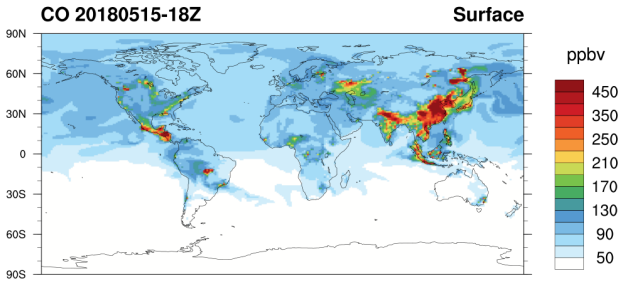
BOXMOX = box model with chemistry as represented in many 3-d chemistry transport models



Examining the Urban/Cloud to Regional Scales

Weather Research and Forecasting model coupled with Chemistry





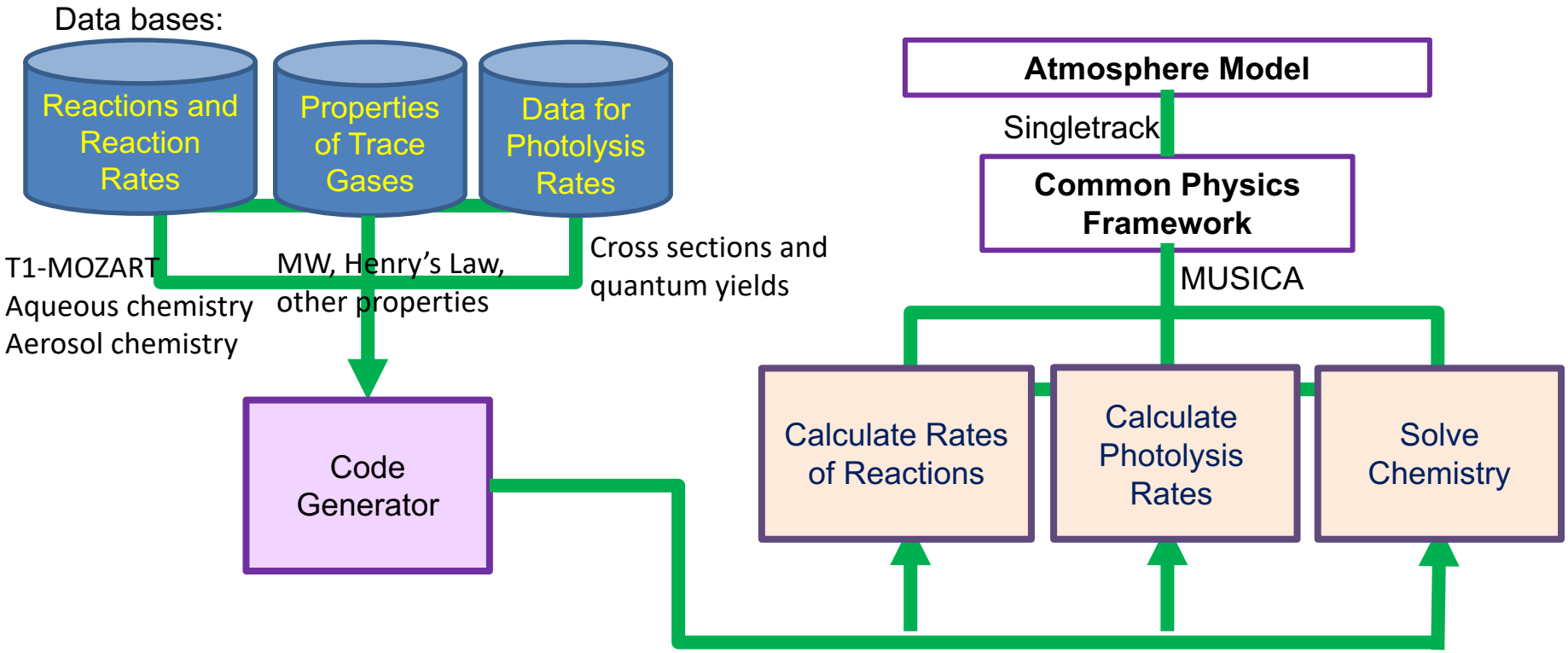
Global Scale Impacts of Atmospheric Chemistry

Community Atmosphere Model with Chemistry

Whole Atmosphere Community Climate Model

Model-Independent Chemistry Module (MICM)

- Same infrastructure for box models, regional-scale models, and global models



Seeking community involvement with MICM and MUSICA
Singletrack is a unified atmosphere modeling system that is being planned
MUSICA is a future global air quality model with regional refinement that is being planned

New Chemistry and Diagnostics for the MOZART Chemistry Suite

- T1-MOZCART chemistry scheme
  - Expands chemistry from MOZARTv4 (Emmons et al., 2010)
  - Still connected to GOCART aerosols
- Henry's Law coefficients
  - Table of coefficients for KH, K1, K2
  - Used in wet deposition (both subgrid and resolved), dry deposition
- Integrated rates of reactions
  - Creates new output for analyzing chemistry

- Model-Independent Chemistry Module
  - Future infrastructure for chemistry modeling at NCAR/ACOM