Overview of the WRF-Chem Modeling System

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WRF-Chem web site - http://wrf-model.org/WG11

Earth System Research Laboratory
SCIENCE, SERVICE & STEWARDSHIP

Structure of talk

- Current capabilities of WRF-Chem
- What is new in WRF-Chem – V3.5.x
- Ongoing and future work

Some general info on the modeling system

WRF-Chem is a community effort: developed nationally and internationally

Largest developer groups for version 3.5:

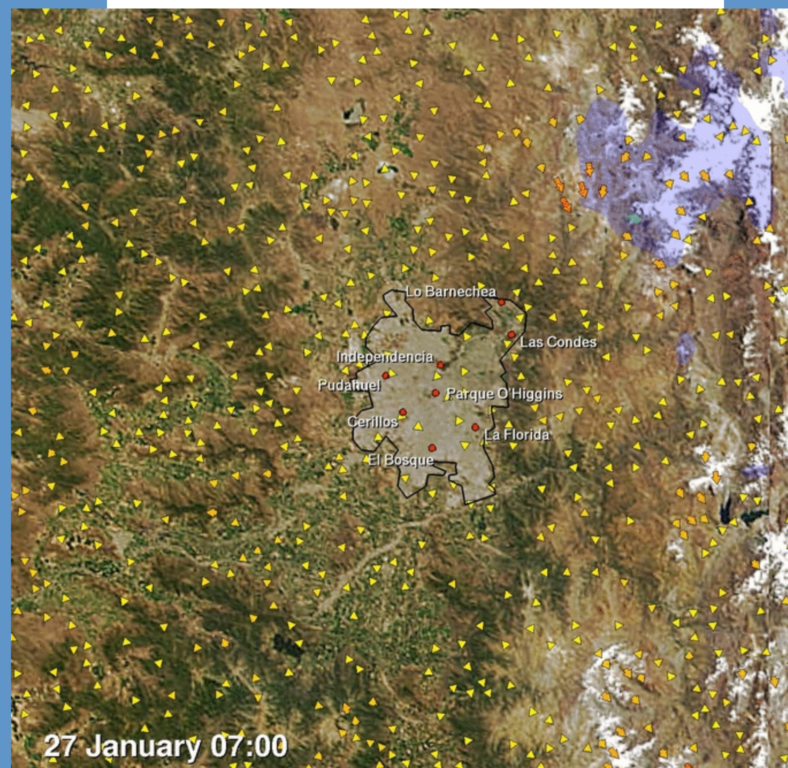
- NOAA/ESRL (wrfchemhelp)
- PNNL
- NCAR

- **Significant recent other contributions:**
- INPE/CPTEC (Brazil)
- L'Aquila (Italy)

WRF-Chem: Online coupling of modeling systems

Weather Data Analysis & Assimilation & Emissions

Simultaneous forecasts of weather and air quality



Chemistry, Aerosols, radiation, clouds, temperature, winds

Weather and AQ-Forecast

Full interaction of meteorology and chemistry

WRF-Chem: wide range of capabilities

- Many different chemical mechanisms (the part of the model that treats the interactions of the chemical species with each other),
- Multiple aerosol models (simple to very complex)
- Aerosol direct and indirect effect included
- Biogenic emissions from BEIS3.14 and MEGAN
- Coupled with a sophisticated fire plumerise model
- Regional to local scale (Large Eddy Simulation and cloud-resolving) applications, 1- and 2-way nesting capabilities
- Volcanic ash and dust, dispersion, and other tracer applications

Applications range from real-time prediction of dispersion, air quality, and weather to challenging and relevant research

Ongoing Real-Time Examples

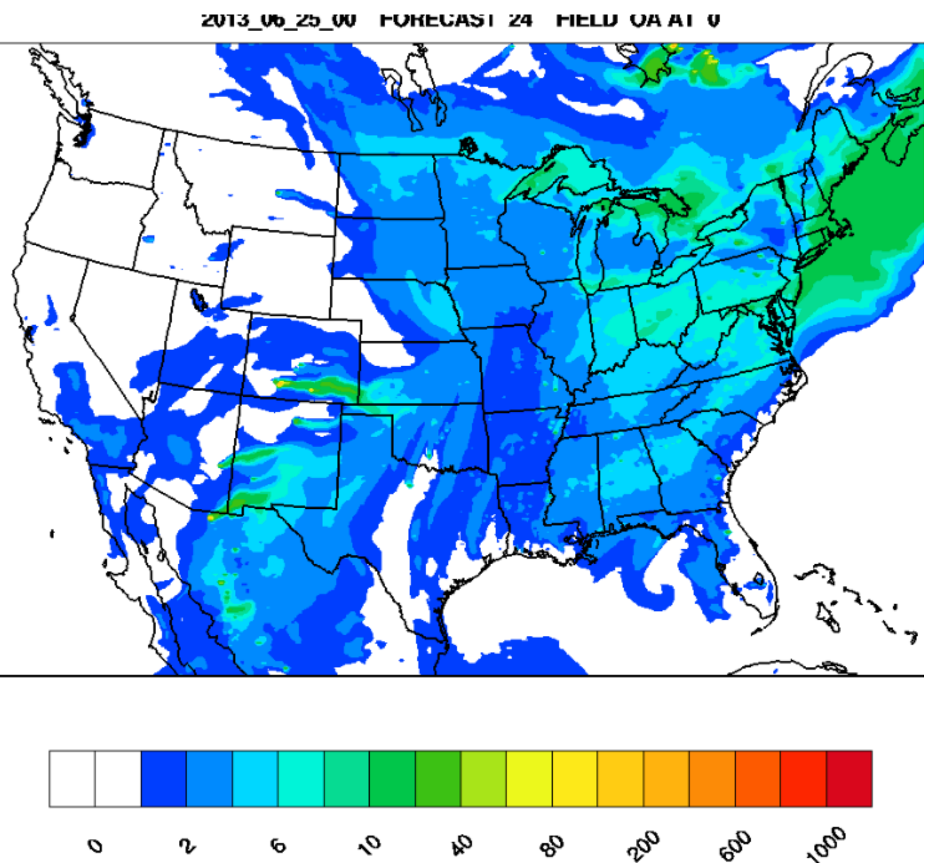
- http://ruc.noaa.gov/wrf/WG11_RT/

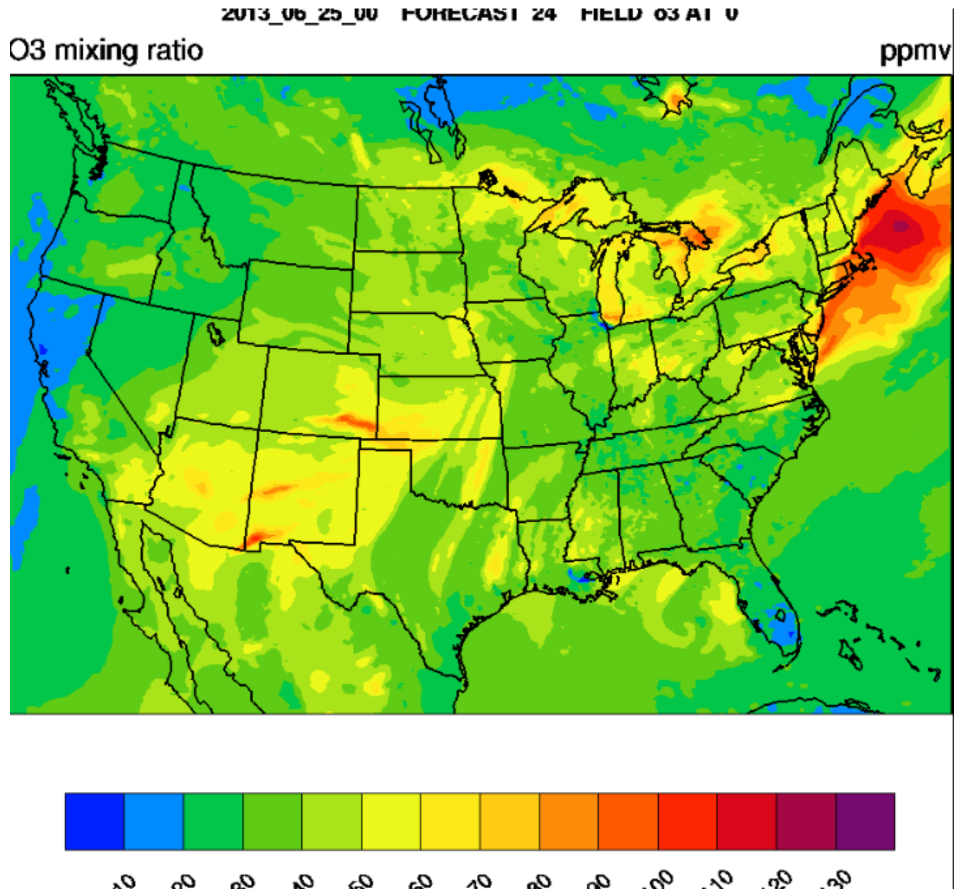
  RR-Chem WEB site, **full ozone chemistry**, aerosols, **VBS for Secondary Organics**, wildfires

- http://ruc.noaa.gov/rr/hrrrchem/

  High Resolution Rapid Refresh (ARW-WRF) with aerosols, wildfires, Western US (dx=3km), including chemical data assimilation

Example Real-Time AQ forecast





Organic aerosols

Ozone

WRF-Chem using MADE/VBS/RACM on Rapid Refresh Domain, DX=13km

Implementation of the Community Atmosphere Model version 5 (CAM5) Physics/Chemistry

- **Includes different physics options for deep and shallow convection, microphysics, boundary layer**
- **Aerosols:** *Liu et al*. (GMD, 2012), Modal Aerosol Model (MAM)
- **Gas-Phase Chemistry:** MOZART used by "CAM-Chem" already implemented in WRF-Chem by NCAR
- **PNNL** has coupled MAM with CBM-Z photochemistry in WRF-Chem

overview paper of CAM5 and coupling of these parameterizations (Rasch et al., 2013)

MAM Overview

- **Size Distribution:**
  - 3-mode version (1= Accumulation, 2 = Aitken, 3 = Coarse), designed for long-term simulations
  - 7-mode version (research version)

$\rightarrow$ Aiken $\rightarrow$ Accumulation | Coarse

nucleation *coagulation*
condensation

- **Species – 3-mode version:**
  - Prognostic: SO_4 (1,2,3) NCL (1,2,3), dust (1,3), H_2O (1,2,3), POM (1), SOA (1,2), BC (1), number (1,2,3)
  - One gas phase specie, *soag*, used for all gaseous SOA precursors
  - Diagnostic: NH_4 (assume SO_4 neutralized to form NH_4HSO_4)
  - Not treated: NO_3 (assumed to be less important on global scales). MOSAIC is being merged with MAM in CAM5 to have a more sophisticated gas-to-particle partitioning and enable NO_3 computation
- **Coupled with Gas-Phase Chemistry:**
  - CBM-Z (in V3.5)
  - MOZART (V3.6 ?)

Example: Compare MAM with other Aerosol Models

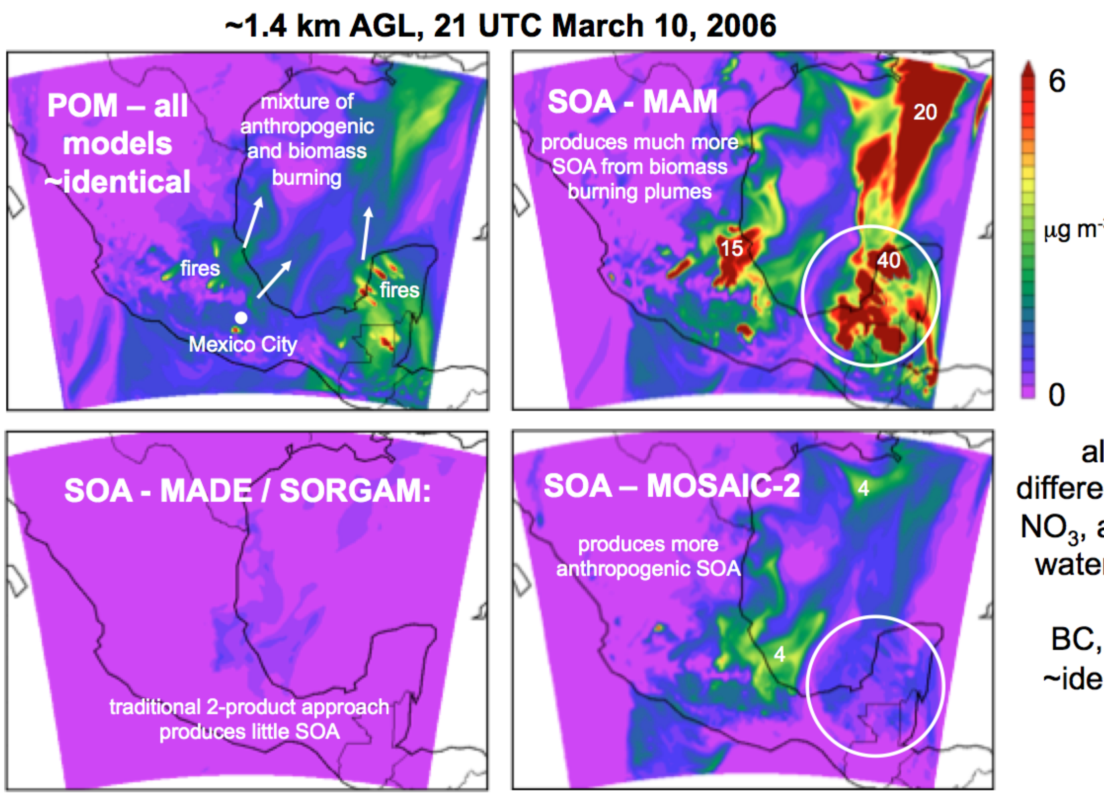
Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

"simple"
MAM
18 species

MADE/SORGAM
38 species
1.2 times slower

"complex"
MOSAIC 4-bin
164 species
3 times slower

MILAGRO Case Study



also differences in NO_3, aerosol water, NH_4

BC, SO_4 ~identical

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Fast et al., 2013. in preparation

Adding More Gas Phase Chemistry and Aerosol Packages for Aerosol Indirect Effect (implemented by **ESRL**)

- New gasphase chemistry packages using the Kinetic Pre Processor (KPP) include
  - Two versiosn of the Regional Atmopsheric Chemistry Mechanism (RACM) coupled with MADE/SORGAM
  - To be used with the aerosol indirect effect and simple aqueous phase chemistry (**CMAQ AQCHEM routine**)
- conv_tr_wetscav will activate wetscavenging in convective transport, DEFAULTS to “1” = “YES”
- conv_tr_aqchem will activate aqueous phase chemistry in parameterized convective transport routine. But only for RADM/RACM/MADE options. DeFAULTS to “1”
- MADE/VBS with this approach may be released in V3.5.1

A new dust model (dust_opt=3)

Was included in V3.4, but additional inputs (sand and clay fields) are now in WRF-WPS

AFWA/AER Dust scheme – modeled after GOCART approach, but included is sand blasting component and clay dependence

- Bulk Vertical Dust Flux Scheme: Based on Marticorena & Bergametti (1995)

- Threshold Friction Velocity (Iversen & White, 1982)):

$$u_{*_t}(D_p) = 0.129 \frac{\left[\frac{\rho_p g D_p}{\rho_a}\right]^{0.5}\left[1 + \frac{0.006}{\rho_p g D_p^{2.5}}\right]^{0.5}}{\left[1.928\left(a D_p^x + b\right)^{0.092} - 1\right]^{0.5}}$$

$$u_{*_t} = u_{*_t}(D_p)\,\frac{f(\text{moisture})}{f(\text{roughness})}$$

- Saltation Flux Over Bare Soil (Kawamura, 1951):

$$H(D_p) = C\frac{\rho_a}{g}u_*^3\left(1 + \frac{u_{*_t}}{u_*}\right)\left(1 - \frac{u_{*_t}^2}{u_*^2}\right)$$

$$G = \sum H(D_p)\,dS_{rel}(D_p)$$

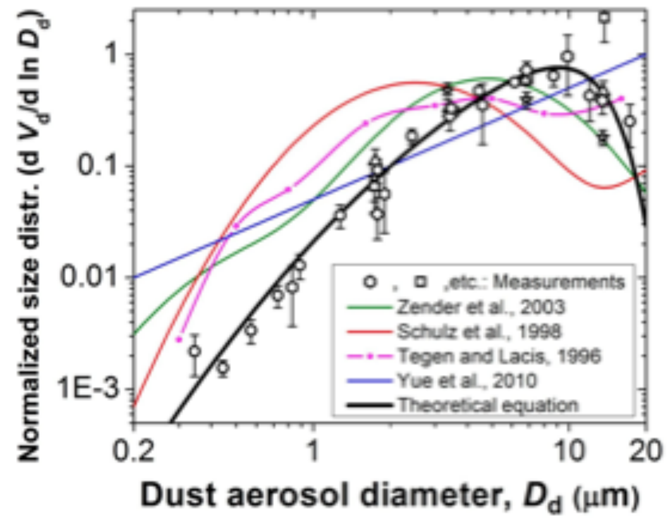
- Bulk Vertical Dust Flux (efficiency factor (α): Gillette, 1979)

$$F_{bulk} = G\alpha \times \text{Erod}$$

$$\alpha = 10^{0.134(\%\text{clay}) - 6}$$

AFWA/AER Dust scheme

- Particle Size Distribution developed by Jasper Kok (NCAR)
  - Brittle material fragmentation theory
  - Kok, 2010
- *f*(roughness) is a drag partition correction
- *f(moisture)* calculated using Fecan's (Fecan et al. 1999) method, incorporates soil texture, increases u^*_t as soil moisture increases



Important to note for GOCART or AFWA/GOCART dust schemes:

Settling is not fully treated –modifications will be necessary, otherwise an over-prediction will most likely result

As of now they only will work fine and as intended for bulk aerosol modules, or if used by themselves (without other aerosol modules)

Fires: What's new in V3.5 and V3.5.1

Previously included in the model: 1-D cloud model to calculate injection height, but with no effect of wind shear on plumes

New in V3.5.1:
The cloud model used to calculate injection height **includes the environmental wind effect**

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial z} = \gamma g B - \frac{2\alpha}{R}w^2 - \delta_{entr} w$$

$$\frac{\partial u}{\partial t} + w\frac{\partial u}{\partial z} = -\frac{2\alpha}{R}|w|(u-u_e) - \delta_{entr}(u-u_e)$$

$$\frac{\partial T}{\partial t} + w\frac{\partial T}{\partial z} = -w\frac{g}{c_p} - \frac{2\alpha}{R}|w|(T-T_e) + \left(\frac{\partial T}{\partial t}\right)_{\substack{micro-\\physics}} - \delta_{entr}(T-T_e)$$

$$\frac{\partial r_v}{\partial t} + w\frac{\partial r_v}{\partial z} = -\frac{2\alpha}{R}|w|(r_v-r_{ve}) + \left(\frac{\partial r_v}{\partial t}\right)_{\substack{micro-\\physics}} - \delta_{entr}(r_v-r_{ve})$$

$$\frac{\partial r_c}{\partial t} + w\frac{\partial r_c}{\partial z} = -\frac{2\alpha}{R}|w|r_c + \left(\frac{\partial r_c}{\partial t}\right)_{\substack{micro-\\physics}} - \delta_{entr} r_c$$

$$\frac{\partial r_{ice,rain}}{\partial t} + w\frac{\partial r_{ice,rain}}{\partial z} = -\frac{2\alpha}{R}|w|r_{ice,rain} + \left(\frac{\partial r_{ice,rain}}{\partial t}\right)_{\substack{micro-\\physics}} + \text{sedim} - \delta_{entr} r_{ice,rain}$$

dynamic entrainment

$$\delta_{entr} = \frac{2}{\pi R}|u_e - u|$$

$$\frac{\partial R}{\partial t} + w\frac{\partial R}{\partial z} = +\frac{6\alpha}{5R}|w|R + \frac{1}{2}\delta_{entr}R$$

$$\left(\frac{\partial \xi}{\partial t}\right)_{\substack{micro-\\physics}} (\xi = T, r_v, r_c, r_{rain}, r_{ice}), \quad \text{sedim} \begin{cases} \textit{bulk microphysics:} \\ \textit{Kessler, 1969; Berry, 1967} \\ \textit{Ogura \& Takahashi, 1971} \end{cases}$$

University of Manchester: completed developments (Lowe et al.), and due for submission for inclusion in WRF-Chem 3.5.1/3.6

- Common Represetative Intermediate Mechanism (CRIMech) (CRIv2-R5; 240 species, 652 rxns) (Watson et al., 2008)
- N_2O_5 heterogeneous chemistry in WRF-Chem sectional aerosol (Bertram & Thornton, 2009)
- Sea-spray emission scheme with organics (Fuentes et al., 2011)
- Organic Partial Derivative Fitted Taylor Expansion (PD-FiTE) added to MOSAIC sectional aerosol (Topping et al., 2009; 2012)

Douglas Lowe, Steven Utembe*, Scott Archer-Nicholls, David Topping, Mark Barley, Gordon McFiggans

Developers are currently in the process of working with us to merge with the latest repository version

What did we do with aerosols in the new GF convective parameterization ?

Step 1:

In G3 parameterization autoconversion from cloud water to rain is constant: c_0=.002

In GF, the equations for conversion of cloud water to rain water are re-derived using the Berry formulation:

$$\left(\frac{\partial r_{rain}}{\partial t}\right)_{\substack{\text{autoconversion} \\ \text{Berry, 1968}}} = \frac{\left(\rho r_c\right)^2}{60\left(5 + \frac{0.0366\ CCN}{\rho r_c m}\right)}$$

What did we do with aerosols in the convective parameterization ?

Step 2:

In GD and G3 parameterization precipitation efficiency depends on wind-shear and sub-cloud humidity

In GF, an empirical study was used to ADD a dependence on aerosols to the calculation of precipitation efficiency

$$PE \sim (I_1)^{\alpha_s - 1}(CCN)^{\zeta} = C_{pr}(I_1)^{\alpha_s - 1}(CCN)^{\zeta},$$

Where for our parameterization α_s and ζ are empirical constants and C_{pr} is a constant of proportionality

Aerosol dependence is included in V3.5, but not turned on !

Various additions to WRF-Chem V3.5

- Lightning from convective parameterizations: this option was generalizedso it can be used for LNO_x emissions as well as meteorological applications (NCAR/ACD)
- Add in MEGAN emissions for CBM-Z,CAM-MAM (NCAR/ACD)
- Correction to the photolysis rates in the Madronich scheme so that they better match current observed values. (ESRL/CSD)
- MODIS landuse can now be used with WRF-Chem
- Many fixes in various routines, some of them significant errors that are posted as bug fixes for V3.4.1

Chemical data assimilation

- NCEP's Grid Point Statistical Interpolation (GSI, 3DVAR) assimilation system can be used with surface chemical data as well as with AOD: Significant improvements in forecasts.
- EnKF assimilation system has been used for WRF-Chem
- Work is on-going with hybrid EnKF/GSI system (ESRL and NCAR)
- Work is also ongoing with WRF-Chem adjoint development (project lead by Greg Carmichael)

WRF-Chem ongoing and future work – PNNL

- Aerosol modeling test bed is still in the works and making progress

http://www.pnl.gov/atmospheric/research/aci/amt/index.stm

- Some of the Analysis Toolkit Software available via the web site
- MILAGRO test bed data is finished,
- CHAPS, VOCALS, ISDAC/ARCTAS, CARES/CalNex integrated datasets (field campaign + routine monitoring) planned for the future

WRF-Chem current and future work – ESRL + other groups

- Using WPS to run WRF-Chem off global FIM-Chem
- 2008 EPA emissions (US)
- Improved global emissions (prep_chem_sources)
- Aerosol-microphysics interactions for RACM_MADE_SOA_VBS
- Including isoropia2 (MADE related aerosol modules)
- NASA: coupling GOCART with microphysics, also with new GODDARD radiation scheme

Other Resources/Information

- ***Publication list now online***

  [***http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.html***](http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.html)

  - ***Please use this list to find papers to read and cite.***
  - ***Please send us your publications too!***

- ***Please make it easy for us If you plan to provide development work back to the community, (provide documentation, follow coding standards)***

Check WRF-Chem web page for model information
http://www.wrf-model.org/WG11

Thank you!