WRF-Chem (V3.5 and 3.5.1) Summary of status and updates

Georg Grell

S. E. Peckham, J. Kazil, R. Ahmadov, S. A. McKeen, (**NOAA/ESRL**), R. Easter, J. D. Fast , W. Gustafson, P.L. Ma, P. Rasch, B. Singh, (**PNNL**), A. Hodzic, M. Barth, G. Pfister, S. Wolters (all **NCAR**), J. Wong (University of Colorado), S. Freitas (**CPTEC, Brazil**), P. Tucella **(L'Aquila ITALY)**

\+ *many more national and international collaborators*

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

Structure of talk

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

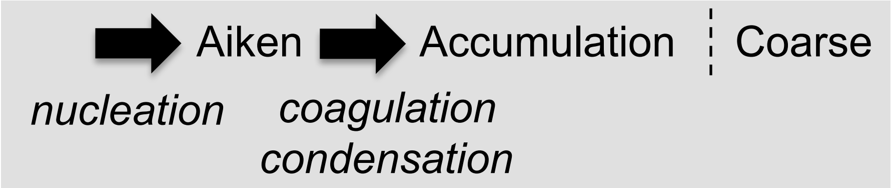
Implementation of the Community Atmosphere Model version 5 (CAM5) Physics/Chemistry, talk 7A.2 by Jerome Fast Thursday Morning

- **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)



- **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 ?)

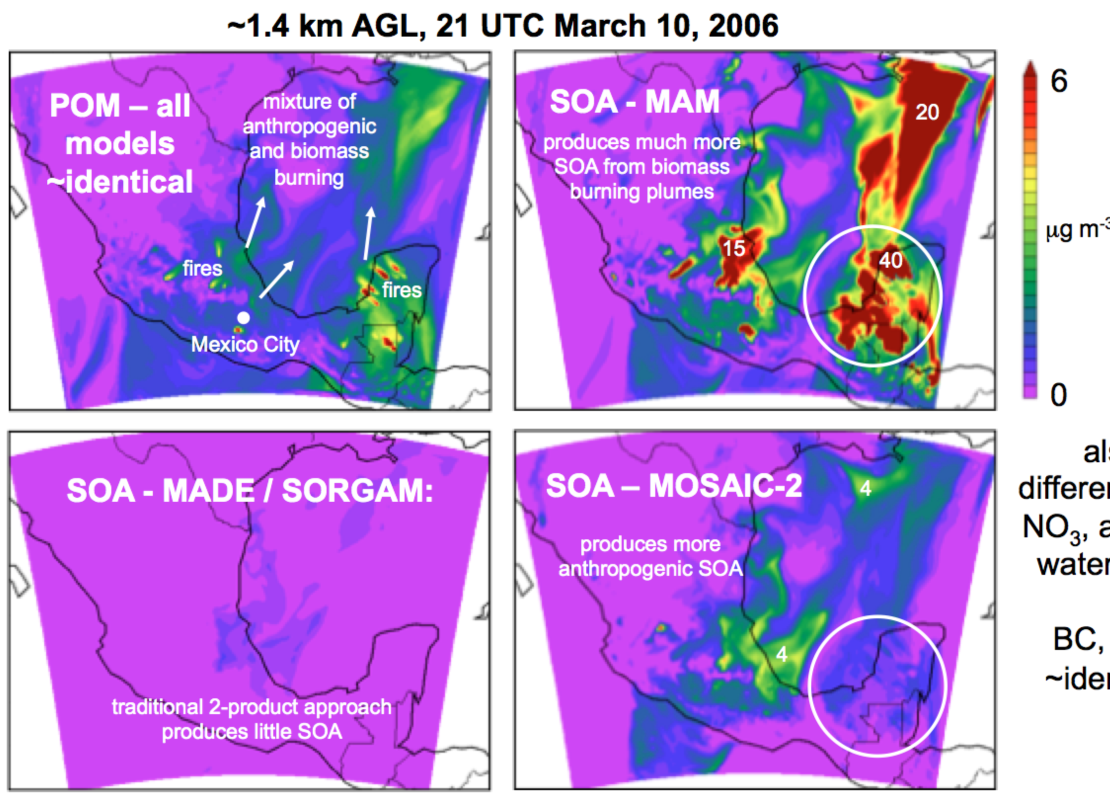
Example: Compare MAM with other Aerosol Models

"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):

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

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

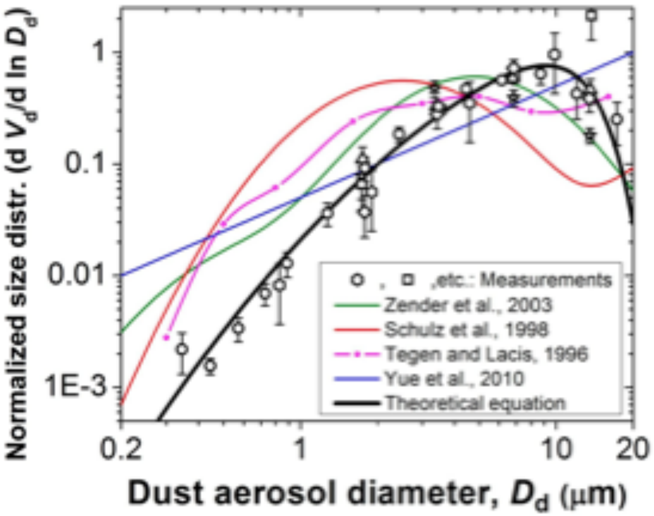
- Bulk Vertical Dust Flux (efficiency factor (α): Gillette, 1979)

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

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

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 –mods will be necessary, otherwise overprediction will 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: 1d cloud model to calculate injection height, but with no effect of wind on plumes

New in V3.5.1:

The 1D cloud model to calculate injection height: **including 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

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

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

$$\left(\frac{\partial \xi}{\partial t}\right)_{\substack{micro-\\physics}} (\xi = T, r_v, r_c, r_{rain}, r_{ice}), \quad \text{sedim}$$

bulk microphysics:
Kessler, 1969; Berry, 1967
Ogura & Takahashi, 1971

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

A scale and aerosol aware convective parameterization

Cu_phys=3, replaces GD

For scale awareness and general description, see talk 9.1 on Thursday afternoon by G. Grell

Application for Hurricane simulations for resolutions of 27, 9, 3, and 1km (!), see poster by E.Grell (P88), Wednesday afternoon

What did we do with aerosols in the 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:

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

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

- Lightning from convective parameterizations: this option was generalized (John Wong and Mary Barth), so it can be used for NO_x emissions as well as meteorological applications
- 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 (see talk by M. Pagowski, 7A.7, Thursday morning in chem session)
- 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

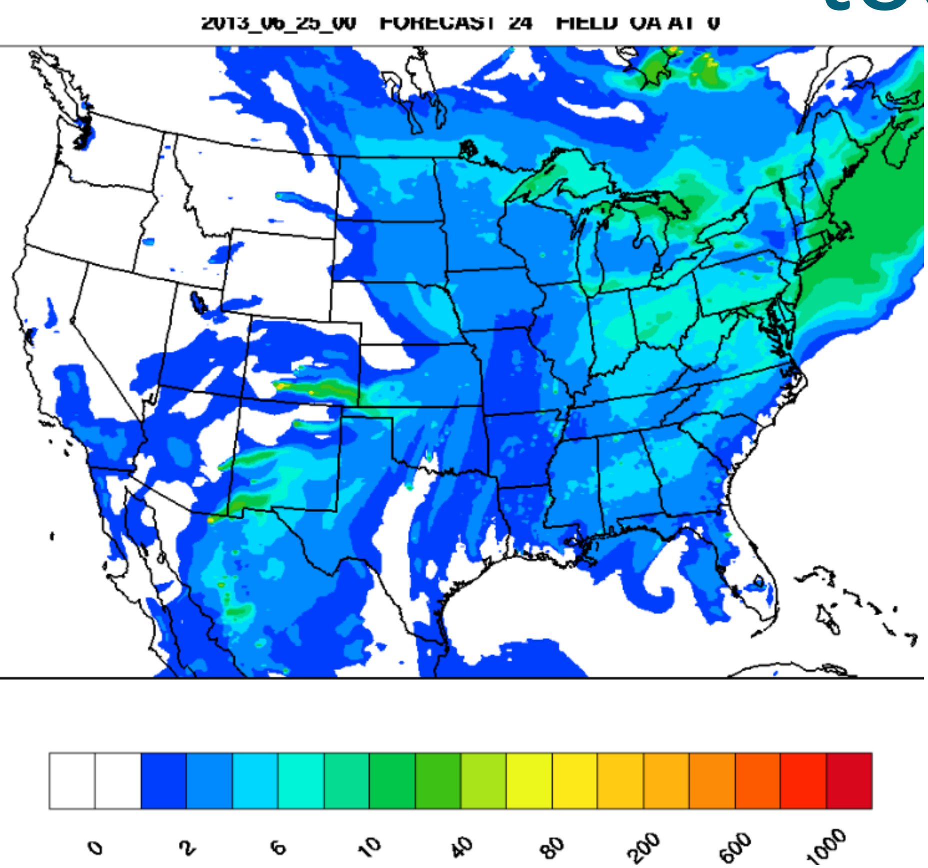
http://www.pnl.gov/atmospheric/research/aci/amt/index.stm

- 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

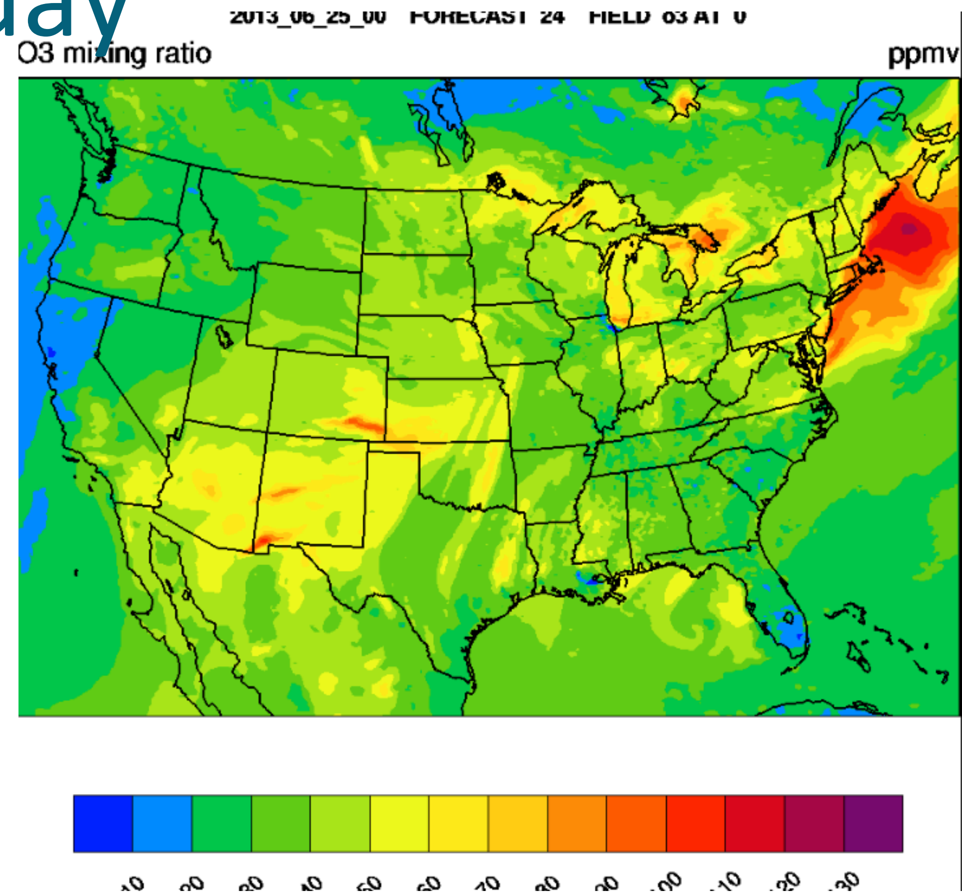
WRF/Chem current and future work – ESRL + other groups

- 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

Your real-time AQ forecast for today



Organic aerosols



Ozone

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

- ***Chemistry session is Thursday morning***
- ***Posters are Wednesday afternoon***
- ***Publication list now online***

http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references.htm

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

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

Thank you!