WRF-Chem: Online vs Offline Atmospheric Chemistry Modeling

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ASP colloquium, NCAR
July 29, 2016
## Meteorology-chemistry interactions

### Meteorology's impact on chemistry

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Impact on Chemistry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>Modulates chemical reaction and photolytic rates, modulates biogenic emissions (isoprene, terpenes, dimethyl sulfide, etc.), influences biogenic emissions (isoprene, monoterpenes), influences the volatility of chemical species, determines aerosol dynamics (coagulation, condensation, nucleation)</td>
</tr>
<tr>
<td>Temperature vertical gradients</td>
<td>Determines vertical diffusion intensity</td>
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<tr>
<td>Temperature &amp; humidity</td>
<td>Affect aerosol thermodynamics (e.g., gas-particle partitioning, secondary aerosol formation)</td>
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<tr>
<td>Water vapour</td>
<td>Modulates OH radicals, size of hydrophilic aerosol</td>
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<tr>
<td>Liquid water</td>
<td>Determines wet scavenging and atmospheric composition</td>
</tr>
<tr>
<td>Cloud processes</td>
<td>Affects mixing, transformation and scavenging of chemical compounds</td>
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<tr>
<td>Precipitation</td>
<td>Determines the wet removal of trace gases and aerosol</td>
</tr>
<tr>
<td>Land surface parameterization (soil type and vegetation cover, soil moisture, leaf area)</td>
<td>Affects natural emissions (e.g., dust, BVOCs) and dry deposition</td>
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<tr>
<td>Lightning</td>
<td>Determines free troposphere NOx emissions</td>
</tr>
<tr>
<td>Radiation</td>
<td>Determines photolysis rates and influences many chemical reaction rates, influences isoprene emissions</td>
</tr>
<tr>
<td>Wind speed and direction</td>
<td>Determines horizontal transport and vertical mixing of chemical species, influences dust and sea-salt emissions</td>
</tr>
<tr>
<td>ABL height</td>
<td>Influences concentrations</td>
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</tbody>
</table>

### Chemistry's impact on meteorology

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Impact on Meteorology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aerosols</td>
<td>Modulate radiation transfers (SW scattering/absorption, LW absorption, LW scattering by large particles like dust), affect boundary layer meteorology (temperature, humidity, wind speed and direction, ABL height, stability), extraordinary high concentrations can affect stability and wind speed, influence cloud formation, since they act as cloud condensation nuclei</td>
</tr>
<tr>
<td>Aerosols physical properties (size distribution, mass and number concentrations, hygroscopicity)</td>
<td>Influence cloud droplet and crystal number and hence cloud optical depth and hence radiation, modulate cloud morphology (e.g., reflectance), influence precipitation (runoff, intensity), influence haze formation and atmospheric humidity, influence scattering/absorption</td>
</tr>
<tr>
<td>Soot deposited on ice</td>
<td>Influences albedo</td>
</tr>
<tr>
<td>Radiatively active gases</td>
<td>Modulate radiation transfers</td>
</tr>
</tbody>
</table>

These processes are parameterized in various air quality models with different complexity. Some of the processes are not treated or poorly parameterized in models.

Baklanov et al., ACP 2014
Advantages of online coupled models:

- The online approach represents the atmosphere more realistically, since in reality the processes are all intertwined. The errors introduced by the offline approach for air quality forecasting can be quite substantial as the resolution is increased.

- For air quality forecasting, the online approach is numerically more consistent. No interpolation in time or space is required, although some time interpolation could be added to gain a computational advantage. Physical parameterizations as well as atmospheric transport are the same. This is especially significant for studies of the aerosol indirect effect or when aqueous phase processes are of importance. Feedback mechanisms can be considered.

- For weather forecasting, inclusion of online chemistry may directly improve the medium range forecasts (1 to 5 days). It may also indirectly improve the forecasts through improving the assimilation of meteorological data.

- The needed closer interaction between atmospheric physicists and chemists will lead to improvements in both the NWP as well as the atmospheric chemistry modeling approaches.

Advantages of offline models:

- Low computational cost, esp. if meteorological output is already available from a forecast run or observations. This is of particular interest for regulatory agencies that need to perform many simulations with different chemical assumptions (such as emissions input). This is also of interest on coarser resolutions.

- There exists more flexibility in specifying ensembles with lower computational cost in an offline approach. This is probably most significant for regulatory agencies, but also for emergency response, where a multitude of ensembles can quickly be run.

Grell and Baklanov et al., AE 2011
Offline: A chemical transport model is run using output from meteorological model

Single or two different numerical models
  Weather forecast completed, then chemistry
Wind fields and thermodynamic fields are interpolated
  Space: different computational grids
  Time: often using weather from hourly output
Different physical parameterizations
No feedback to meteorology
Computationally cheaper if running chemistry repeatedly with same meteorology
  with higher and higher resolution:
Convective storms more and more resolved by met-model: Scale separation does not exist, and offline run does not have the time resolution to estimate the vertical mass flux
Increasing variability in meteorological fields
No feedback to meteorology
History of the development of atmospheric chemistry models

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<td>Global</td>
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<td>Regional/Urban/Local</td>
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<td>O₃ and/or other gases</td>
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<td>Aerosols</td>
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<td>Tropo. O₃, CO, CH₄</td>
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<td>Global-to-urban treatments</td>
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<td>Exposure/health effects</td>
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<td>SO₂ direct radiation</td>
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<td>Atmosphere-Land-Ocean-Chemistry</td>
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→ → indicate the time and treatments in global and regional models, respectively.

Zhang Y., ACP 2008
Some examples of online and offline models

- **Regional online models**: MM5-Chem, WRF-Chem, BRAMS
- **Global online models**: Fim-Chem, AM3, MPAS, CAM-Chem, GEM-MACH, C-IFS (ECMWF)
- **Online access models**: WRF-CMAQ, COSMO-MUSCAT

- **Regional offline models**: CMAQ, CAMx, CHIMERE
- **Global offline models**: GEOG-Chem, MOZART, TM5
- **Lagrangian dispersion models**: FLEXPART, HYSPLIT, STILT

+ Many other models that you're going to learn about at this colloquium!

I am going to present some applications of the MM5-Chem and WRF-Chem models to demonstrate advantages of online coupling.
MM5-Chem model (predecessor of WRF-CHEM)

MM5-Chem (Grell et al. 2000)

- No mass conservation
- 1-way and 2-way nesting capable
- Height-based vertical coordinate

Chemistry:

- Online
  - Model-based grid-scale transport
  - Subgrid-scale transport by turbulence
  - Subgrid-scale transport by convection

- Dry deposition (Wesley)
- Biogenic emissions (Guenther et al.)
- RADM2 chemical mechanism
- Photolysis (Madronich)
- MADE/SORGAM aerosols
Weather Research and Forecasting coupled with Chemistry (WRF-Chem)
http://ruc.noaa.gov/wrf/WG11/

- Chemistry is online, completely embedded within WRF CI
- Consistent: all transport done by meteorological model
  - Same vertical and horizontal coordinates (no horizontal and vertical interpolation)
  - Same physics parameterization for subgrid scale transport
  - No interpolation in time
- Easy handling (Data management)
- Ideally suited to study feedbacks between chemistry and meteorology
- Ideally suited for air quality forecasting on regional to cloud resolving scales
Main features and capabilities of the WRF-Chem model
http://ruc.noaa.gov/wrf/WG11/

1. Advection and diffusion (all done by WRF)
2. Sub-grid scale transport (WRF parameterizations, PBL, convection)
3. Some processes that are specific for chemical constituents, but need meteorology: emissions (biogenic, fire, sea salt, dust, volcanic, anthropogenic), dry deposition, wet scavenging
4. Treatment of chemical reactions, aqueous phase chemistry, gas phase species and aerosols
5. “Chemical” radiation routines (photolysis routines) that provide photolysis rates necessary for (4)
6. Capability of feedback from chemistry to meteorology (meteorological radiation and microphysics parameterizations, possibly also convective parameterizations)
METHODOLOGY

- Use MM5-Chemistry and WRF-Chemistry model
- 1 online simulation each
  - Winds (u,v,w) output every time interval
- Several offline simulations each
  - Meteorology and chemistry coupled at different time intervals
    - Meteorological fields are time averaged, therefore mass consistent
    - Linearly interpolated meteorology between coupling times
SIMULATION DOMAINS MM5-CHEM

D01 (Domain 1)
110x135 @ 27 km horiz. res.

D02 (Domain 2)
88x82 @ 9-km horiz. res.

D03 (Domain 3)
100x110 @ 3-km horiz. res.

29 Vertical levels
Vertical stretched
~7m @ lowest level
~300 m @ 2 km AGL

Cloud Resolving Simulation
SIMULATION DOMAIN FOR WRF-CHEM

- D01 (Domain 1)
  - 171x181 @ 12 km horiz. res.

- 35 Vertical levels
  - Vertical stretched
    - ~7 m @ lowest level
    - ~300 m @ 2 km AGL

Not completely cloud resolving resolution, but compatible to resolution used by current operational models
Online simulation coupling interval
  10 s (MM5/chem), 60s (WRF/Chem)

Offline Meteorological coupling intervals
  1 h
  \( \frac{1}{2} \) h
  10 min

Saved wind data every time step
  Purpose: frequency analysis
What is the effective resolution of Eulerian models?

Grell and Baklanov et al., ACP 2011

Fig. 1. Energy power spectrum from a WRF forecast with 10-km horizontal resolution (dashed black line) and analytic results from Lindborg (1999).
Let’s look at extreme case: Cloud resolving, front moving through the area
FREQUENCY ANALYSIS

- Fixed Height
  - Around 500 m AGL
- horizontal 4 h time period
  - 1700 to 2100 UTC
- Large variations at short time scales
- MM5 uses time/space numerical filters
Fraction of total variability that is captured (x1000), level 10

1h

MM5/Chem,
dx=3km

10 min
ONLINE VS OFFLINE SIMULATIONS

Average CO and O$_3$ mixing ratios

Significant differences even using 10 min meteorological updates

MM5/Chem, dx=3km
E-W cross section of difference in ozone concentrations, online/offline, 1-hr 18Z
Spectra for three different models: MM5, COAMPS and WRF

**MM5 AMPS /Antarctica**
20 Sept 2003, dx = 10 km

**COAMPS BAMEX**
2 June 2003, dx = 10 km

**WRF-ARW BAMEX**
1 – 3 June 2003, dx = 10 km
Fraction of captured variability using WRF/Chem, dx=12km, centered at 14Z

60 min

10 min

Level 10, “normal” day, no severe convection
WRF-Chem modeled carbon monoxide time series, averaged over an area
WRF-Chem modeled ozone time series, averaged over an area
Studying chemistry-weather feedback using WRF-Chem

AOD during March 2006 for MILAGRO Field Campaign

MODIS AOD, ~1930 UTC March 10

Simulated AOD using MOSAIC

Fast J. WRF-Chem tutorial presentation, 2015
Available at http://ruc.noaa.gov/wrf/WG11/Tutorial.html
Studying chemistry-weather feedback using WRF-Chem

- WRF-Chem simulation, which includes direct and indirect feedback, and the state-of-the-art secondary organic aerosol (SOA) parameterization based on the volatility basis set approach, with direct and indirect cloud feedback, evaluated in Europe with data from a field campaign (Tuccella et al., GMD, 2015)

The 17–19 May 2008 averages of droplet effective radius at cloud top (first row), retrieved using MODIS-aqua observations (first column), predicted by model in the reference run (CTRL, second column), and sensitivity test without SOA (NOSOA, third column).
Wildfires in Alaska, 2004

No feedback

With feedback

Fig. 4. Observed (black) and predicted (blue) sounding for Fairbanks, Alaska, on 4 July, 00:00 UTC. Shown is temperature (solid), dew points (dashed-dotted) and wind barbs for runs without fires (a) and runs with fires (b). A moist adiabat based on a mixed parcel for the lowerst 100 mb of the observed (simulated) sounding is dashed in red (magenta).

Grell et al., ACP (2011)
Studying chemistry-weather feedback using WRF-Chem

Difference between the model cases with and w/o fires for an area over Alaska

Fig. 6. Hydrometeor properties averaged over Box A (shown in Fig. 5). Displayed is the difference (dashed line) in droplet number density (a), the sum of rain water, snow, and graupel mixing ratio (b) and the sum of cloud water and ice mixing ratio (c) for the run with fires minus the run witho put fires. Shown also on all 3 panels is the total PM$\text{_{2.5}}$ concentration (solid line) for the run with fires.
To calculate plume rise we need to know heat flux. The traditional approach in WRF-Chem to calculate plume rise:
Use constant fire released heat flux numbers for a given land use class, e.g. Tropical Forest: min and max heat flux = 30, 80 kW/m2

New approach recently implemented in WRF-Chem:
Heat flux \~ FRP/ burnt_area
FRP measured by satellites
Burnt_area is determined by using fire size

Example in the model:
- Flaming emission
- Smoldering emission

Diurnal cycle of the burning for S. America:
\[ E_\eta (t) = r(t) E_\eta \]

Freitas et al. (2011)
Another application of a coupled AQ model (wildfires and air quality)

- Based on the WRF-Chem model, run with two tracers emitted as PM2.5 from wildfires and anthropogenic emissions
- Run in real-time at NOAA Earth System Research Laboratory in Boulder
- 3km resolution CONUS domain
- 1080x1059 grid cells, 50 vertical levels
- Biomass burning emissions are calculated in real-time using VIIRS Fire Radiative Power data
- Biomass burning emissions are calculated on the same grid as WRF-Chem
- Meteorological input and boundary fields come from another real-time meteorological runs (with data assimilation) using the same domain and settings.

The High-Resolution Rapid Refresh (HRRR) – Smoke modeling system

http://rapidrefresh.noaa.gov/HRRRsmoke/
Smoke forecast for yesterday morning

No need to interpolate BB emissions, meteorological fields from other global models. Fire plume rise is simulated in an online mode using simulated meteorology on the same grid! Smoke impact on numerical weather prediction will be studied.

Several advantages of using an online model for such application!
The highest ozone pollution in the US during 2013 was detected during winter over the Uinta Basin, UT!
The dry deposition and photolysis schemes in WRF-Chem were modified to take into account the effect of snow cover.

<table>
<thead>
<tr>
<th>Description</th>
<th>Details</th>
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<tbody>
<tr>
<td>Horizontal resolution</td>
<td>12 and 4 km nested domains</td>
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<tr>
<td>Vertical resolution</td>
<td>60 layers (18 within lowest 500 m)</td>
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<tr>
<td>Meteorological input</td>
<td>NAM analysis</td>
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<tr>
<td>Microphysics</td>
<td>WRF Single-Moment 5-class</td>
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<td>Shortwave and longwave radiation</td>
<td>RRTMG</td>
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<td>Gas-phase chemistry</td>
<td>RACM_ESRL</td>
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<td>Transport of species</td>
<td>advection and vertical mixing</td>
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<td>Advection option for chemical variables</td>
<td>Monotonic</td>
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To accurately simulate such multi-day stagnant weather conditions, tight coupling between meteorology and chemistry is necessary.
O$_3$ distribution over a surface site on February 5th, 2013
Needs and future directions in development of online models

- Online anthropogenic emissions processing using simulated meteorology (e.g. plume rise)
- Inline mixing of chemical species in boundary layer and cumulus parameterizations
- Vertical mixing of chemical species by shallow convection parameterizations
- Development of new parametrizations for biogenic VOCs fluxes that are more consistent with meteorological parameterizations (e.g. using the same land use and vegetation greenness maps for meteorological and chemistry parameterizations)
- Feedback of resolved and sub-grid clouds on simulated photolysis rates
- Refinement of parameterizations chemistry-weather interactions (aerosol-cloud feedback in resolved and sub-grid parameterizations)
- Possible improvement of numerical weather prediction by including chemistry-weather feedback processes in the models
- Moving towards next generation coupled global coupled meteorology-chemistry models (e.g. NGGPS initiative by NOAA, USA), using one modeling framework for both global and regional applications
HRRR-CONUS domain (terrain)