Aerosol in WRF/Chem

Jan Kazil

University of Colorado / NOAA Earth System Research Laboratory
Part I - Introduction

- Overview of ...
  - Aerosol types
  - How aerosols are treated in atmospheric models
  - Aerosol processes
  - WRF/Chem aerosol schemes

Part II – Details

- Representing the aerosol size distribution
- WRF/Chem aerosol schemes
  - How they work and what they do
  - Coupling to other processes
    - Gas phase chemistry
    - Clouds and aqueous chemistry
    - Wet deposition
- How to tell WRF/Chem what to do
- Resources
Part I – Introduction
Aerosol processes

Particle diameter

~ 0.3 nm  ~ 1 nm  ~ 3 nm  ~ 3-50 nm  >50 nm

UV radiation

Nucleation

Condensation, coagulation

Activation, aqueous chemistry, wet scavenging

OH

OH + SO₂

H₂O

H₂SO₄

Organic molecules

Loss onto aerosol particles from surface emissions, dry deposition

Surface emissions
How aerosols are treated in atmospheric models

**Aerosol microphysics schemes describe:**
- The aerosol size distribution
- Microphysical processes between aerosol particles

**Aerosol chemistry schemes describe:**
- Chemical processes in and on the aerosol
- Gas/partical partitioning

**Coupled to:**
- **Gas phase chemistry:** gas phase molecules can condense onto aerosol (depends on the aerosol surface area)
- **Aerosol nucleation:** Gas phase molecules can stick together and form new aerosol particles (depends on concentrations of gas phase species)
- **Radiation:** Aerosol particles scatter radiation (depends on number and size of aerosol particles)
- **Cloud microphysics:** Cloud drop number (depends on the number and size of aerosol particles)
WRF/Chem aerosol schemes

- **An efficient aerosol scheme from the GOCART model**
  - No size information for sulfate, BC, OC
  - Size information for dust and sea salt
  - No secondary organic aerosol (SOA)

- **The Modal Aerosol Dynamics Model for Europe – MADE**
  - 3 log-normal modes
  - Inorganic, organic aerosol, SOA

- **The Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)**
  - Sectional model, 4 or 8 bins
  - Inorganic, organic aerosol, SOA

- **Simple scheme for volcanic ash aerosol**
Part II – The details
Bulk aerosol schemes

- Only total mass of aerosol compounds is known
- No information on
  - Particle number
  - Aerosol size distribution

Aerosol size distribution needs to be assumed for:
- radiative transfer
- response of cloud properties to aerosol number

- Numerically efficient
- Useful when focus is on complex gas phase chemistry

→ GOCART (+ size resolved dust and sea salt)
Modal aerosol schemes

Twin Otter data (black)
Modal aerosol schemes

\[
\frac{dN}{dD} = \frac{N}{\sqrt{2\pi \ln(\sigma) D}} e^{-\frac{1}{2} \left( \frac{\ln(D/\mu)}{\ln(\sigma)} \right)^2}
\]

- \( \frac{dN}{dD} \rightarrow N = 8195 \text{ cm}^{-3} \)
  - \( \mu = 18.22 \text{ nm} \)
  - \( \sigma = 1.42 \)

- \( \frac{dN}{dD} \rightarrow N = 12732 \text{ cm}^{-3} \)
  - \( \mu = 68.44 \text{ nm} \)
  - \( \sigma = 1.57 \)

- \( \frac{dN}{dD} \rightarrow N = 3140 \text{ cm}^{-3} \)
  - \( \mu = 164.41 \text{ nm} \)
  - \( \sigma = 1.28 \)
Modal aerosol schemes

\[ \frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD} \]
Modal aerosol schemes

Twin Otter data (black)

$\rightarrow$ MADE aerosol module
Sectional aerosol schemes

Twin Otter data (black)

→ MOSAIC aerosol module
• Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport model (Chin et al., JGR, 2000)

  ■ **Bulk aerosol:**
    - Hydrophobic black carbon (fresh soot)
    - Hydrophilic black carbon (aged/coated soot)
    - Hydrophobic organic carbon (fresh burnt biomass)
    - Hydrophilic organic carbon (aged/coated burnt biomass)
      ◦ Fresh $\rightarrow$ aged conversion time 2.5 days
    - Other GOCART primary PM2.5
    - Other GOCART primary PM10
    - Sulfate (only secondary aerosol species)

  ■ **Sectional scheme for dust and sea salt:**
    - Dust: 0.5, 1.4, 2.4, 4.5, 8.0 μm effective radius
    - Sea salt: 0.3, 1.0, 3.2, 7.5 μm effective radius
GOCART comes with sulfur gas phase chemistry:

- DMS + OH $\rightarrow$ SO$_2$ + ...
- DMS + OH $\rightarrow$ MSA + ...
- DMS + NO$_3$ $\rightarrow$ SO$_2$ + ...
- SO$_2$ + OH $\rightarrow$ SO$_4$ $^2-$ + ...

Extended gas phase chemistry can be used:

- MOZART (with KPP)
- RACM (with KPP)
- RADM (with and without KPP)
GOCART aerosol module

- **Interaction with radiation:**
  - Direct effect for some model setups
  - Effect on photochemistry

- **Interaction with clouds:**
  - Aqueous chemistry
    - $\text{SO}_2 + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{\text{2-}}$
    - $\text{SO}_2 + \text{O}_3 \rightarrow \text{SO}_4^{\text{2-}}$
  - No indirect effect
  - No wet scavenging/deposition

- **No secondary organic aerosol (SOA)**
Modal Aerosol Dynamics Model for Europe (Ackermann et al., Atm. Env., 1998)

- 3 log-normal aerosol modes: Aitken, accumulation, coarse
- Mode width $\sigma$ is fixed
- Aerosol number and mass variable
- (Currently no nucleation mode)

Interaction with radiation:
- Direct aerosol effect
- Effect on photolysis

Interaction with clouds:
- Aerosol number determines cloud drop number and size
- Radiative response $\rightarrow$ 1st indirect effect
  - only for grid-scale ("dynamically resolved") clouds
- Aqueous chemistry
- Wet removal (scavenging)
Aerosol composition in the Aitken and accumulation modes

- $\text{SO}_4^2$, $\text{NH}_4^+$, $\text{NO}_3^-$, $\text{H}_2\text{O}$
- $\text{NaCl}$ (sea salt)
- Anthropogenic SOA from oxidation of ...
  - Alkanes
  - Alkenes
  - Aromatics
- Biogenic SOA from oxidation of ...
  - Alpha-pinene
  - Limonene
  - Isoprene
- Anthropogenic POA
- Elemental carbon (soot)
- Primary PM2.5
Aerosol composition in the coarse mode

- Anthropogenic primary aerosol – e.g. from
  - Coal combustion
  - Cement manufacturing
  - Metallurgy
  - Waste incineration
- Sea salt
- Soil derived particles (mineral dust)
MADE aerosol coupling with chemistry

- **Gas phase chemistry:**
  - RADM2 *(Regional Acid Deposition Model version 2)*
  - RACM *(Regional Atmospheric Chemistry Mechanism)*
  - CBMZ *(Carbon-Bond Mechanism version Z)*
    - Hard-wired version, no indirect effect

- **Gas phase/particle partitioning (aerosol chemistry):**
  - MARS *(Model for an Aerosol Reacting System)*
  - SORGAM *(Secondary Organic Aerosol Model)*
  - VBS *(Volatility Basis Set)*

- **Aqueous chemistry:**
  - CMU aqueous chemistry
  - CMAQ (EPA) aqueous chemistry
  - Only for Aitken and accumulation mode
  - Only for selected gas phase chemistry options
MARS (Model for an Aerosol Reacting System), Saxena et al., Atm. Env., 1986
**MADE/SORGAM**

**Gas phase scheme (RADM2, RACM)**

- **Alkanes**
- **Alkenes**
- **Toluene**
- **Xylene, cresole, ...**
- **Isoprene**
- **Sesquiterpene**
- **Alpha-pinene, limonene**

**OH, O₃, NO₃**

**Semi-volatile organics**

\[ X_1, X_2, X_3, X_4, X_5, \ldots, X_n \]

**SOA**

- \( \text{H}_3\text{O}^+ \)
- \( \text{HSO}_4^- \)
- \( \text{NH}_4\text{HSO}_4 \)
- \( \text{H}_2\text{O} \)
- \( \text{SO}_4^{2-} = (\text{NH}_4)^+ \text{SO}_4 \)
- \( \text{NO}_3^- \)
- \( \text{SO}_4^{2-} = \text{NH}_4^+ \)
- \( \text{NaCl} \)

**SORGAM** (Secondary Organic Aerosol Model), Schell et al., JGR, 2001
MADE/VBS (Volatile Basis Set)

- **Gas phase scheme (RACM)**
- **Alkanes**
- **Alkenes**
- **Toluene**
- **Xylene, cresole, ...**
- **Isoprene**
- **Sesquiterpene**
- **Alpha-pinene, limonene**

Products

- OH, O₃, NO₃

Volatile

Semi-volatile

Volatility

Ahmadov et al., JGR 2012
Organic aerosol mass in the surface layer (August - September 2006)

Ahmadov et al., JGR 2012
MADE and aqueous chemistry

- **CMU aqueous chemistry** (Fahey & Pandis, Atm. Env., 2001)
  - Only for Sc clouds
  - Slow
  - Does not conserve mass

- **CMAQ (EPA) aqueous chemistry** (Walcek & Taylor, JAS, 1986)
  - For both Sc and Cu clouds
  - Relatively fast
  - Conserves mass very well
  - Can be enabled for Cu together with the CMU scheme for Sc

- **MADE and aqueous chemistry for selected gas phase chemistry options**

- **KPP versions of gas phase chemistry schemes: watch for bug fixes on WRF/Chem web site**
Aqueous chemistry:
• Treatment depends on cloud type

Stratocumulus

Cumulus

Cumulonimbus

\[ O(10\text{km}) \]

\[ O(100\text{m}) \]

\[ O(1\text{km}) \]
MADE aerosol and wet deposition

Wet removal:
- Activated aerosol
- Dissolved gas phase species
- Treatment depends on cloud type

No regeneration, but uptake of $\text{H}_2\text{SO}_4$, $\text{H}_2\text{O}_2$, $\text{SO}_2$

Regeneration, but no uptake from gas phase

$\text{SO}_4^{\text{2-}}$, $\text{NO}_3^-$
MADE aerosol and wet deposition

**NADP SO₄²⁻ wet deposition (mg m⁻² month⁻¹)**

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<table>
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<th>SO₄²⁻ wet dep.</th>
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<td>r</td>
<td>model/obs.</td>
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<td>0.86</td>
<td>0.53</td>
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May-September 2006
(National Atmospheric Deposition Program)
MOSAIC aerosol module

Model for Simulating Aerosol Interactions and Chemistry (Zaveri et al., JGR, 2008)

- Most modern aerosol scheme in WRF/Chem
- 4 or 8 aerosol size sections (bins) 39 nm – 10 μm
- (Lower bin boundary of 39 nm too large for nucleation)

Interaction with radiation:
- Direct aerosol effect
- Effect on photolysis

Interaction with clouds:
- Aerosol number determines cloud drop number and size
- Radiative response → 1st indirect effect
- Aqueous chemistry
- Wet removal (scavenging)
- only for grid-scale (“dynamically resolved”) clouds
Aerosol composition

- $\text{SO}_4^{2-}$, $\text{NH}_4^+$, $\text{NO}_3^-$, $\text{H}_2\text{O}$
- $\text{NaCl}$ (sea salt)
- $\text{CH}_3\text{SO}_3$ (methanesulfonate)
- carbonate ($\text{CO}_3^-$)
- calcium (Ca)
- black carbon (BC)
- primary organic mass (OC)
- other inorganic mass (minerals, trace metals)
MOSAIC aerosol coupling with chemistry

- **Gas phase chemistry:**
  - **CBMZ** *(Carbon-Bond Mechanism version Z)*
    - "Standard" gas phase chemical scheme for MOSAIC
  - **SAPRC99** (extensive VOC chemistry)
    - Works with the VBS SOA scheme
  - **MOZART** *(Model for Ozone and Related chem. Tracers)*
    - Works with the VBS SOA scheme

- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MTEM** *(Multicomponent Taylor Expansion Method)*
  - **MESA** *(Multicomponent Equilibrium Solver for Aerosols)*
  - **VBS** *(Volatility Basis Set)*

- **Aqueous chemistry:**
  - CMU aqueous chemistry, only for grid-scale (dynamically resolved) clouds
  - Not with KPP versions of gas phase chemistry schemes
MOSAIC, MTEM, and MESA

MTEM calculates activity coefficients
MESA solves ion-equilibria in the liquid phase
For SOA: VBS (Volatility Basis Set) scheme

MTEM (Multicomponent Taylor Expansion Method), Zaveri et al., JGR 2005a
MESA (Multicomponent Equilibrium Solver for Aerosols), Zaveri et al., JGR 2005b
• 10 bins for volcanic ash aerosol
• Transport, settling, dry deposition
• Currently no other aerosol
• Single active volcano
• 1535 volcanoes (latitude, longitude, height)
• SO$_2$ degassing from the volcano on/off
How to tell WRF/Chem what to do

..WRFV3/test/em_real/real.exe

..WRFV3/test/em_real/namelist.input

..WRFV3/test/em_real/

..WRFV3/test/em_real/

&chem
chem_opt = 42
photdt = 0.25
chemdt = 0

...aerchem_onoff = 1
...conv_tr_aqchem = 1

MADE/SORGAM
CMAQ (EPA) aq. chemistry

Switches all aerosol processes on/off
CMAQ (EPA) aq. chemistry in Cu
Resources

- **WRF/Chem User's Guide**
  - Model options (namelist parameters)
  - Combinations of physical/chemical schemes
  - ...
- **Papers referenced in the WRF/Chem User's Guide**
- **WRF/Chem source code**
  - **WRF/Chem Help** ([wrfchemhelp.gsd@noaa.gov](mailto:wrfchemhelp.gsd@noaa.gov))
  - **Yours truly** ([jan.kazil@noaa.gov](mailto:jan.kazil@noaa.gov))