WET DEPOSITION OF FINE PARTICULATE MATTER IN WRF-CHEM

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OUTLINE

- Sulfate and removal processes
- Parameterization of wet removal processes in WRF-CHEM
- Evaluation of rain, concentration and the removal rates for sulfate particles using WRF-CHEM3.1.1 with aqueous chemistry
- Preliminary results using WRF-CHEM3.3 with Grell convective rainfall/wet removal
- Concluding remarks
SULFUR SOURCE-SINK RELATIONSHIP

- CEMS emissions for SO2
- NADP for wet removal
- Surface networks – STN, IMPROVE

Seinfeld and Pandis, 2006
Available Wet Deposition Tools in WRF-Chem3.3

1) Simple wet removal scheme (G. Grell):
   *computationally very efficient, limited evaluation, scavenging parameters need tuning,*
   *only for the resolved clouds!*

2) Full aqueous chemistry scheme (PNNL, ref. Fahey and Pandis, 2001)
   *computationally very expensive, only for the resolved clouds!*

3) Wet removal within convective mixing (G. Grell)
   *computationally efficient, scavenging parameters need tuning, only for sub-grid clouds!*

4) Aqueous chemistry parameterization from CMAQ (ref. Walcek & Taylor, 1986), implemented by J. Kazil (NOAA/CSD)
   *faster than the full aq. chem (2), only for the sub-grid clouds, not in the official version!*
DAILY SULFATE CONCENTRATIONS – STN OBSERVATIONS

Observations, 24hr mean - SO4A
130 STN sites, 08/04/06 through 09/28/06

SO4A, μg/m³
med.(all sites): 3.31
med.(all data): 3.30

- <0.8
- 0.8 to 1.6
- 1.6 to 5.8
- >5.8
DAILY SULFATE CONCENTRATIONS – MODEL/OBS.

WRF-CHEM settings:
Version 3.1.1
RACM_ESRL gas chemistry:
GOCART SO2->SO4 conversion
Cloud fraction
No wet removal!

Model obs. comparison for 24hr mean - SO4A
130 STN sites, 08/04/06 through 09/28/06

med. ratio
med.(all sites): 1.23
med.(all data): 1.22

<0.3
0.3 to 0.7
0.7 to 1.3
>1.3
NADP OBSERVED SULFATE WET REMOVAL, AUGUST, 2006, (mg/m²/month)
NADP NETWORK, EVALUATION OF RAINFALL

Model/Observed Total Rainfall (August 2006)
MODEL-OBSERVED SO4 WET DEPOSITION (AUGUST 2006)

WRF-CHEM settings:
Version 3.1.1
Gas chemistry:
RADM_KPP
CMAQ aqueous chemistry
with wet removal
## WET REMOVAL STATISTICS FOR MAY-SEPTEMBER, 2006

<table>
<thead>
<tr>
<th>Month</th>
<th>Precipitation r coeff.</th>
<th>Precipitation mod/ob median</th>
<th>SO4 wet dep. r coeff.</th>
<th>SO4 wet dep. mod/ob median</th>
</tr>
</thead>
<tbody>
<tr>
<td>May</td>
<td>0.66</td>
<td>1.35</td>
<td>0.73</td>
<td>0.61</td>
</tr>
<tr>
<td>June</td>
<td>0.78</td>
<td>1.30</td>
<td>0.76</td>
<td>0.47</td>
</tr>
<tr>
<td>July</td>
<td>0.67</td>
<td>1.12</td>
<td>0.78</td>
<td>0.41</td>
</tr>
<tr>
<td>August</td>
<td>0.51</td>
<td>1.51</td>
<td>0.67</td>
<td>0.54</td>
</tr>
<tr>
<td>September</td>
<td>0.72</td>
<td>0.98</td>
<td>0.70</td>
<td>0.56</td>
</tr>
<tr>
<td>May-Sept.</td>
<td>0.81</td>
<td>1.25</td>
<td>0.86</td>
<td>0.55</td>
</tr>
</tbody>
</table>
Model obs. comparison for 24hr mean - SO4A
130 STN sites, 08/04/06 through 09/28/06

- med. ratio
- med.(all sites): 0.46
- med.(all data): 0.46

Legend:
- <0.3
- 0.3 to 0.7
- 0.7 to 1.3
- >1.3
SULFATE WET REMOVAL, AUGUST, 2006 (mg/m²/month)

Observations

WRF-CHEM3.3, convective wet removal (Grell scheme)
MODEL-OBSERVED SO4 WET DEPOSITION (AUGUST 2006)

August 2006 total SO4 dep.
Linear Fit, Model = -17.014 + 0.602*Obs
r-coefficient = 0.64

median(mod./obs.)=0.30

WRF-CHEM 3.3 with convective only wet removal (Grell scheme)
CONCLUDING REMARKS

- Reasonable correlations for rain and wet removal, still sulfate removal and concentrations are under-estimated
- Strong need for extensive evaluation of wet removal in WRF-CHEM different scales, resolved and sub-grid precipitation
- Improvement of sulfate simulations – cloud phase conversion, wet and dry removal
- CMAQ aqueous chemistry needs to be coupled to resolved clouds as well
- Role of cloud fraction (SO2->SO4 conversion, feedback on radiation and photolysis)
- Implementation of wet removal for other gaseous and particle species
Model obs. comparison for 24hr mean - SO4A
126 STN sites, August, 2006

r coef.
med.(all sites): 0.54
all data: 0.48

- Blue <0.5
- Green 0.5 to 0.71
- Yellow 0.71 to 0.87
- Red >0.87
July 2006 rainfall totals

From NADP/NTN network

Convective plus Nonconvective

From Jan’s 20km WRF/Chem
Convective plus Nonconvective
August 2006 total precip.
Fit through zero, Model = 1.421 \times \text{Obs}
\text{r-coefficient} = 0.54
Model/Observed Total Rainfall (July 2006)
July 2006 SO4 wet deposition

From Jan Kazil 20km WRF/Chem

From NADP/NTN network

mg/m²/month
Model/Observed SO4 wet deposition (July 2006)

Rainwater so4wd
Model/Obs. ratio
- 0.02 to 0.1
- 0.1 to 0.33
- 0.33 to 0.5
- 0.5 to 0.8
- 0.8 to 3.99

Number of points = 172
Median = 0.3915

July 2006 total SO4 dep.:
Linear Fit: Model = -0.453 + 0.419 * Obs
r-coefficient = 0.79
July 2006 SO4 average rainwater concentration

From Jan Kazil 20km WRF/Chem

From NADP/NTN network
Model/Observed SO4 rainwater concentration (July 2006)

Rainwater SO4
Model/Obs. ratio
- 0.02 to 0.1
- 0.1 to 0.33
- 0.33 to 0.5
- 0.5 to 0.8
- 0.8 to 1.92

Number of points= 172
Median=0.34005

July 2006 average conc.
Linear Fit, Model= 0 + 0.383*Obs
r-coefficient = 0.71
Model/Observed Total Rainfall (September 2006)

Number of points = 245
Median = 0.9118

September 2006 total precip.
Fit through zero, Model = 0.925 * Obs
r-coefficient = 0.65
Model/Observed SO4 wet deposition (May through September 2006)
Model/Observed SO4 rainwater concentration (May through September 2006)

May-Sept. 2006 average conc.
Linear Fit, Model = 0.222 + 0.369*Obs
r-coefficient = 0.63