A “new” Direct Coupled Meteorology and Chemistry Model — WRF-chemT

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Outline of Presentation

- What is WRF-chemT?
- How is it different from WRF-chem?
- Some thoughts on “online model”
WRF-chemT
A NEW DIRECT COUPLED METEOROLOGY AND CHEMISTRY MODEL

- It is derived from WRF-chem
- The philosophical departure is to focus on selected options and improvements of only those options.
- At NCU we assume responsibilities for correct operations of this “reduced and modified” model.
- When useful, our submodels will be offered to WRF-chem working group for consideration for the “mother” model.
WRF-chem development

- Original WRF-chem is WRF + RADM2 + ... mostly ported from offline models.
- Some of the major issues are:
  1. Computationally slow
      It is desirable to be faster
  2. Incomplete direct coupling of emissions
      Not really “online”
  3. Incomplete direct coupling of other processes
      Version 2.2 is much improved
Computational efficiency of WRF-chem ver. 2.1.2

For a particular five day simulation over a East Asian domain (Taiwan)

Using 128 CPUs

WRF  
(meteorology only): 939 sec

WRF-chem  
(met. and gas chemistry): 3905 sec

No aerosol or aqueous chemistry!
Comparison of two models

WRF-CHEM  RADM2 - QSSA
Quasi Steady State Approximation (QSSA) Solver

WRF-CHEM T  RADM2 - NCU
NCU fast chemistry (NCU) Solver
<table>
<thead>
<tr>
<th>Group No</th>
<th>CASE No.</th>
<th>Version</th>
<th>Condition</th>
<th>Time used(sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CASE-2</td>
<td>QSSA</td>
<td>dtcmin=0.05min, dt = 45 sec, chemdt = 0.75min</td>
<td>1458.912</td>
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<tr>
<td></td>
<td>CASE-6</td>
<td>NCU</td>
<td>dt = 45 sec,chemdt = 0.75min</td>
<td>695.490</td>
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<tr>
<td>2</td>
<td>CASE-3</td>
<td>QSSA</td>
<td>dtcmin=0.05min, dt = 45 sec, chemdt = 1.5min</td>
<td>1419.405</td>
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<tr>
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<td>CASE-7</td>
<td>NCU</td>
<td>dt = 45 sec,chemdt = 1.5min</td>
<td>428.857</td>
</tr>
<tr>
<td>3</td>
<td>CASE-4</td>
<td>QSSA</td>
<td>dtcmin=0.05min, dt = 45 sec, chemdt = 4.5min</td>
<td>1300.592</td>
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<tr>
<td></td>
<td>CASE-8</td>
<td>NCU</td>
<td>dt = 45 sec,chemdt = 4.5min</td>
<td>316.076</td>
</tr>
</tbody>
</table>

Chemistry Computation Performance

- **2 times faster**
- **3 times faster**
- **4 times faster**
## Test Case

<table>
<thead>
<tr>
<th>No.</th>
<th>Version</th>
<th>Condition</th>
<th>Time used(sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CASE-1</td>
<td>WRF-CHEM(QSSA)</td>
<td>dt = 45 sec, Meteorology Only</td>
<td>939.364</td>
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<tr>
<td>CASE-2</td>
<td>WRF-CHEM(QSSA)</td>
<td>dtcmin=0.05min, dt = 45 sec, chemdt = 0.75min</td>
<td>3904.848</td>
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<tr>
<td>CASE-3</td>
<td>WRF-CHEM(QSSA)</td>
<td>dtcmin=0.05min, dt = 45 sec, chemdt = 1.5min</td>
<td>3865.341</td>
</tr>
<tr>
<td>CASE-4</td>
<td>WRF-CHEM(QSSA)</td>
<td>dtcmin=0.05min, dt = 45 sec, chemdt = 4.5min</td>
<td>3746.528</td>
</tr>
<tr>
<td>CASE-5</td>
<td>WRF-CHEM(QSSA)</td>
<td>dtcmin=0.016666667min, dt = 45 sec, chemdt = 4.5min</td>
<td>5028.567</td>
</tr>
<tr>
<td>CASE-6</td>
<td>WRF-CHEM(NCU)</td>
<td>dt = 45 sec, chemdt = 0.75min</td>
<td>3141.426</td>
</tr>
<tr>
<td>CASE-7</td>
<td>WRF-CHEM(NCU)</td>
<td>dt = 45 sec, chemdt = 1.5min</td>
<td>2874.793</td>
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<td>CASE-8</td>
<td>WRF-CHEM(NCU)</td>
<td>dt = 45 sec, chemdt = 4.5min</td>
<td>2762.012</td>
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<td>CASE-9</td>
<td>WRF-CHEM(NCU)</td>
<td>dt = 45 sec, chemdt = 0.75min, No Chem, Transport Only</td>
<td>2445.936</td>
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<td>CASE-T3</td>
<td>WRF-CHEM(NCU)</td>
<td>dt = 45 sec, chemdt = 4.5min, Transport=2.25</td>
<td>2019.926</td>
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</tbody>
</table>
WRF-chem and WRF-chemT Performances

![Bar chart showing time used (sec) for different case numbers.](chart.png)
Structure in original QSSA module_radm.F

radm_driver: Initialization and return chemistry data to parent sequence.

radm: Calculate rate constants (rk and rj) and control dt.

predraten: Calculate reaction rate (crk, crj, dvc).

producn: Calculate production and loss.

setdtc: Set integration time step.

integln: QSSA solver.
Structure in new NCU module_radm.F

radm_driver
  Initialization and return chemistry data to parent sequence

radm
  Calculate rate constants (rk and rj)

chem_solver
  NCU solver for RADM2

  crjk
    Calculate reaction rate

  prodloss
    Calculate production and loss

  daynox
    Calculate NO₂, NO, O₃, O¹P, O¹D

  dayhox
    Calculate HO, HO₂, HONO, HNO₄

  panx
    Calculate PAN and ACO3

  nozt
    Calculate NO₃ and N₂O₅

  ebi
    Calculate other species
Impact of operator splitting on chemical solver time step size

Box model

\[ dtc^n \rightarrow \text{error estimate} \rightarrow \text{larger } dtc^{n+1} \rightarrow \text{Error estimate} \rightarrow \text{larger } dtc^{n+2} \]

3-D model with operator splitting

\[ dtc^n \rightarrow \text{error estimate} \rightarrow \text{other operator} \rightarrow \text{accuracy test fails} \rightarrow \text{no change in } dtc^{n+1} \]

(Huang and Chang, JGR, 106, 2001)
**Online Emissions IO**

- `med_read_wrf_chem_emiss`
  - `io_style_emissions = 0`: No emissions input
  - `io_style_emissions = 1`: Emissions are read in from two 12 hour files
  - `io_style_emissions = 2`: Emissions are read in from files identified by date
  - `io_style_emissions = 3`: Online emissions input

**Initial processor**:
- Do at first time step:
  1. Save time profiles in memory
  2. Save point source record in memory
  3. Write out area and line source emission (grided)
  4. Save biogenic source record in memory

- Read area and line source every single hour
Online Emission Processing

chem_driver
  → emission_driver
  → emission_driver_NCU
    → emi_p_plume_rise
      → emi_b
        → emi_alp_combin
          → emi_alpb_combin
            → add_realtime_emissions
        → Combin point, area, line and biogenic emissions and map onto grid system
          → Add emissions into chem

Original emissions driver
Call at set steps
Do point source plume rise (record to grid)
Do biogenic emissions online (TBEIS)
STRUCTURE IN NEW DRY DEPOSITION ROUTINES

**dry_dep_driver**
- Driver of dry deposition

**wesely_driver**
- Calculate dry deposition velocity

**cblcalc**
- Calculate convective boundary layer

**vmix**
- Calculate vertical mixing under CBL (ACM)

**vertmx**
- Calculate vertical diffusion above CBL
Some thoughts on Online modeling

- Gas-phase and aqueous chemistry mechanisms are **lumped** approximations in VOCs.

- **Cloud impact** on actinic flux should be consistent with WRF cloud-aerosol submodel used, not just moisture parameterization.

- All chemical species emissions must be **direct coupled** to WRF meteorology.

- Secondary aerosol processes must be linked consistently through **aerosol-radiation-chemistry-cloud interactions**.
Thank you for your attention!