WRF/Chem forecasting of boundary layer meteorology and $O_3$

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Nov. 22$^{\text{th}}$ 2013
Importance of O$_3$, Aerosols

- Have adverse effects on human health and environments
- Reduce visibility
- Play an important role in climate changes
  - Direct effect
  - Indirect effects
Boundary layer meteorology simulation is most important for air quality forecasting. PBL schemes are most critical for boundary layer meteorological simulation.
Outline

• Current status of performance of PBL schemes in terms of wind and $O_3$

• Results of WRF model with chemistry (WRF/Chem) for an episode from the Joint Urban 2003 field campaign

• Future plan regarding improving vertical mixing in WRF/Chem
Current status of performance of PBL schemes

• Errors and uncertainties associated with PBL schemes still remain one of the primary sources of inaccuracies of model simulations.

• While much progress has been made in simulating daytime convective boundary layer (CBL), progress with the modeling of nighttime boundary layer has been slower.

PBL schemes play critical roles for simulation of wind, turbulence, and air quality in the boundary layer.
Systematic over-estimations of near-surface winds during stable conditions with several models

WRFV3.3 with YSU (Zhang et al., 2013)

WRF (Wolff and Harrold, 2013)
Over-estimation of near-surface winds during stable conditions (2)

Systematic positive model biases for surface wind speed during nighttime.

Performance of 5 meteorological models (Vautard et al., 2012)
Over-estimations of near-surface winds during stable conditions (3)

Performance of MM5 applied in Sweden (Miao et al., 2008)
Overestimation of nighttime surface $O_3$

MM5-CMAQ (Mao et al., 2006)
Summary of current status

– A few models face the problem of overestimation of near-surface wind and $O_3$ during nighttime.

– Previous studies did not identify the exact cause and solution.

– PBL schemes play critical roles for simulation of wind, and air quality in the boundary layer. Would PBL schemes be fully responsible for the problems?
Past evaluation of the YSU PBL scheme
One of the mostly widely used schemes

Longstanding problem with YSU in WRF:
simulating weaker and higher LLJs (Floors et al., 2013)
Past evaluation of YSU (2)

(Schumacher et al., 2013)
Simulations from CAPS 2010 Spring Experiment
Past evaluation of YSU (3)

Time-height diagram of wind speed (Storm et al., 2009)
Updates of YSU from V3.4 to V3.4.1

\[ Eddy\ diffusivity\quad K_m = k w_s z (1 - \frac{Z}{h'})^2 \]

Velocity scale
\[ w_s = u_*/\phi_m \]

Version 3.4 and earlier
\[ \phi_m = 1 + 5 \frac{Z}{L} \cdot \frac{h'}{h} \]

Version 3.4.1
\[ \phi_m = 1 + 5 \frac{Z}{L} \]

h' is diagnosed using a critical Richardson # of 0 while h is diagnosed using Ri # of 0.25
Vertical profiles of $K_m$ under different stabilities

\[ \phi_m = 1 + \frac{5z}{L} \cdot \frac{h'}{h}, \quad \frac{h'}{h} = 0.05 \]

\[ \phi_m = 1 + \frac{5z}{L} \]

Old YSU in earlier WRF (i.e., 3.4 and earlier)
Updated YSU in WRF 3.4.1

Vertical mixing simulated by the updated YSU in WRF is reduced
Objectives of this study

– Document the impact of YSU updates on the boundary layer prediction.
– Evaluate PBL schemes for wind resource and air quality assessments.
– Diagnose possible reasons for the often reported overestimation problem for near-surface wind and $O_3$
### Numerical experiments with WRF/Chem

<table>
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<tr>
<th>Abbreviation</th>
<th>WRF version</th>
<th>PBL scheme</th>
<th>Surface layer scheme* (option number in WRF)</th>
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<tbody>
<tr>
<td>YSU3.4</td>
<td>3.4</td>
<td>old YSU</td>
<td>MM5 similarity (1)</td>
</tr>
<tr>
<td>YSU3.4+</td>
<td>3.4</td>
<td>updated YSU</td>
<td>MM5 similarity (1)</td>
</tr>
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<td>YSU3.4.1</td>
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<td>MYJ</td>
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<td>MYNN2</td>
<td>3.4.1</td>
<td>MYNN2</td>
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<td>BouLac</td>
<td>3.4.1</td>
<td>BouLac</td>
<td>Eta similarity (2)</td>
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<td>QNSE</td>
<td>3.4.1</td>
<td>QNSE</td>
<td>QNSE (4)</td>
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<tr>
<td>UW</td>
<td>3.4.1</td>
<td>UW</td>
<td>Eta similarity (2)</td>
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To isolate the impact of YSU update, the updated YSU from WRF3.4.1 is implemented into WRF3.4. The experiment with this version is referred to as YSU3.4+.
Domain configuration and observation sites around OKC

Resolution: 22.5->4.5km
Episode: July 17-19, 2003
Initial conditions
  meteo: FNL
  chemical: MOZART
Emission: NEI2005
YSU3.4 overestimates nighttime T2
YSU3.4 stands out during nighttime, BouLac has a similar but less severe problem. The nighttime performance is improved with the updated YSU.
YSU3.4 and BouLac overestimates nighttime wind speed at 10 m AGL
Improvement for nighttime wind

The update of YSU did not affect daytime simulation but improved performance during nighttime.
The updated YSU better reproduces LLJs.
YSU3.4 simulated too weak and elevated LLJs. The updated YSU simulates lower and stronger LLJs, showing a better agreement with observation.
Root cause of the improvement

The updated YSU reduces nighttime vertical mixing

The BouLac has a similar problem as the old YSU
Improvement in vertical thermal structure

The old YSU simulates too neutral boundary layer, while the updated YSU simulates a more stable boundary layer.
Reduced heat flux leads to improved T2

Reduced downward heat flux during nighttime leads to lower T2.
The nighttime performance is improved with the updated YSU.
The improvement in the presence of strong LLJs is prominent while it is less prominent for weak wind regimes (e.g., in the absence of LLJ).
The old YSU and BouLac significantly underestimate the shear exponent during nighttime.
Improvement of nighttime $O_3$

Previously nighttime $O_3$ overestimation was attributed to dry deposition and emissions.

The updated YSU improved predictions of the early evening decline of $O_3$. 
Impact on vertical distribution of O$_3$

The updated YSU reduces the downward transport of O$_3$ during nighttime
Vertical mixing of chemical species is treated with a simple 1\textsuperscript{st} order closure scheme using the $K$ diagnosed by PBL schemes.

$$\overline{w'c'} = -K_c \frac{\partial c}{\partial z}$$
Conclusions (1)

1. The update of the YSU scheme in WRF3.4.1 improved predictions of the nighttime boundary layer and can thus provide better wind resource assessments.

2. The BouLac scheme gives the strongest vertical mixing in the nighttime boundary layer. It consequently overestimates near-surface wind and temperature and underestimates the wind shear exponent at night.
3. Overestimation of nighttime O\textsubscript{3} is related to overestimation of surface winds, both of which can be partially attributed to excessive vertical mixing

- This has wide implications for the previously often reported overestimation of surface winds and O\textsubscript{3} from many models. Vertical mixing might be the cause and should be carefully considered.
Outline

• Current status of performance of PBL schemes
• Results of WRF model with chemistry (WRF/Chem) for an episode from the Joint Urban 2003 field campaign
• Future plan regarding improving vertical mixing in WRF/Chem
Improvement of vertical mixing of chemical species

Current treatment: \[ \overline{w'c'} = -K_c \frac{\partial c}{\partial z} \]

Proposed: \[
\overline{w'c'} = -K_c \left( \frac{\partial c}{\partial z} - \gamma_c \right) + \overline{(w'c')}_h \left( \frac{z}{h} \right)^3
\]

\[
\overline{(w'c')}_h = -A \overline{w_m}^3 / h
\]

\[
\overline{w_m}^3 = \overline{w_*}^3 + B \overline{u_*}^3
\]
Test of SCM WRF

1999-10-24_08:00:00 YSU

1999-10-24_08:00:00 BouLac+Chem

Height, km

Wind speed, m s⁻¹
References


5. Wolff, J., and M. Harrold, (2013), Tracking WRF performance: how do the three most recent versions compare? the 14th Annual WRF Users' Workshop, paper 2.6