Evaluation/improvement of PBL Schemes for meteorology and air quality simulations

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- Part 1: Daytime
 - a) Evaluate three PBL schemes in the WRF model
 - b) Improve PBL schemes through EnKF parameter estimation
 - c) Use L-Band radiosonde to improve PBL stability
- Part 2: Nighttime

Three PBL schemes in WRF MYJ, YSU, ACM2

• MYJ: local, down gradient

 YSU, ACM2: local+non-local (YSU implicit, ACM2 explicit)

YSU: the Yonsei University scheme MYJ: the Mellor–Yamada–Janjic scheme ACM2: the asymmetric convective model scheme, v2



Configurations

Episode & Resolution

- Period: July Sept., 2005
- Resolution: 108km, 36km, 12km, 4km
- Grids: 53×43, 97×76, 145×100, 166×184

Model Configurations

- YSU, ACM2, MYJ PBL schemes
- WSM 6-class graupel scheme
- NOAH land-surface model (LSM)
- Dudhia short wave radiation
- RRTM long wave radiation
- Grell-Devenyi ensemble cumulus scheme



Domains and TCEQ, NWS/FAA sites

T2 and Td over 211 NWS/FAA sites



MYJ gives the coldest and moistest biases near the surface

Mean PBL Height



MYJ underpredicts PBL height over most sites

Difference of T2 and HFX between simulations with YSU and MYJ

Mean over TCEQ sites (YSU-MYJ)



Difference of sensible heat flux (HFX) cannot explain difference of T2

Mean profiles of T and moisture



MYJ doesn't mix as high as YSU and ACM2 during daytime

Mean temperature profile difference from 9 to 11 CST



Normalized Kz profile due to different p



Profiles of T and q from runs with altered p



The similarity between the sensitivity of WRF to varied mixing strength and the sensitivity of WRF to different PBL schemes confirms that much of the sensitivity of WRF to different PBL schemes is attributable to their different vertical mixing strengths.

Mean profiles of T and moisture



MYJ doesn't mix as high as YSU and ACM2 during daytime

Conclusions

- The YSU and ACM2 schemes both tend to predict higher T and lower moisture, and thus smaller biases, than the MYJ scheme in the lower atmosphere during daytime because of their stronger vertical mixing.
 The above conclusion is verified by the experiments with the WRF model with altered
 - vertical mixing strength.

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b) Improve PBL schemes through EnKF parameter estimation

Sources of model errors:

Structural: model equations have a different functional form from the true laws governing the system

Parametric: the parameters used in model equations are not accurate

Test parameter sensitivity in ACM2

	Parameter name	ACM2 value	Plausible range	Role of parameter
p		2	1–3	Structure of local mixing within PBL
P	Prandtl No.	1	0.9–1.5	Nominal ratio of momentum/heat diffusion
0.1 <i>a</i>		0.72	0-large	Controls proportion of nonlocal mixing
R i _{crit}	Critical Richardson No.	0.25	0.2–1.2	Affects calculation of height of PBL
b		8.5	0–10	Controls excess buoyancy of surface plumes
r		5	4.5–7	Affects stable mixing in dimensionless profile
Rc	Critical Richardson No.	0.25	0.2-1.0	Governs flow dependence of stable turbulence
λ		80 m	40–120 m	Asymptotic value of turbulent length scale
V		1	0–1	Formulation for K_{zo}
K_v		0.001	0.0003-0.006	Proportional to minimum K_z as function of layer thickness

TABLE 1. Potentially identifiable ACM2 parameters

EnKF can only calibrate those most identifiable parameters with the attributes of 1) observability, 2) simplicity, and 3) distinguishability

WSP sensitivity to 10 parameters in ACM2



Correlation between parameters & WSP



WSP shows the largest correlation with *p*, Rc. Thus *p*, Rc have the largest identifiability

Sensitivity to p

 $K_z(z) = k \frac{u_*}{\phi} z (1 - z/h)^p$



Lower *p* => stronger vertical mixing => higher PBL height.

Use EnKF to update p, Rc

- Deterministic simulation (NoDA)
- Regular EnKF (NoPE)
- Parameter estimation EnKF (SSPE)
 - Update *p*, *Rc* simultaneously as updating regular states
 - Assimilate wind profiler data only every 6-hour between Aug. 30-Sept. 2, 2006 over Texas
- Deterministic simulation with estimated parameters (NoDAnew)

Wind vectors at Sept 1, 10 CST



SSPE shows the best agreement for surface wind.





SSPE predicts higher PBLH to match profiler data.

Evolution of *p*



During most of time, SSPE predicts *p* value lower than 2.0 (default).

Bias and error of T2



SSPE predicts the least cold bias.

Conclusions

- 1. PBL schemes remain one of the primary sources of inaccuracies in model simulation. Vertical mixing strength plays an important role in performance of PBL schemes
- 2. Real-data experiments show that simultaneous state and parameter estimation with EnKF performs better than deterministic simulation and regular EnKF by providing optimized flow dependent parameters in the PBL scheme

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CBL structure, 1st order K-theory



1st order K-theory: $\overline{w'\theta'} = -K_h \cdot \frac{\partial \overline{\theta}}{\partial z}$

1st order K-theory is widely used

1st order K-theory: $\overline{w'\theta'} = -K_h \cdot \frac{\partial \overline{\theta}}{\partial z}$

Table I Results of model survey.

GCM	Total levels	PBL Levels	Closure
BMRC	9	2	$\mathbf{K}(R_i)$
Canadian Climate Centre	15	2-3	$\mathbf{K}(R_i)$
ECMWF	19	4	$\mathbf{K}(R_i)$
GFDL-Manabe	30	6	$K(R_i)$ -MY-2.5
GFDL-Miyakoda	18	4	$K(R_i)$ -MY-2.5
GLA	17	2-3	MY-2.5
Los Alamos	20	$\Delta z_s = 30 \mathrm{m}$	$\mathbf{K}(R_i)$
NCAR-CCM1	12	1	$\mathbf{K}(R_i)$
NMC-MRF		3-4	$\mathbf{K}(R_i)$
NMC-eta		$\Delta z_s = 30 \mathrm{mb}$	$K(R_i)$ -MY-2.5
NMC-NGM	16	5	N. Phillips
Oregon State		$\Delta z_s = 20 - 50$ m	K-profile
U.K. Meteorological Office		2	$\mathbf{K}(R_i)$
U. Hamburg	19	4	$K(R_i)$
U. Maryland	18	3–4	$K(R_i)$
UCLA-CSU		1	mixed-layer model

TABLE II Model name, use, type and reference.

Model	Use	Туре	Ref
ECMWF	Operational	1st order	Beljaars and Viterbo (1998)
ECMWF-MO	Operational-test	1st order	
NOAA-NCEP	Operational	1st order	Hong and Pan (1996)
MeteoFrance	Operational	1st order	Louis et al. (1982)
JMA	Operational	1st order	Mellor and Yamada (1974)
MetOffice	Operational	1st order	Louis (1979)
MetOffice-res	Research	1st order	Williams (2002)
WageningenU	Research	1st order	Duynkerke (1991)
Cuxart et al. (2006)			

Ayotte et al. (1996)

But it has problem!!!!

Slightly stable upper CBL, early evidence



Fig. 5. This graph shows the average potential temperature for each run on 12 June 1961, plotted as a function of height. The uncertainty between the two points marked is of the order of 0.1 deg due to a range change in the thermometer used.

Telford and Warner (1964)

FIG. 1. The mean state of the atmosphere during the measurement runs on 25 April 1968. Lenschow 1970

Slightly stable upper CBL, early evidence



Figure 4. Potential temperature and mixing ratio obtained from soundings made at positions A and C as shown in Fig. 1. The dashed lines represent observations made while the aircraft was ascending, the full lines those while the aircraft was descending immediately afterwards and in the same air position as the ascent.

<u>Warner 1971</u>

Slightly stable upper CBLs justify countergradient term



Uncertainties in instantaneous soundings: Beijing



Using limited number of soundings to infer CBL structure and calibrate γ has substantial uncertainties

$$\overline{w'\theta'} = -K_h \cdot \left(\frac{\partial\theta}{\partial z} - \gamma\right)$$

Uncertainties in instantaneous soundings: Beltsville



Thus, we use large amount of afternoon soundings (**only available in China!**) to calibrate PBL schemes

Long-term L-Band radiosondes confirm slightly stable CBL



YSU vs. Shin-Hong to simulate CBL



Shin-Hong loses the capability to simulate the slightly stable CBL
Quasi-steady-state analytical solutions to a K-profile PBL model (<u>Stevens, 2000</u>)

$$\overline{w'\theta'} = -K_h \cdot \left(\frac{\partial\theta}{\partial z} - \gamma\right) \qquad \qquad K_h = kz(1-z)^2$$



The countergradient term γ is critical to simulate the slightly stable CBL

Testing Shin-Hong and YSU in 1D WRF



 f_{nl} and z_{*SL} are critical to simulate the CBL structure

Parameterized fluxes with different f_{nl} and z_{*SL}





Evaluation of 3D WRF for 14 cases

Roughly capture individual cases

Zoom in individual cases



Uncertainties in instantaneous soundings: Beltsville



LES: instantaneous vs. ensemble mean



Improve Shin-Hong to simulate real CBLs



Composite profile of the 14 cases: calibrated Shin-Hong has the best performance Hu, Xue, Li (2019, MWR, conditionally accepted)

Conclusions

1. The Shin-Hong scheme is improved to simulate the slightly stable upper CBL 2. The improved Shin-Hong simulates a lower level of neutral stability

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Outline

- Current status of performance of PBL schemes in terms of wind and O₃
- Results of WRF/Chem for an episode from the Joint Urban 2003 field campaign
- Future plan to improve vertical mixing in WRF/Chem

Current status 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 CBLs, 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

Overestimations of nighttime surface winds with several models



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

WRF (Wolff and Harrold, 2013)

Overestimation of surface winds during stable conditions (2)



Systematic positive model biases for surface wind speed during nighttime.

Overestimations of surface winds during stable conditions (3)



Performance of MM5 applied in Sweden (Miao et al., 2008)

Overestimation of nighttime surface O₃



Summary of current status

- A few models face the problem of overestimation of near-surface wind and O₃ 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 scheme one of the mostly widely used schemes



Past evaluation of YSU (2)



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
$$K_m = kW_s Z(1 - \frac{Z}{h})^2$$

Velocity scale $W_s = \mathcal{U}_* / \phi_m$
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 Ri # of 0 while h is diagnosed using Ri # of 0.25

Vertical profiles of K_m under different stabilities



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 O₃

Numerical experiments with WRF/Chem

Abbreviation	WRF version	PBL scheme	Surface layer scheme*
			(option number in WRF)
YSU3.4	3.4	old YSU	MM5 similarity (1)
YSU3.4 +	3.4	updated YSU	MM5 similarity (1)
YSU3.4.1	3.4.1	updated YSU	MM5 similarity (1)
MYJ	3.4.1	MYJ	Eta similarity (2)
MYNN2	3.4.1	MYNN2	Eta similarity (2)
BouLac	3.4.1	BouLac	Eta similarity (2)
QNSE	3.4.1	QNSE	QNSE (4)
UW	3.4.1	UW	Eta similarity (2)

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



Temporal variation of T2



YSU3.4 stands out during nighttime, BouLac has a similar but less severe problem The nighttime performance is improved with the updated YSU.

Improvement for nighttime wind





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 YSU3.4+ YSU3.4 YSU3.4.1 1.5 -7-19_03 UTC - -7-19_04 UTC -7-19_05 UTC •••7-19_06 UTC Height, km .5 a b 0 ΜYJ **BouLac** PNNL obs 1.5



The old YSU simulates too neutral boundary layer, while the updated YSU simulates a more stable boundary layer.

Temporal variation of T2



The nighttime performance is improved with the updated YSU.

Improvement of nighttime O₃

Previously nighttime O₃ overestimation was attributed to dry deposition and emissions



Impact on vertical distribution of O₃



The updated YSU reduces the downward transport of O₃ during nighttime

Limitation of vertical mixing of chemical species in current WRF/Chem



$$\overline{w'c'} = -K_c \,\frac{\partial c}{\partial z}$$

Vertical mixing of chemical species is treated with a simple 1^{st} order closure scheme using the *K* diagnosed by PBL schemes

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.
Conclusions (2)

- 3. Overestimation of nighttime O_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 O₃ 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: $\overline{w'c'} = -K_c \left(\frac{\partial c}{\partial z} - \gamma_c\right) + \overline{(w'c')_h} (\frac{z}{h})^3$
 $\overline{(w'c')_h} = -Aw_m^3/h$
 $w_m^3 = w_*^3 + Bu_*^3$

Test of SCM WRF



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