P1.8 **SENSITIVITY OF WRF/CHEM PREDICTIONS TO METEOROLOGICAL SCHEMES**

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1. INTRODUCTION

Three-dimensional (3-D) atmospheric models are an important tool in studying meteorological variables and their impacts on chemical species. Understanding the effects of meteorological parameterizations on meteorological and chemical predictions of 3-D models is necessary to the use of appropriate parameterizations for simulating different episodes. Performance of these schemes may vary from episode to episode, and may be highly dependent upon the horizontal grid spacing and time resolution used. The accuracy of predicted meteorological variables (e.g., temperature (T), relative humidity (RH), wind speed and direction, and planetary boundary layer (PBL) height) is a prerequisite for accurate predictions of chemical species and depends on the performance of meteorological parameterizations.

Operating online, the Weather Research and Forecasting/Chemistry (WRF/Chem) model uses the state of the science WRF meteorological model and integrates the simulation of chemical species formation and transport simultaneously with meteorological predictions. The objectives of this study are to examine the simulated meteorological variables using different combinations of land-surface models (LSMs) and planetary boundary layer (PBL) parameterizations, and the effects of the simulated meteorology on chemical predictions.

WRF/Chem offers several options for meteorological physics, as well as several gas-phase mechanisms, and aerosol modules. Two options critical to WRF/Chem simulations are the LSM and PBL schemes. This study evaluates several well known meteorological schemes including two LSMs (the Noah (Ek et al., 2003) and slab soil (Dudhia, 1996) and two PBL schemes (the Yonsei University (YSU) (Hong and Dudhia, 2003) and Mellor-Yamada-Janjic (Mellor and Yamada, 1982; Janjic, 1994) (MYJ) PBL schemes). The Noah LSM is a popular scheme developed jointly by the National Center for Environmental Prediction, Oregon State University, the Air Force, and the Hydrologic Research Lab. The five-layer slab soil model provides an improvement to the two-layer scheme used in MM5. Both the YSU and MYJ PBL schemes are turbulence parameterizations commonly employed in several operational meteorological models. The MYJ is a PBL scheme that explicitly defines turbulent quantities, using a conservation of turbulent kinetic energy (TKE). The YSU scheme, however, is a modification of the Medium Range Forecast (MRF) PBL scheme, using an explicit treatment of entrainment rather than implicit. The MYJ scheme defines the PBL height using TKE, while the YSU scheme is dependent upon the bulk Richardson number.

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2. DOMAIN AND MODEL CONFIGURATION

WRF/Chem is applied with a 12-km horizontal grid spacing for a 5-day (28 August through 2 September 2000) episode from the Texas Air

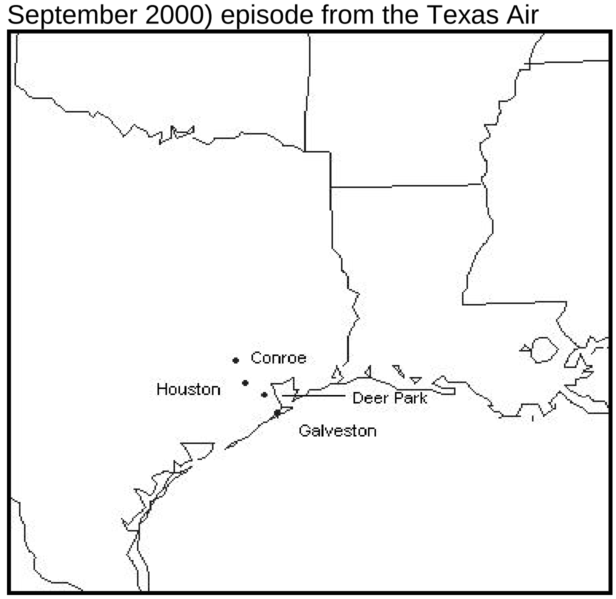

Figure 1. Map of WRF/Chem simulation domain for 28 August - 2 September 2000 TexAQS-2000 episode.

Quality Study 2000 (TexAQS-2000) in the southern U.S. The domain for this study centers on the Houston-Galveston area in eastern Texas, as shown in Figure 1.

The chemistry used in this study consists of the Second Generation Regional Acid Deposition Model (RADM2) gas-phase mechanism (Stockwell et al., 1990), the Modal Aerosol Dynamics Model (MADE) with the Secondary Organic Aerosol Model (SORGAM)(Ackermann et al., 1998; Schell et al., 2001).

To examine the effects of different meteorological schemes on chemical simulations, a base simulation with the Noah LSM coupled with the YSU PBL scheme (hereafter referred to as SOR_NOAH) is conducted to provide a benchmark to two sensitivity simulations in which

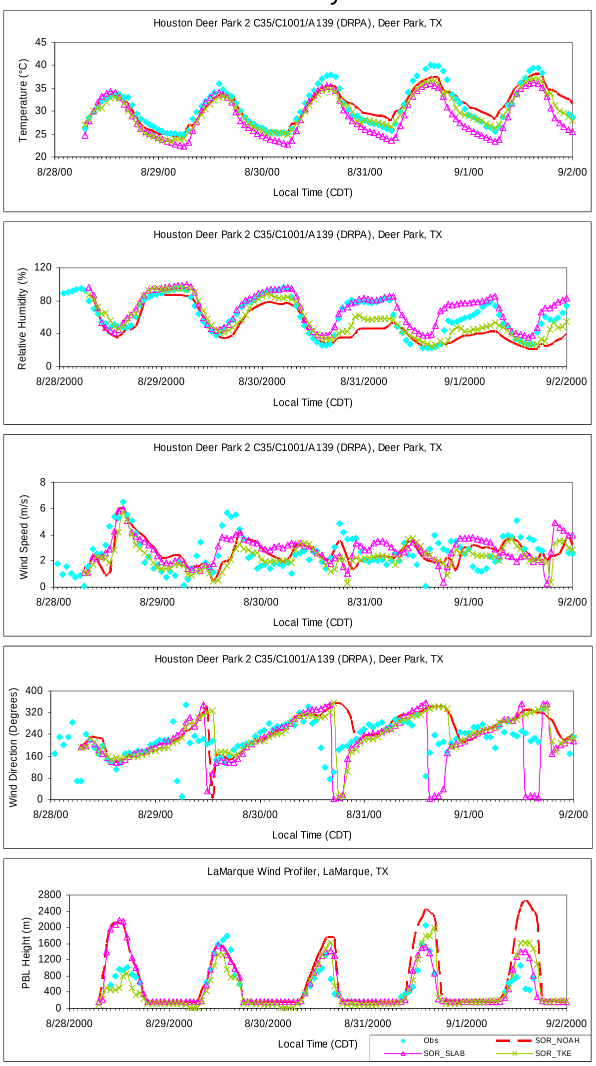

Figure 2. Temporal distributions of (a) T, (b) RH, (c) wind speed, and (d) wind direction at Deer Park, Texas; and (e) PBL height at LaMarque, Texas during 28 August - 2 September, 2000.

different combinations of meteorological schemes are used. The slab LSM and the YSU PBL scheme are used in the first sensitivity simulation and the Noah LSM and MYJ PBL scheme are used in the second sensitivity simulation (hereafter referred to as SOR_SLAB and SOR_TKE, respectively).

3. MODEL EVALUATION

3.1 *Meteorological Variables*

The meteorological predictions of WRF/Chem are compared against observations from TexAQS-2000. The analysis consists mainly of temporal and statistical analysis. Figure 2 shows the temporal distributions of temperature, wind speed and direction, and RH at Deer Park, Texas and PBL height at LaMarque, Texas, a location with observations near Deer Park. The predicted meteorological variables correspond well with observed values for the first two days at most locations, especially in the case of temperature and RH. During days three through five, model deviations grow significantly away from observed values for all simulations. This can be attributed to the lack of a data assimilation system in the version of WRF used here, which is currently under development. In general, each model simulation underpredicts the daily maximum temperature. The SOR_NOAH simulation overpredicts nighttime temperatures at most locations, while SOR_SLAB shows a general underprediction at nearly all times during days three through five. The SOR_SLAB simulation also gives RH more accurately than SOR_TKE and SOR_NOAH, as the latter two grossly underpredict nighttime values by up to 58% of the observed value during days 3-5. All three simulations reproduce the observed wind speed relatively well at all locations and during most hours. Overall, wind direction simulations showed significant deviations from observed values during nighttime hours. However, one limitation of evaluating wind directions is that because wind direction is a vector, the numeric values of differences between the observations and predictions may not reflect well the actual differences in wind rose plots when the numeric differences are greater than 180°. For example, at 6:00AM LST on August 29 at Deer Park, the observed wind direction is 11°, and the predicted wind directions from the three model runs range from 228.3° to 254.1°. The numerical differences range from 217.3° to 243.1°, whereas the actual differences on wind rose plots range from 142.7°

Table 1. Performance statistics for T at 2-meter height (T2), RH, PBL height (1A) and wind speed and direction (1B).

1A	**T2**			**RH**			**PBL Height**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	31.2	31.2	31.2	62.5	62.5	62.5	1089.3	1089.3	1089.3
MeanMod	30.9	28.9	29.9	45.2	66.2	52.6	1519.4	1288.6	913.4
Number	3502	3502	3502	795	795	795	203	203	203
Corr	.88	.91	.91	.70	.75	.74	.66	.77	.64
NMB (%)	-1	-7	-4	-28	6	-16	39	18	-16
NME (%)	5	8	6	31	20	23	45	29	30

1B	**WSP**			**WDR**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	2.9	2.9	2.9	210	210	210
MeanMod	3	2.9	2.6	228.5	223.7	223.7
Number	3502	3502	3502	3391	3391	3391
Corr	0.35	0.30	0.47	0.46	0.40	0.46
NMB (%)	3	-1	-12	9	7	7
NME (%)	0.42	0.42	0.37	0.21	0.23	0.21

to 116.9°, respectively. For PBL height predictions at most locations, both SOR_NOAH and SOR_SLAB overpredict values for day one at all locations. During days two through five, SOR_TKE and SOR_SLAB give a closer agreement to the observed PBL heights, with SOR_TKE showing a slight overprediction and SOR_NOAH showing consistent overprediction during most time periods. All simulations, however, represent the early development of the PBL height relatively well at all locations. Temporal analyses also show that model discrepancies grow significantly larger during days three through five, mainly because of the lack of a data assimilation system in WRF, as mentioned previously.

Several statistical metrics suggested by Yu et al. (2003) are calculated to evaluate overall model performance. Tables 1A and 1B show several statistical parameters for meteorological predictions. In terms of normalized mean bias (NMB), the SOR_SLAB simulation gives better performance than SOR_NOAH and SOR_TKE for RH (5.8% vs. -27.8% and -15.9%) and wind speed (-0.5% vs. 2.6% and -12.2%). Both SOR_TKE and SOR_SLAB slightly outperform SOR_NOAH for wind direction (both 6.5% vs. 8.8%). Statistically, SOR_TKE predicts PBL height more accurately than SOR_NOAH and SOR_SLAB (-16.1% vs. 39.5% and 18.3%). The general underprediction of the MYJ scheme is generally consistent with results from past studies (e.g., Fast, 2005). Due to the implicit nature of the boundary layer depth in the YSU scheme, errors within variables used to calculate vertical motions can cause errors in simulated depths, whereas the MYJ scheme (which uses more complete physics) seems to have less bias (Alapaty et al., 1996). However, as shown in Figure 2, SOR_SLAB may seem to outperform SOR_NOAH and SOR_TKE during days two through five, but the magnitude of the overprediction on day one dominates the overall statistical performance of the simulation. Because SOR_TKE is relatively closer to observations at all days, it shows less bias than SOR_SLAB, even though SOR_SLAB performs better on Days 4-5. SOR_NOAH, though, outperforms SOR_SLAB and SOR_TKE at forecasting temperature (-1.1% vs. -7.4% and -4.1%).

3.2 *Chemical Species*

The model chemical predictions are also evaluated using observed chemical data taken from the TexAQS-2000. The mixing ratios of O_3 and CO, as well as the concentrations of fine particulate matter ($PM_{2.5}$) and sulfate (SO_4^{2-}) are the initial foci of our analyses. Temporal and statistical analyses are conducted (where data were available), along with an intercomparison among three sets of model results.

Figure 3 shows the temporal distribution of chemical species at Deer Park, Texas. For O_3, all three model simulations predict daytime concentrations relatively well, with the exception of some sites (as shown in Figure 3 at Deer Park) where deviations are 41-52% less than the maximum observed values on days 3-4. Each simulation significantly overpredicts nighttime concentrations, by as much as 200% of the observed value in some cases. Of the three simulations, however, SOR_TKE more adequately replicates nighttime O_3, with the lowest NMB.

Analyses of the CO plot shows that SOR_TKE gives mixing ratios that are closer to the observations than the other two simulations. One possible explanation for this is that SOR_TKE gives lower PBL heights on days 1-3 than SOR_NOAH and SOR_SLAB, which allows less volume for CO to mix out. Large model deviations exist for CO predictions during nighttime. At night, the MYJ scheme simulates a shallower boundary layer, which would explain the higher predictions of CO during nighttime by SOR_TKE. For $PM_{2.5}$ and SO_4^{2-}, the results from the three model simulations are quite similar during most time periods. At most locations, SO_2 concentrations predicted by SOR_SLAB are greater than those predicted by either SOR_NOAH or SOR_TKE, which leads to higher predicted SO_4^{2-} concentrations. Relatively minor differences among model simulations exist for $PM_{2.5}$ with the exception of higher simulated daily maximum values by the SOR_SLAB simulation.

Table 2. Performance statistics for predictions of O_3, CO, NO, NO_2, and $PM_{2.5}$.

O_3	**Daytime**			**Nighttime**			**Daily**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	54.5	54.5	54.4	24.8	24.8	24.8	39.4	39.4	39.4
MeanMod	58.7	59.7	57.1	46.2	48.1	33.9	52.1	53.6	45
Number	3270	3270	3270	3139	3139	3139	6123	6123	6123
Corr	.62	.57	.63	.61	.54	.60	.70	.60	.70
NMB (%)	8	9	5	87	94	37	30	40	10
NME (%)	28	30	29	93	101	59	50	40	40
CO	**Daytime**			**Nighttime**			**Daily**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	390.4	390.4	390.4	433.6	433.6	433.6	411.8	411.8	411.8
MeanMod	257.8	309.5	343.4	236.3	273.5	338.7	247.1	291.6	341.1
Number	667	667	667	658	658	658	1325	1325	1325
Corr	.13	.17	.17	.04	.06	.07	.10	.10	.10
NMB (%)	-34	-21	-12	-46	-37	-22	-40	-30	-20
NME (%)	52	54	58	59	58	61	60	60	60
NO	**Daytime**			**Nighttime**			**Daily**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	3.6	3.6	3.6	11.7	11.7	11.7	7.5	7.5	7.5
MeanMod	3.1	3.5	5.2	.02	.02	.08	1.6	1.8	2.8
Number	395	395	395	363	363	363	758	758	758
Corr	.36	.36	.57	.29	.32	.27	-.07	-.07	-.02
NMB (%)	-13	-4	45	-100	-100	-99	-78	-76	-63
NME (%)	79	83	100	100	100	99	94	96	99
NO_2	**Daytime**			**Nighttime**			**Daily**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	11.9	11.9	11.9	14.7	14.7	14.7	13.2	13.2	13.2
MeanMod	13.3	16.1	18.0	29.5	32.4	40.4	21.0	23.9	28.7
Number	805	805	805	730	730	730	1535	1535	1535
Corr	.32	.31	.32	.17	.21	.21	.28	.30	.30
NMB (%)	12	36	52	100	120	170	89	80	120
NME (%)	84	98	1.04	130	140	190	110	120	150
$PM_{2.5}$	**Daytime**			**Nighttime**			**Daily**		
	NOAH	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**	**NOAH**	**SLAB**	**TKE**
MeanObs	10.3	10.3	10.3	10.4	10.4	10.4	10.3	10.3	10.3
MeanMod	14.1	15.3	16.2	11.1	12.1	12.2	12.7	13.8	14.3
Number	886	886	886	811	811	811	1697	1697	1697
Corr	0.26	0.33	0.37	0.16	0.18	0.2	0.2	0.3	0.3
NMB (%)	36	48	56	7	17	18	20	30	40
NME (%)	66	70	74	51	54	54	60	60	60

For SO_4^{2-}, SOR_TKE simulates values 25-30% higher than SOR_NOAH or SOR_SLAB on day 1 at most locations (as seen in Figure 3), while SOR_SLAB simulates higher maximum concentrations by near 50% at most locations for days 4-5. The simulation results with SOR_NOAH are similar to those of SOR_TKE at most locations. Table 2 shows the performance statistics for O_3, CO, NO, NO_2, and $PM_{2.5}$ for daytime and nighttime, as well as daily values. For hourly predictions throughout a day, SOR_TKE performs better for O_3 (14.3% vs. 32.3% and 36.0%) and CO (-17.2% vs. -40.0% and -29.2%) mixing ratios in terms of NMB as compared to SOR_NOAH and SOR_SLAB. SOR_NOAH performs better for $PM_{2.5}$ than SOR_SLAB and SOR_TKE (22.4% vs. 33.3% and 38.0%). While all model simulations reproduce observed daytime O_3 mixing ratios reasonably well (with NMBs of 5-9%), they all significantly overpredict nighttime O_3 mixing ratios (with NMBs of 37-94%). This can be partially attributed to the significant underprediction of nighttime NO (as a result of overprediction of mixing at night), which titrates less amounts of O_3 in the nocturnal PBL. While the CO mixing ratios during some time periods (e.g., 7:00AM to 10:00AM LST on days 1-5) are overpredicted, those during other periods are underpredicted. The underpredictions dominate, resulting in a net negative bias. While NO mixing ratios are significantly underpredicted (by 63-78%), NO_2 mixing ratios are significantly overpredicted (80-120%), with much larger deviations occurring at night for both species. In addition to inaccuracies in the meteorological predictions, the equilibrium assumption made in simulating nitrogen chemistry in the RADM2 gas-phase mechanism may not represent the ambient conditions simulated for this particular episode, which may contribute to the larger model biases for NO_x predictions. An interesting observation is that each model shows a lower NMB during daytime simulations of O_3, CO, NO and NO_2, but daytime biases for $PM_{2.5}$ are higher than those at night. While the secondary PM species may have been well reproduced during daytime, the larger uncertainties may be likely due to the uncertainties in the emissions of primary PM species such as BC and OM. Among the three model simulations, SOR_TKE gives the best performance for O_3, CO, and NO, and SOR_NOAH gives the best performance for NO_2 and $PM_{2.5}$. It is noted that differences between observations and model predictions from the three simulations are larger than differences among model results. This indicates that uncertainties other than meteorology (e.g., emissions) may also be important factors for the discrepancies between observations and predictions.

4. SUMMARY

Our evaluation has shown, for this particular episode, that meteorological schemes play an important role in the simulation of chemical species. It appears that the use of different PBL parameterization and land-surface schemes affects chemical predictions for this scenario. When comparing the performance of the models in terms of meteorological variables and chemical species, the SOR_SLAB simulation performs better in terms of temporal and statistical analyses than either SOR_NOAH or SOR_TKE, with the exception of SOR_NOAH predicting surface temperature more accurately. Although SOR_SLAB gives better meteorological predictions, SOR_TKE performs better than SOR_NOAH and SOR_SLAB for O_3 and CO predictions. A better representation of daytime

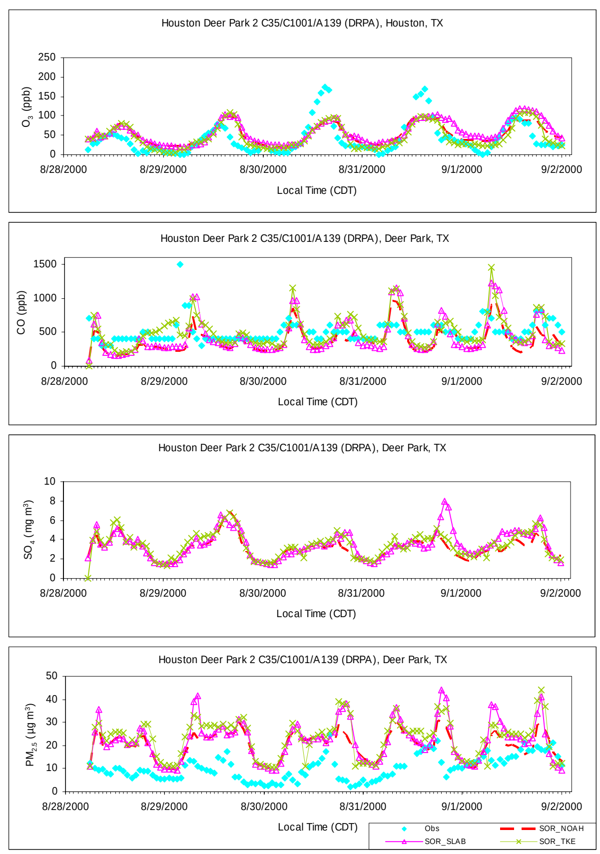

Figure 3. Temporal distributions of (a) O_3, (b) CO, (c) SO_4^{2-}, and (d) $PM_{2.5}$ at Deer Park, Texas, during 28 August - 2 September 2000 (Observed SO_4^{2-} data was not available during this time period).

and nocturnal PBL heights by the TKE PBL scheme gives better predictions for primary species such as CO and NO (higher than those predicted by the YSU scheme). Compared to SOR_NOAH, higher NO mixing ratios predicted by SOR_TKE titrate more O_3 at night, resulting in a lower NMB in nighttime O_3 predictions (and thus overall O_3 predictions because of the dominancy of the nighttime NMB). For NO_2 and $PM_{2.5}$, SOR_NOAH gives the best overall performance.

A strong correlation has typically been considered between temperature and mixing ratios of O_3. An interesting finding of this study, however, shows that better temperature predictions do not necessarily give a better O_3 performance. While SOR_NOAH simulates temperature more accurately than either SOR_SLAB or SOR_TKE, its O_3 performance is not as good as that of SOR_TKE (with a NMB of 32.3% and 14.3%, respectively). This is because the O_3 performance for this episode is dominated by the poor O_3 performance at night, rather than daytime. The poor O_3 performance at night by SOR_NOAH is due partially to the fact that the YSU scheme gives poorer representation of the nocturnal PBL than the TKE scheme.

Further study is necessary to fully understand the impacts of meteorological variables on the formation and transport of chemical species and all major likely causes for the discrepancies in meteorological and chemical predictions with different meteorological schemes.

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