ABSTRACT

MISENIS, CHRISTOPHER ALLEN. An Examination of WRF/Chem: Physical Parameterizations, Nesting Options, and Grid Resolutions. (Under the direction of Dr. Yang Zhang).

The accurate representation of meteorological processes in the boundary and surface layers, as well as the interaction between the two, is crucial to the accurate simulation of meteorological variables and chemical species. This work focuses on several facets of simulating atmospheric processes: (1) planetary boundary layer (PBL) parameterizations, (2) land surface models (LSM), (3) horizontal grid spacing, and (4) one- and two-way nesting options. A modeling study utilizing the Weather Research and Forecast model with Chemistry (WRF/Chem) is conducted for a five-day period beginning 12 UTC (7AM CDT) 28 August through 6 UTC (1AM CDT) 2 September 2000. The modeling domain is centered over the Houston-Galveston area in Texas. Sensitivity studies for PBL and LSM options are conducted using a 12-km horizontal grid spacing. For analysis of horizontal grid spacing and nesting options, both 12- and 4-km horizontal grid spacings are used, each utilizing both one- and two-way nesting.

For the PBL sensitivities, two parameterizations are chosen: Yonsei University (YSU) and the Mellor-Yamada-Janjic (MYJ) 2.5 order TKE closure. These simulations will both use the National Center for Environmental Prediction, Oregon State University, Air Force, and the Hydrologic Research Lab’s (NOAH) LSM. For simplicity, we will refer to these simulations as N_Y and N_M, respectively. Sensitivities to different LSMs are also studied with three parameterizations: NOAH, simple thermal diffusion scheme (slab), and Rapid Update Cycle (RUC), using the same PBL scheme (YSU) (referred to as N_Y, S_Y, and R_Y). The nesting and horizontal grid spacing sensitivities will utilize the same
physical setup as the N_Y simulation. Four simulations are evaluated: one-way nesting at 12-km (1W12), one-way nesting at 4-km (1W4), two-way nesting at 12-km (2W12), and two-way nesting at 4-km (2W4).

Results from these simulations are compared with observations taken during the 2000 Texas Air Quality Study (TexAQS-2000). A comprehensive, regional field campaign included more than 20 sites measuring meteorological variables and chemical species. Measurements taken from NOAA’s Electra aircraft are compared with simulated vertical profiles.

Results show that overall, model simulations are quite sensitive to changes in physical parameterizations. For instance, if simulated sensible heat fluxes from an LSM are lower, simulated surface temperatures are lower, RH is higher, and PBL depth is shallower. Also, differences in simulated PBL depths and wind fields can cause differences in simulated chemical species. Theoretically, lower PBL heights will limit vertical mixing, and variations in wind fields can reintroduce pollutants. However, the latter hypothesis was not confirmed in this study. Model simulations are also sensitive to nesting and horizontal grid spacing. The most significant differences occur at 4-km using different nesting options. When analyzing the 12-km simulations, it was interesting to note that two-way nesting had no appreciable benefit to simulated values.

Overall, results give a good indication of the current status of development for WRF/Chem and its future use as an operational forecasting tool. These results also serve to reinforce the need for future research into the use of various physical parameterizations and nesting options as they relate to air quality modeling and forecasting.
An Examination of WRF/Chem: Physical Parameterizations, Nesting Options, and Grid Resolutions

by

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BIOGRAPHY

Chris Misenis was born in Raleigh, NC and raised in rural Johnston County. As a student at North Johnston High School, Chris developed a fond interest in meteorology, selecting it as a career to pursue. He was selected into N.C. State University’s Meteorology program in the Fall of 2000. Upon graduation from high school in 2001, Chris enrolled as full-time student at N.C. State. The first research experience Chris was involved in was performing small projects with Greg Fishel at WRAL-TV. After this position, he was given the opportunity to work with Dr. Yang Zhang as an undergraduate research assistant in the Air Quality Forecasting Lab. In this capacity, he worked on model evaluation, first with CMAQ and subsequently, WRF/Chem. Also, Chris was charged with the initial development of the AQFL website (http://www.meas.ncsu.edu/aqforecasting). Chris graduated from N.C. State with a B.S. in Meteorology and Minor in Statistics in May 2005. He then worked as a research assistant in the summer of 2005 in the AQFL and enrolled in the Master’s program in the Fall, with a concentration in Air Quality Modeling and Forecasting.
I would first like to acknowledge my committee members, Drs. Yang Zhang, Jerry Davis, and Pal Arya. Each has provided great insight and knowledge (in graduate years and earlier) to me in the aid of completion of this degree. More importantly, I would like to thank Dr. Zhang for the opportunities she has given me to further my research through academics, as well as through various outside research experiences.

There are numerous people who deserve credit and notice here. I will try my level best to include all of those that I can remember. In no particular order: Drs. Georg Grell and Steven Peckham of NOAA, ESRL; Dr. Jerome Fast, PNNL; Dr. Shaocai Yu, NOAA Atmospheric Sciences Modeling Division; Dr. Darrel Baumgardner, Universidad Nacional Autonoma de Mexico; Dr. Russell Philbrick, Pennsylvania State University; Dr. Jianping Huang, Yale University. Certainly, I wish to thank the funding of this research and my academic career: National Science Foundation Award No. Atm-0348819; Department of Marine, Earth, and Atmospheric Sciences, N.C. State.

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1.1 Background and Motivation

Three-dimensional (3-D) atmospheric models are important tools in studying and understanding meteorological variables and their effects on chemical species. Current state-of-the-science models use various physical parameterizations to simulate meteorological processes. The most notable reason for the use of such approximations is to reduce computational time required to simulate these processes. Although the effects of parameterizations vary from episode-to-episode, the understanding of each option and how they affect meteorological and chemical predictions is important to improve current treatments in atmospheric models.

Two important parameterizations involved in atmospheric modeling include planetary boundary layer (PBL) schemes and land-surface models (LSMs). The PBL is defined as the lower portion of the atmosphere (on the order of 1 km) that exists due to the interactions between the atmosphere and the surface on timescales of less than a day (Arya, 2001). Several important small-scale atmospheric processes occur in this portion of the atmosphere, such as entrainment of free atmospheric air, generation of turbulence, vertical mixing, and resulting fluxes of heat, mass and momentum. It is the accuracy of the representation of these processes in large-scale atmospheric models that influence resultant predictions of meteorological variables, in turn affecting simulated chemical species.

LSMs have a similar task in trying to represent processes that occur at the interface between the surface and the atmosphere. Such microscale processes include sensible and
latent heat fluxes, long and shortwave radiations, as well as transfer through subsurface medium. Other processes involved are water’s phase change from liquid to gas (evaporation), evaporation from plants (transpiration), and the sum of both (evapotranspiration).

One important factor to note when examining atmospheric simulations using such parameterizations is the presence of feedback between schemes. For example, PBL schemes and LSMs have a semi-circular feedback. Simulated values of temperature and mixing ratio are used as input into land-surface processes. Likewise, simulated values of sensible and latent heat fluxes by the LSM serve to influence processes within the PBL (Figure 1.1).

The interplay between these two model components has significant bearing on the simulation of atmospheric chemistry. As surface-layer variables (e.g., temperature, humidity, wind speed) are simulated within the PBL scheme, they are fed back into the LSM for incorporation. Likewise, as the LSM simulates outgoing radiation and soil moisture, these values are integrated within the PBL scheme for further simulation.

Typically, atmospheric modelers are interested in knowing where the most interesting or dangerous weather is likely to occur. However, air quality episodes are typically associated with relatively calm weather conditions (Dabberdt et al., 2004). This work attempts to examine the effectiveness of a state-of-the-science modeling system by comparing simulated values with a relatively high resolution observational dataset consisting of meteorological variables and chemical species (e.g., ozone (O$_3$) and fine particulate matter (PM$_{2.5}$)).

Recent advancements in computational power have allowed for tremendous progress in terms of numerical prediction. One such sign of progress involves the use of finer (12-km
or less) horizontal grid spacing domains and nesting (Mass and Kuo, 1998; Mass et al., 2002). Meteorology and atmospheric chemistry are inundated with processes that occur on a wide range of spatial and temporal scales. There are varying opinions on the ability of atmospheric models running at a smaller resolution to accurately simulate atmospheric processes. Mass et al. (2002) cite several studies which indicate that performance of models using finer horizontal resolutions can provide better, worse, or similar results to models using coarser grid spacing. Further information on such studies will be provided later. By utilizing a state-of-the-science atmospheric model, an examination of the use of finer horizontal grid spacing as it relates to meteorological variables and chemical species will be presented.
Figure 1.1. The interactions among various parameterizations within numerical models (from United Corporation for Atmospheric Research (UCAR)). http://www.mmm.ucar.edu/mm5/documents/MM5_tut_Web_notes/MM5/mm5.htm; SH – sensible heat, LH – latent heat, SW – shortwave, LW – longwave, T – temperature, Q_v – water vapor mixing ratio.
2.1 Effects of Parameterizations on Meteorological Simulations

When simulating meteorological variables and chemical species using 3-D numerical models, one must understand that parameterizations used within the model framework are not fully independent. By this, it is implied that feedback from one scheme to another can lead to changes in both (Jankov et al., 2005). A review of various effects of parameterizations on the simulation of meteorological variables and thus, chemical species, is given below.

2.1.1 Planetary Boundary Layer (PBL)

The simulation of the atmospheric boundary layer is extremely important in terms of meteorology and chemistry. The PBL is known as the lowest level of the Earth’s atmosphere (3000 m and lower), which is directly influenced by surface characteristics, on a timescale of an hour or less (Stull, 1988). The fact that surface forcing influences the PBL makes it extremely difficult to simulate numerically, due to small-scale turbulent motions. To simulate the PBL accurately, one must have an accurate representation of turbulent fluxes of moisture, heat and momentum, and short and longwave radiation fluxes (Shafran et al., 2000). In order to better understand the effects of various parameterizations on atmospheric chemistry, an examination of the sensitivity of meteorological predictions to PBL parameterization schemes must be conducted.
Initially, PBL schemes were simple, bulk models of the atmosphere (half-order closure). The bulk method of simulating PBL processes has been used for several decades, mostly due to its simplicity and general accuracy (Stull, 1988). Some variations of the bulk method remain popular and in use even today (Kara et al., 1999; Braun and Tao, 2000; Ahlgrimm and Randall, 2006). However, various small-scale processes (e.g., turbulent eddies) exist in the boundary layer that cannot be accounted for by the simple bulk method.

The next available option for simulating the PBL is the use of K-theory (first-order closure) (Garratt, 1992). K-theory (or gradient-transport theory) assumes that turbulent fluxes are transported down the local gradient. First-order closure works well in near-neutral and stably stratified PBLs, but becomes questionable as convection dominates in the production of turbulence. Two types of turbulence closure schemes exist in atmospheric models: local and nonlocal closure. In local closure schemes, turbulent fluxes at various height levels in the boundary layer are related to vertical gradients of mean variables at the same heights. Nonlocal closure works much in the same way, but it estimates the fluxes at a certain point by analyzing the mean profiles over the entire domain of turbulent mixing (the PBL). In doing so, nonlocal schemes are able to account for multiple-size eddies, making them more applicable to convective, unstable boundary layers (Bright and Mullen, 2002).

Several studies have been conducted on the effects of various PBL parameterizations on simulated meteorological variables (Bright and Mullen, 2002; Jankov et al., 2005; Deng and Stauffer, 2006; Gallus and Bresch, 2006; Mao et al., 2006; Misenis et al., 2006). Hong and Pan (1996) noted that by using nonlocal closure schemes, a more accurate representation of temperature and relative humidity is achieved. They also noted that PBL depth was simulated to be lower than observed when a local closure scheme was implemented. Mao et
al. (2006) found that the largest variation in terms of meteorological variables when using various PBL schemes was found in determining PBL depth. They also found that, with the exception of mixing depth, no particular scheme resulted in particularly good or poor model performance. Consequently, no appreciable differences were found in the simulation of atmospheric pollutants by varying PBL parameterizations. These results are similar to what was found by Misenis et al. (2006) in terms of the biases in PBL depth. The inability of the local closure schemes to simulate the effects of large eddies is the most logical reasoning for the low PBL height bias observed in most studies.

Notable changes are also evident with varying parameterizations in terms of convective precipitation. Jankov et al. (2005) found that when changing from a nonlocal closure scheme to a local closure scheme, the PBL became wetter, though this had no significant impact on the ability of the schemes to simulate more accurate rainfall. The most important finding of the study was that varying PBL and microphysics had appreciable differences on simulated convective precipitation. However, neither method provided a statistically significant improvement over the other.

The simulation and development of the PBL can also affect formation and transport of chemical species. Numerous studies have been conducted on the effects of boundary layer processes on atmospheric chemistry (Giannakopoulos et al., 2004; Olerud et al., 2004; Pino et al., 2004; Bao et al., 2005; Mao et al., 2006; Misenis et al., 2006). The effects of simulated temperature, precipitation, and other meteorological variables can have wide-ranging impacts on atmospheric chemistry.

One notable impact of meteorological variables on chemical species is the simulated height of the PBL. Theoretically, the depth of the PBL is determined to be a well-mixed
volume, the height of which indicates the boundary constituting the free atmosphere. In
general, it is observed that chemical species within the boundary layer tend to remain there.
Therefore, lower PBL heights would essentially result in a lower effective mixing volume.
One would hypothesize that in instances where a less deep PBL is simulated, concentrations
or mixing ratios of atmospheric pollutants would increase. This decreased mixing volume
has been suggested previously (Olerud et al., 2004; Misenis et al., 2006).

The ability of the PBL scheme to accurately simulate wind speed and direction at
various levels is also of great importance. Wind speed and direction are crucial in
determining downwind transport of chemical species, especially in areas where complex
geography plays a crucial role in meteorological simulations. For example, the eastern coast
of Texas borders the Gulf of Mexico. As the day progresses, it is not uncommon to observe a
coastal front move inland over the Houston metropolitan area (Banta et al., 2005; Darby,
2005). Daum et al. (2003) observed that O$_3$ transportation from over the Gulf of Mexico
back into urban areas was directly responsible for several non-attainment days. They
discovered that as pollutants from the ship channel were transported downwind, they were
trapped underneath a boundary layer and transported inland with the advance of the late
afternoon coastal front.

Table 2.1 shows several popular PBL schemes currently used in atmospheric models.
With large variations that seem to occur due to the implementation of a nonlocal closure
scheme versus local closure, an examination of simulations using each type should be
performed. By simulating meteorological variables and chemical species using each method
of closure, the effects nonlocal versus local closures can be examined.
2.1.2 Land Surface Model (LSM)

An important aspect of simulating atmospheric conditions is the correct parameterization of surface-level processes. It is well known that the ability to reproduce an accurate representation of the atmospheric feedbacks in terms of heat fluxes to the boundary layer must be correctly accounted for by land-surface parameterizations. The earliest attempt at incorporating an LSM into atmospheric models was done using a simple bucket scheme by Manabe (1969). This model provided no biophysical controls on water or heat fluxes, and merely placed precipitation into a “bucket.” Manabe’s (1969) scheme was developed mainly around the availability of soil water. Later, advancements in technology and scientific understanding allowed for the explicit simulation of the effects of vegetation on atmospheric processes (Sellers et al., 1986). Today, computational advancements, coupled with high-resolution land use datasets have enabled scientists to better simulate surface-atmosphere interactions (Pielke et al., 1997).

Studies have shown that differences in soil moisture, temperature, land use, and vegetation types can have profound effects on meteorological conditions and climate (Entekhabi et al., 1992; Bouttier et al., 1993; Zhang and Ding, 1999; Pielke, 2001; Yoo, 2001; Roy and Avissar, 2002; Zhang and Frederiksen, 2003). The effect of evaporation and transpiration in LSMS is capable of drastically affecting the PBL structure (Alapaty et al., 1997; Chen and Dudhia, 2001). Increased evaporation simulated by land surface models can lead to higher simulated PBL heights due to increased sensible heat flux.

In terms of meteorological conditions, different methods of simulating land-surface processes are extremely important. The depth of the PBL is driven by several factors. Some
of these factors are directly influenced by land-surface characteristics and dynamical processes. More specifically, surface sensible and latent heat fluxes can alter the structure of the atmospheric boundary layer (Chen and Dudhia, 2001).

Large uncertainties exist, however, in terms of the model’s ability to reproduce precipitation. Studies have shown that incorrect soil moisture initialization within an LSM can have detrimental effects on precipitation forecasts (Betts et al., 1997). The effect of incorrect soil moisture transport is also very obvious in terms of convective precipitation. Holt et al. (2006) found that using an LSM with a better representation of soil transpiration and moisture transport leads to more accurate forecasts of convective precipitation.

High resolution and physically complex LSMS also have interesting effects on the simulated surface temperature. One can hypothesize that with a more accurate representation of land use and vegetation, a more accurate depiction of the atmosphere could be simulated (Xian and Crane, 2006). In fact, the inclusion of physically rigorous surface characteristics such as vegetation allows the model to be able to better simulate evapotranspiration. The inclusion of evapotranspiration can lead to better simulated soil moisture, thus leading to more accurate surface fluxes (Verseghy, 1996; Dupont et al., 2004).

The effects of various LSM options are not limited to meteorology alone. Seaman (2003) recognized that to effectively simulate atmospheric chemistry, parameterizations that simulate meteorological conditions must be examined and overhauled. Recent studies have shown that various physical parameterizations can lead to differences in simulations of chemical species as well (Jang et al., 2006; Misenis et al., 2006). In fact, Misenis et al. (2006) found that utilization of a more physically complex LSM may not necessarily lead to better simulation of meteorological variables or chemical species.
It can also be noted that different land use or land type can have an effect on the simulated chemistry. Tegen et al. (2002) conclude that atmospheric dust emissions are extremely sensitive to vegetation cover and land use at the time of simulation. The accurate prediction of these emissions can have significant effects on the simulation of various chemical species.

These differences are not limited to particulate species alone. Tarasick and Bottenheim (2002) studied ozone depletion at the surface in the Arctic and Antarctic. The differences in ozone depletion at different sites were eventually found to be driven mostly by surface meteorological variables (Tarasick and Bottenheim, 2002). The cold surface temperatures served as a form of catalyst for bromine to bromide reactions, which are detrimental to surface ozone (Tarasick and Bottenheim, 2002).

Table 2.2 shows a brief list of some popular LSMs currently used in atmospheric models. The LSMs chosen for study in this evaluation each have various characteristics in terms of simulating surface meteorological characteristics. By comparing simulations using various LSM options, the sensitivity of model simulations to various schemes can be analyzed.

2.2 **Effect of Horizontal Grid Spacing**

Over the past decade, computational advancements in terms of numerical modeling have been tremendous. The ability to better resolve small-scale meteorological and atmospheric chemistry phenomena would theoretically provide a better understanding of and a more realistic simulation of atmospheric processes. Because of this rapid advancement in
computing power, atmospheric scientists have been able to take advantage of the finer resolution simulations that these computing systems are able to perform. Today’s operational meteorological models typically operate at a horizontal resolution of 12-km (Mass et al., 2002), down from hundreds of kilometers in the late 1950s. Even so, models currently under development and slated for operational use within the next few years are designed to operate at even finer resolution (e.g., Weather Research and Forecast (WRF) model at 1 to 10-km (Michalakes et al., 2001)). While Mass et al. (2002) state that increasing the resolution of atmospheric models may lead to better reproduction of fine-scale processes, they also find that this may not necessarily correlate to better model accuracy, as seen in more recent studies (Gego et al., 2005). However, Jimenez et al. (2006) provide one such study centered over the Iberian Peninsula, where an accurate reproduction of sea breeze processes is important. Fine scale simulations were able to reproduce the sea breeze conditions more accurately than coarse resolutions. This ability to better simulate wind fields using finer resolution was also observed in previous studies (Liu and Westphal, 2001).

Past studies (Jang et al., 1995a and b; Jimenez et al., 2006) have shown that increasing the resolution for the simulation of chemical species is also beneficial. Jimenez et al. (2006) found that by increasing the horizontal resolution of model to 2-km, better model performance was achieved in terms of the critical success index (CSI), false alarm rate (FAR) and probability of detection (POD). The formation and transport of chemical species occur at a range of small scales and lead one to conclude that both fine-scale input and resolution are necessary to accurately simulate chemical processes (Jang et al., 1995a; Jimenez et al., 2005). Other studies have been aimed at understanding the impacts increased resolution of meteorological processes (e.g., turbulence, wind speed and direction) have on chemical
species formation and transport (Jang et al., 1995a and b; Salvador et al., 1999; Baklanov et al., 2002). Jang et al. (1995a) state that the relationship between highly-reactive chemical species and grid spacing is nonlinear as the simulation of chemical species on finer scales is different from those on coarser scales. Non-reactive species, however, are affected mostly by transport, which is linearly related to horizontal grid spacing (Jang et al., 1995a).

It is interesting to note that studies also examined the effect of vertical grid spacing on model performance (Jimenez et al., 2006; Jimenez et al., 2005; Jang et al., 1995a and b). It was found that by increasing the vertical resolution, simulations were able to reproduce more accurate values and distributions of $O_3$ concentrations at ground-level (Jimenez et al., 2006) in terms of statistical parameters. While examining the effect of vertical resolution is not a part of this study, it is important to state that horizontal resolution alone may not necessarily lead to better reproduction of meteorological variables and chemical species.

While the benefits of using finer horizontal resolution are apparent, there are still uncertainties which exist when utilizing such resolutions (< 5-km). Evaluation of smaller horizontal grid-spacing must be completed with an abundance of observational data to compare with simulations (Colle et al., 2000).

As noted previously, the impacts of the sea breeze circulations on geographic areas near large bodies of water are very important to the simulation of meteorological variables and chemical species (Daum et al., 2003; Daum et al., 2004; Jimenez et al., 2006). By comparing finer resolution simulations to simulations conducted using a coarser grid, sensitivity of model simulations to horizontal grid spacing can be analyzed.

In addition to simply decreasing the horizontal grid-spacing, today’s numerical models are capable of using a technique known as nesting. Nesting involves the use of a
finer grid within a coarse domain. Pleim et al. (1991) indicated the need for multiple, smaller domains within a coarse domain to be able to simulate chemistry more accurately, due to the wide range of spatial scales on which processes occur. Two types of nesting exist; one-way nesting uses the output of a coarser resolution as input for the fine resolution simulations. Two-way nesting involves feedback from the fine domain to the coarse domain and vice versa. By implementing the use of nesting, one can evaluate model performance regarding the feedback between large and small temporal and spatial scales (Jakobs et al., 1995).

Studies have shown that using nested domains can lead to more accurate predictions of chemical species (Wang et al., 2001; Gego et al., 2005). Though the simulations may produce more detailed information in simulated values, one must be able to compare simulated values with observations from a relatively fine resolution dataset (Gego et al., 2005). By using both methods of nesting, the effects of two- or one-way nesting on model simulations can be evaluated.
Table 2.1. Prominent PBL schemes that are currently used in major meteorological models.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Closure</th>
<th>Features</th>
<th>Application</th>
<th>Reference(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Medium-Range Forecast (MRF)</td>
<td>Non-local</td>
<td>Implicit vertical diffusion</td>
<td>Coarse to fine resolution</td>
<td>Hong and Pan (1996)</td>
</tr>
<tr>
<td>Mellor-Yamada-Janjic (MYJ)</td>
<td>Local</td>
<td>Explicitly calculates TKE</td>
<td>Coarse to fine resolution</td>
<td>Janjic (1994)</td>
</tr>
<tr>
<td>Yonsei University (YSU)</td>
<td>Non-local</td>
<td>Explicit treatment of entrainment</td>
<td>Coarse to fine resolution</td>
<td>Hong and Dudhia (2003); Hong et al., (2006)</td>
</tr>
<tr>
<td>Pleim-Chang (P-C)</td>
<td>Hybrid (Non-local/local)</td>
<td>Developed for use with specific LSM</td>
<td>Coarse to fine resolution</td>
<td>Pleim and Chang (1992)</td>
</tr>
</tbody>
</table>
Table 2.2  Some prominent land-surface models used in atmospheric modeling.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Soil-Layers</th>
<th>Theory</th>
<th>Application</th>
<th>Reference(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slab</td>
<td>5 (1-, 2-, 4-, 8-, and 16-cm layers)</td>
<td>Blackadar, Force-Restore</td>
<td>Coarse to fine resolution</td>
<td>Dudhia (1996)</td>
</tr>
<tr>
<td>NOAH</td>
<td>4 (10-, 30-, 60-, and 100-cm)</td>
<td>Similarity Theory</td>
<td>Coarse to fine resolution</td>
<td>Chen and Dudhia (2001)</td>
</tr>
<tr>
<td>Pleim-Xiu (P-X)</td>
<td>2 (1-cm soil, and 100-cm root zone)</td>
<td>Interactions among Soil, Biosphere, and Atmosphere (ISBA)</td>
<td>Coarse to fine resolution</td>
<td>Xiu and Pleim (2000)</td>
</tr>
</tbody>
</table>

3.1 The 2000 Texas Air Quality Study (TexAQS-2000)

The Houston-Galveston region in Texas is a highly populated, industrial-oriented region with more than 4-million people. With the abundance of fossil-fuel refining plants and urban industry, there is an abundance of NO\textsubscript{x} and volatile organic compound (VOC) emissions. Coupled with a warm, moist climate makes this region susceptible to significant levels of air pollution and appropriate for air quality-related research.

The meteorology and atmospheric chemistry in the Houston-Galveston area in Texas are extremely complex. With coastal flows impacting meteorological variables, there is much to understand before one begins to simulate and analyze air quality in this region. Recent studies have shown the impacts of large- and small-scale meteorological forcings on the formation and transportation of chemical species within this area (Daum et al., 2004; Banta et al., 2005). Additionally, modeling studies have been conducted to determine how accurately state-of-the-science atmospheric models can reproduce chemical formation in a geographically complex area (Bao et al., 2005; Jiang and Fast, 2004).

For six weeks that spanned August and September in 2000, the state of Texas underwent the largest air quality study in its history. A multi-organizational collaborative effort was made to better understand the atmospheric chemistry in and around the Houston-Galveston area. As many as 250 scientists and engineers participated in the study. Goals of
the study were to ultimately assimilate the data into atmospheric models in order to better understand the impact of atmospheric chemistry on humans and the environment, as well as coming into attainment with the National Ambient Air Quality Standards (NAAQS).

The study consisted of several sets of measurements. Ground-level observations of meteorological variables and chemical species were made at around 20 sites throughout eastern Texas. The National Oceanic and Atmospheric Administration (NOAA) also equipped aircraft with the necessary instrumentation to record upper-level observations of atmospheric pollutants and meteorological variables simultaneously.

3.1.1 TexAQS-2000 Episode during 28 August – 2 September

This study focuses on the evaluation of the modeling performance during 28 August – 2 September. One motivation for choosing this time period is the overall availability of observational data. The collaborative effort started on the 14th of August, running for six weeks, as mentioned previously. The locations of the ground-level observation stations are shown in Figure 3.1. Additionally, measurements at the surface and aloft were made by several other organizations such as the Texas Commission on Environmental Quality (TCEQ) and NOAA.

Secondly, when examining the maximum one-hour average ozone values, there were a notable number of exceedances (O₃ concentrations > 120 ppbv). More specifically, the maximum values for hourly-averaged ozone at any of the sites were 112, 146, 199, 168, 124 and 125 ppb on 28 August – 2 September, respectively (see http://www.tceq.state.tx.us/cgi-bin/compliance/monops/peak_monthly for more details). The 199 ppbv measurement on 30
August was the highest hourly-averaged ozone concentration of the entire study. The magnitudes of these values indicate that this was a significant ozone event, making it worthy of study.

Synoptically, a surface area of high pressure centered over southern Texas and the Gulf of Mexico dominated this time period. The location of the surface high varies minimally over the time period of interest. This lack of movement can be attributed to a subtropical ridge in the upper levels of the atmosphere. Eastward progression of the ridge was limited during this time, indicative of the stagnant surface and upper-level patterns which persisted over Houston. Formation of ozone is most likely to occur within warm, moist atmospheres of high pressure and relatively calm winds where there is an abundance of emitted NO$_x$ and VOC emissions.

Additionally, the daytime evolution of sea breeze circulations occurred several times throughout the time period. Most notably, sea breeze circulations were clearly observed on 29 – 31 August, with winds shifting from southwesterly to more southeasterly, causing pollution which had been advec ted over the Gulf to be transported back over the Houston-Galveston area (Daum et al., 2003). Daytime maximum temperatures over the domain of interest during this time period typically varied from 35°C to as a high as 42°C, with nighttime minimums ranging from 20°C to 25°C. Average surface temperatures ranged from 28°C to 34°C. According to reanalysis, this event was generally void of precipitation occurrences.
3.2 Modeling System

The Weather Research and Forecast (WRF) modeling system is developed jointly through several governmental agencies (see http://www.wrf-model.org for more information). These groups include, but are not limited to, the National Center for Atmospheric Research (NCAR), the National Center for Environmental Prediction (NCEP), and the Federal Aviation Administration (FAA), among others.

The motivation behind the development of WRF was to establish a completely new code aimed at simulating atmospheric conditions at the 1-10 km horizontal grid scale. As a new atmospheric model, WRF is to eventually supersede other popular atmospheric models (such as PSU/NCAR’s Mesoscale Model, also known as MM5) for research and operational forecasting needs (Michalakes et al., 2001). One notable impact of the architecture of the modeling system is the fact that the code is designed to be extremely flexible and portable across several computing platforms. This flexibility is a key characteristic in terms of model development and implementation.

WRF is a fully-compressible, nonhydrostatic, mass-conserving modeling system with several available dynamical cores. The two most used cores are known as the Advanced Research WRF (ARW) and the non-hydrostatic mesoscale model (NMM). WRF development started from 2000. Further technical details and information on the equations used in the WRF modeling system can be found in Skamarock et al. (2005).
3.2.1 WRF/Chem

Until recently, the feedback between atmospheric chemistry and meteorology were not taken into account as the two were treated independently (such as in the Community Multi-scale Air Quality (CMAQ) model (Byun and Ching, 1999)). WRF with chemistry (WRF/Chem) (Grell et al., 2005) simulates meteorological variables as well as trace gases and particulates “on-line” or simultaneously. By being able to simulate the formation and transport of chemical species at the same time as meteorological variables, we are more capable of analyzing the interactions between them. The motivation for development of WRF/Chem is associated with the expected use of the WRF modeling system as the operational and research model in the future. It follows that the future generation of atmospheric chemistry models includes the WRF modeling system.

The implementation of chemistry into mesoscale models was first introduced in 2000 at the “Workshop on Modeling Chemistry in Cloud and Mesoscale Models.” Following this meeting, the first available version of WRF/Chem was released in 2002 (see http://ruc.fsl.noaa.gov/wrf/WG11/ for more details). Grell et al. (2005) state that current chemistry architecture of WRF/Chem was derived mostly from MM5/Chem (Grell et al., 2000), which was evaluated in several studies even during the development of WRF/Chem (McKeen et al., 2003; Eder et al., 2005). As the WRF model underwent changes during development, these improvements had to be implemented into WRF/Chem as well. A summary of changes from version 2.0.3 through the current version 2.2 is shown in Table 3.1. The version used for evaluation in this study is 2.1.1. The most recent version can be
downloaded by contacting Dr. Georg Grell (georg.a.grell@noaa.gov) or Dr. Steven Peckham (steven.peckham@noaa.gov).

3.2.2 Application

WRF/Chem is applied for a five-day period beginning 28 August 2000 at 12Z through 2 September 2000 at 06Z from the TexAQS-2000 episode. A description of the model configurations and simulation designs follows.

3.2.2.1 WRF/Chem Configurations

As this study will focus on the evaluation of WRF/Chem using various physical parameterizations, horizontal grid spacing and nesting options, there naturally must be several options which remain constant among the simulations. This section will serve to introduce these options. Such options include the gas-phase and aerosol-phase mechanisms, surface layer schemes, radiation schemes, etc. A summary of the following options is provided in Table 3.2.

In terms of meteorology, there are several options within the configuration which remain constant throughout the evaluation. In terms of the surface layer parameterization, this study will utilize Monin-Obukhov similarity theory (Monin and Obukhov, 1954), similar to what is used in MM5.

Radiation is also an important factor when simulating atmospheric conditions. Accurate parameterizations of incoming (shortwave) and outgoing (longwave) radiation are
important aspects which are used in the PBL and land-surface models. Shortwave radiation scheme employed in this study is the simple Dudhia (1989) scheme taken from MM5. This parameterization accounts for clear-air scattering and water absorption within the atmosphere (Lacis and Hansen, 1974). The longwave radiation scheme used in conjunction with Dudhia shortwave is the Rapid Radiative Transfer Model (RRTM) from MM5, which is based on Mlawer et al. (1997). Using look-up tables, this scheme can account for the presence of several chemical species, as well as water vapor and cloud optical depth.

Due to a lack of precipitation and clouds for this particular episode, the cumulus parameterization scheme (CPS) used may not be as important as other parameterizations. However, it is still important to note which scheme will be employed. For this study the Kain-Fritsch CPS will be used. The KF scheme (Kain and Fritsch, 1990; Kain and Fritsch, 1993) uses mass flux and vertical momentum to determine whether instability exists for cloud formation. The version of KF in the WRF/Chem model is an update on previous versions, as described in Kain (2004). As mentioned previously, microphysics may not necessarily play a large role in this study. Therefore, all microphysics have been turned off.

The gas-phase mechanism to be employed in this study was developed by Stockwell et al. (1990) for its application to the second generation Regional Acid Deposition Model (RADM2). RADM2 is a fairly popular mechanism in the atmospheric chemistry modeling community. Grell et al. (2005) notes the ability of the mechanism to be computationally efficient while not totally sacrificing the accuracy of simulated chemical species.

The Modal Aerosol Dynamics model for Europe (MADE) with the Secondary Organic Aerosol Module (SORGAM). Derived from the Regional Particulate Model (Binkowski and Shankar, 1995), MADE was developed by Ackermann et al. (1998).
Secondary organic aerosols (SOA) were coded into MADE by Schell et al. (2001). MADE/SORGAM simulates particulates using a modal method, assuming a log-normal distribution within each mode (Aitken, accumulation, and coarse mode). MADE/SORGAM also employs the modified model for an aerosol reacting system (MARS-A, Binkowski and Shankar, 1995) for thermodynamics of inorganic species. This scheme assumes a thermodynamic equilibrium for gas/particle mass transfer and simulates significant dynamic processes (nucleation, condensation, and coagulation) associated with SOA.

3.2.2.2 Simulation Design

This study will consist of several simulations that will be utilized in the evaluation of several facets of the WRF/Chem modeling system. A summary of the options chosen for each simulation is shown in Table 3.3.

First, the design of the simulations used to evaluate sensitivity to physical parameterizations will be discussed. All simulations used for analysis of parameterization sensitivity will be conducted using a 12-km horizontal grid spacing with a 60-s time step centered over the Houston-Galveston region in eastern Texas (Figure 3.2). Initial and boundary conditions (IC and BC, respectively) for meteorological variables were derived from the North American Regional Reanalysis (NARR) (http://www.emc.ncep.noaa.gov/mmb/rreanl/). ICs and initial BCs for chemical species are both horizontally homogeneous. Emissions for these simulations were taken from the Texas Commission on Environmental Quality (TCEQ) for gaseous species and from the EPA’s
The baseline simulation (N_Y) coupled the National Center for Environmental Prediction, Oregon State University, Air Force, and Hydrologic Research Lab’s (NOAH) LSM (Chen and Dudhia, 2001a, 2001b; Ek et al., 2003) with the Yonsei University (YSU) PBL scheme (Hong and Dudhia, 2003; Hong et al., 2006), based on improvements to the Medium-Range Forecast (MRF) scheme (Hang and Pan, 1996). The NOAH LSM is a 4-layer soil model which incorporates canopy moisture, vegetation effects, runoff and drainage, as well as snow cover. Fluxes calculated within this scheme include sensible and latent heat fluxes to the PBL. The YSU PBL parameterization utilizes nonlocal mixing as described by Troen and Mahrt (1986). This scheme takes into account the effect of large eddies by bulk properties of the PBL, rather than local properties. The height of the PBL is determined using a critical bulk Richardson number of 0. However, this may not be applicable for typical nighttime simulations, where the Richardson number is equal to zero at the surface. In this way, the height of the PBL is dependent only on the buoyancy profile. Entrainment at the top of the PBL is handled explicitly, rather than implicitly (Noh et al., 2003) and set proportional to the surface buoyancy flux.

The YSU PBL scheme will be used in conjunction with two other LSMs to examine the sensitivity of WRF/Chem to various land-surface parameterizations. The first sensitivity pair (S_Y) couples the YSU scheme with the simple thermal diffusion (slab) scheme described by Dudhia (1996). The slab LSM is a simple five-layer soil model built upon slight improvements to the force-restore method. For calculating surface fluxes, this scheme uses a one-dimensional equation for heat flux,
\[ F = -K \rho_s c_s \frac{\partial T_z}{\partial z}, \]

where \( F \) is surface heat flux (W m\(^{-2}\)), \( K \) is thermal diffusivity of the soil (m\(^2\) s\(^{-1}\)), \( \rho_s \) is soil density (kg m\(^{-3}\)), \( c_s \) is the specific heat capacity of the soil (J kg\(^{-1}\) K\(^{-1}\)), and \( \frac{\partial T_z}{\partial z} \) is the temperature gradient of the soil (K m\(^{-1}\)). One possible area of uncertainty with this scheme is the initialization of the soil temperature profile. The slab scheme applies a linear profile based on model parameters, though ideally it should be determined from the previous day’s conditions (Dudhia, 1996).

The last simulation (R_Y) to compare the sensitivity of WRF/Chem simulations to LSM options is the coupling of the Rapid Update Cycle (RUC) LSM (Smirnova et al., 2000) with the YSU scheme. Similar in physical complexity to the NOAH LSM (RUC also simulates canopy moisture, vegetation, etc.), one major difference is the inclusion of two additional soil layers (i.e., six rather than four in NOAH).

For analyzing the sensitivity of WRF/Chem to various PBL parameterizations, the options are limited. In addition to the YSU PBL scheme mentioned previously, the only other PBL option in the WRF modeling which works with the chemistry framework is the Mellor-Yamada-Janjic (MYJ) 1.5 order turbulent kinetic energy (TKE) closure scheme described by Janjic (1994; 2002) and developed from Mellor and Yamada (1982). This scheme imposes a limit on the master scale over which mixing can occur, which is determined by TKE, buoyancy and shear. In doing so, this scheme determines the height of the PBL to be the lowest level at which TKE approaches its lower bound.
Another area of investigation regarding the performance of WRF/Chem is the use of higher resolution and one- and two-way nesting. Figure 3.2 shows the original domain used for the previous sensitivity tests, as well as the nested 4-km domain.

Because simulating atmospheric processes at a higher resolution requires model input of higher resolution, emissions data for the smaller domain are needed. Emission datasets for use in WRF/Chem must have followed the speciation of the gas-phase and aerosol modules used during simulation. A 12-km emission dataset was readily available for use with the initial simulations, while 4-km following RADM2-MADE/SORGAM speciation was not (Fast, personal communication, November 2006). Not utilizing a 4-km emission file would make analyzing differences in nesting and grid resolution meaningless. However, 12- and 4-km emissions data for simulations using the Carbon Bond Mechanism version Z (CBMZ) and the Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) were available. These files had to be converted for use with RADM2-MADE/SORGAM.

The largest difference between the two files was the approach used for aerosols. MOSAIC utilizes the sectional approach, while MADE/SORGAM is modal. By comparing the original 12-km emissions for RADM2-MADE/SORGAM with the 12-km emissions for CBMZ-MOSAIC, the necessary factors were calculated to create the emission files needed for use with RADM2-MADE/SORGAM at 12- and 4-km.

Nearly all the gaseous species from both sets were the same. One notable difference is the absence of acetaldehydes and other higher aldehydes in the new emissions files. This discrepancy could lead to changes in the amount of simulated $O_3$ as compared with the earlier simulations. Table 3.4 shows the mapping used for generating the new emissions files.
For the aforementioned reasoning regarding emissions, the baseline simulation (N_Y) was conducted using the new 12-km emissions data. In order to compare the effect of grid resolution and nesting options on model performance, all the following simulations will utilize the same physical schemes as the base case. The first simulation (1WAY) aimed to see the effects of one-way nesting on model performance. One-way nesting is defined as completing a simulation at a finer resolution by using the output from the coarse domain as initial and boundary conditions for the smaller domain. WRF/Chem has a built-in scaling program which creates the necessary initial and boundary conditions from the 12-km output. In this program, the forecast from the coarse parent domain is interpolated down to form the initial and boundary conditions for the fine domain.

WRF/Chem also has the ability to perform two-way nesting simulations. Two-way nesting allows the user to observe influences of finer resolution on the coarse domain by simulating both simultaneously. The final simulation used in this study (2WAY) simulates both the 12- and 4-km grids simultaneously. This requires no scaling down of the 12-km output for initial and boundary conditions at 4-km.

3.3 Evaluation Methods

In order to provide a scientifically insightful analysis of the information presented, one would need to employ several methods of evaluation. Because WRF/Chem is a 3-D atmospheric model, it would be beneficial to not only examine surface-level conditions, but also the vertical distribution of chemical species.
3.3.1. Surface Level

3.3.1.1 Temporal

Analyzing model output temporally allows us to examine how well the model simulates meteorological variables and chemical species at specific sites for specific days. Because the geographic makeup of the domain under consideration is so complex, temporal analyses may provide better insight into how well the model handles this issue. Sites were chosen based on the abundance of observational data available (i.e., more complete meteorological and chemical observations) and location (e.g., urban coastal, urban inland, etc.). Temporal analyses are performed for meteorological variables (e.g., temperature (T2), relative humidity (RH), wind speed and direction (WSP and WDR), and PBL height (PBLH)) and chemical species (e.g., O$_3$, CO, NO, NO$_2$, PM$_{2.5}$ and PM$_{2.5}$ composition). A temporal analysis is also beneficial due to the ability to better examine differences in the simulation of meteorological variables and chemical species during daytime and nighttime.

3.3.1.2 Spatial

Comparisons of spatial distributions of chemical species across both the 12- and 4-km domains are also completed. Using the NCAR Command Language (NCL), hourly-averaged simulation plots are created. By comparing the distribution of several chemical species, we may better understand how each parameterization handles transport and formation of chemical species in a domain-wide sense. In examining these plots, we may better
understand the sensitivity of certain areas within the domain to changing parameterizations. A comparison of spatial plots for the 12- and 4-km horizontal grid spacings will allow us to determine whether or not the model can reproduce small-scale meteorological and chemical processes given a finer resolution.

3.3.1.3 Statistical

Statistical comparisons are completed and expressed in terms of several statistical parameters: correlation coefficient (corr), mean bias (MB), mean absolute gross error (MAGE) root mean-square error (RMSE), mean normalized bias (MNB), mean normalized absolute error (MNAE), normalized mean bias (NMB), normalized mean error (NME), fractional bias (FB), fractional absolute error (FAE), normalized mean bias factor (NMBF), and normalized mean error factor (NMEF). Formulas for the aforementioned parameters are provided in Yu et al. (2006) as follows:
corr = \[ \frac{\sum(M_i - \bar{M})(O_i - \bar{O})}{\left(\sum(M_i - \bar{M})^2 \sum(O_i - \bar{O})^2\right)^{\frac{1}{2}}} \]

MB = \[\frac{1}{N} \sum (M_i - O_i)\]

MAGE = \[\frac{1}{N} \sum |M_i - O_i|\]

RMSE = \[\left(\frac{1}{N} \sum (M_i - O_i)^2\right)^{\frac{1}{2}}\]

MNB = \[\frac{1}{N} \sum \left(\frac{M_i - O_i}{O_i}\right)\]

MNAE = \[\frac{1}{N} \sum \left(\frac{|M_i - O_i|}{O_i}\right)\]

\[
\begin{align*}
NMB & = \frac{\sum (M_i - O_i)}{\sum O_i} \\
NME & = \frac{\sum |M_i - O_i|}{\sum O_i}
\end{align*}
\]
\[ FB = \frac{1}{N} \sum \frac{(M_i - O_i)}{(M_i + O_i) / 2} \]

\[ FAE = \frac{1}{N} \sum \frac{|M_i - O_i|}{(M_i + O_i) / 2} \]

\[ NMBF = \sum \frac{(M_i - O_i)}{\sum M_i} \]

\[ NMEF = \sum \frac{|M_i - O_i|}{\sum M_i} \]

where \( M_i \) and \( O_i \) are the model simulated and observed values of a particular parameter at any time/location, \( i \), up to \( N \) number of simulated and observed pairs. All summations in the previous equations are from \( i = 1 \) to \( N \).

These statistical parameters will be used to evaluate the model performance when simulating the aforementioned meteorological variables and chemical species. NMB allows us to examine the ability of the model simulations to accurately reproduce observational data in terms of over-prediction or under-prediction. One must also note that because NMB is the summation of the differences between simulated and observed values, cancellations may occur that would give misleading information regarding model performance. For this reason, NME is utilized. Because NMEs take the absolute value of the difference, we can see actual magnitudes of model discrepancy, though we cannot determine whether over-predictions or under-predictions occur. The above statistical parameters will be calculated for meteorological variables (e.g., T2, RH, WSP, WDR, U, V, and PBLH) and chemical species (e.g., O3, NO, NO2, CO, and PM2.5).
3.3.2 Vertical Profile

An analysis of the vertical distribution of chemical species in the atmosphere over Houston-Galveston is also completed. During the time period of interest, there were three scheduled aircraft measurement flights. In-situ measurements of mixing ratios and concentrations of chemical species were obtained during takeoff and in flight. By examining the observations made during takeoff of the aircraft, we can compare model simulated vertical distributions of chemical species, although nearly instantaneous values of observed parameters at different heights may not be comparable to grid-volume averages of the model. The analysis provided by this evaluation method allows us to see how well different model parameterizations perform at various levels.

Observations were made using the NOAA/NCAR Electra aircraft. Data was sampled at a time resolution of 1-s for O\textsubscript{3}, NO, and CO, and at 3-s for NO\textsubscript{2}. Additionally, the method of comparing aircraft data to model-simulated values should be discussed. During aircraft takeoff, we assume the observations of meteorological variables and chemical species to be similar to a vertical profile. Unlike a sonde, the aircraft is moving quickly in the horizontal direction relative to the vertical. For this purpose, it makes it a little more challenging to compare with grid-averaged simulated values. For the purposes of this study and the lack of significant processing tools, some liberties were taken with the comparison. Latitude and longitude data made available by the aircraft were averaged to find the average position of the aircraft during the flight time. Using this information, the corresponding grid cell was found and the vertical profiles of meteorological variables and chemical species from that
cell were used to compare with the vertical measurements made by the aircraft. This has several limitations in that the aircraft observations and model simulations are not on the same time scale and also not from the same latitude and longitude positions. Other methods of comparing this data are currently being investigated.
Table 3.1. Major updates to the recently released versions of WRF/Chem.

<table>
<thead>
<tr>
<th>WRF/Chem Version</th>
<th>Notable Changes</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0.3</td>
<td>Two-way Nesting added; Prototype Moving Nest; Compiles with RSL and RSL_Lite</td>
</tr>
<tr>
<td>2.1</td>
<td>YSU PBL Scheme added officially; Memory Optimization; Earth System Modeling Framework (ESMF) ready</td>
</tr>
<tr>
<td>2.1.1</td>
<td>Bug fixed for nesting interpolation; Bug fixes to some microphysics, cumulus, and radiation schemes</td>
</tr>
<tr>
<td>2.2</td>
<td>Kinetic PreProcessor (KPP) Implemented; NMM Core Implemented; Cloud-Aerosol Interactions available (CBM-Z/MOSAIC only)</td>
</tr>
</tbody>
</table>

Acronyms: RSL – runtime system library; YSU – Yonsei University; PBL – planetary boundary layer; ESMF – Earth System Modeling Framework; CBM-Z – Carbon Bond Mechanism, version Z; MOSAIC - Model for Simulating Aerosol Interactions and Chemistry
Table 3.2. Selected physical options within WRF/Chem used in all model simulations (baseline and sensitivity).

<table>
<thead>
<tr>
<th>WRF/Chem Physics</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shortwave Radiation</td>
<td>Dudhia</td>
</tr>
<tr>
<td>Longwave Radiation</td>
<td>RRTM</td>
</tr>
<tr>
<td>Microphysics</td>
<td>Turned off</td>
</tr>
<tr>
<td>Cumulus</td>
<td>Kain-Fritsch</td>
</tr>
<tr>
<td>Gas-phase Mechanism</td>
<td>RADM2</td>
</tr>
<tr>
<td>Aerosol Module</td>
<td>MADE/SORGAM</td>
</tr>
<tr>
<td>Initial Conditions</td>
<td>Horizontally Homogeneous</td>
</tr>
<tr>
<td>Boundary Conditions</td>
<td>Horizontally Homogeneous</td>
</tr>
</tbody>
</table>

Acronyms: RRTM – Rapid Radiative Transfer Model; RADM2 – Second Generation Regional Acid Deposition Model; MADE/SORGAM – Modal Aerosol Dynamics Model for Europe with Secondary Organic Aerosol Model
Table 3.3. Physical configurations for each simulation used in evaluation.

<table>
<thead>
<tr>
<th>Simulation Name</th>
<th>LSM Option</th>
<th>PBL Option</th>
<th>Nesting</th>
</tr>
</thead>
<tbody>
<tr>
<td>N_Y</td>
<td>NOAH</td>
<td>YSU</td>
<td>None</td>
</tr>
<tr>
<td>S_Y</td>
<td>Slab</td>
<td>YSU</td>
<td>None</td>
</tr>
<tr>
<td>R_Y</td>
<td>RUC</td>
<td>YSU</td>
<td>None</td>
</tr>
<tr>
<td>N_M</td>
<td>NOAH</td>
<td>MYJ</td>
<td>None</td>
</tr>
<tr>
<td>1WAY</td>
<td>NOAH</td>
<td>YSU</td>
<td>One-Way</td>
</tr>
<tr>
<td>2WAY</td>
<td>NOAH</td>
<td>YSU</td>
<td>Two-Way</td>
</tr>
</tbody>
</table>

Acronyms: LSM – Land-surface model; PBL – planetary boundary layer; N_Y – NOAH/YSU pair; S_Y – slab/YSU pair; R_Y – RUC/YSU pair; N_M – NOAH/MYJ pair; 1WAY – One-way nesting; 2WAY – Two-way nesting; NOAH – National Center for Environmental Prediction, Oregon State University, Air Force, National Weather Service’s Hydrologic Research Lab; RUC – Rapid Update Cycle; YSU – Yonsei University; MYJ – Mellor-Yamada-Janji
Table 3.4. Species mapping in emission conversion from CBMZ-MOSAIC to RADM2-MADE/SORGAM.

<table>
<thead>
<tr>
<th>Species</th>
<th>CBMZ-MOSAIC</th>
<th>RADM2-MADE/SORGAM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine Particulate Matter (PM$_{2.5}$)</td>
<td>PM25J</td>
<td>PM$<em>{25I} = 0.15 \times$ PM$</em>{25J}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PM$<em>{25J} = 0.85 \times$ PM$</em>{25J}$</td>
</tr>
<tr>
<td>Sulfate (SO$_4^{2-}$)</td>
<td>SO4J</td>
<td>SO$<em>{4I} = 0.15 \times$ SO$</em>{4J}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>SO$<em>{4J} = 0.85 \times$ SO$</em>{4J}$</td>
</tr>
<tr>
<td>Elemental Carbon (EC)</td>
<td>ECJ</td>
<td>EC$<em>{I} = 0.15 \times$ EC$</em>{J}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>EC$<em>{J} = 0.85 \times$ EC$</em>{J}$</td>
</tr>
<tr>
<td>Organic Aerosols (ORG)</td>
<td>ORGJ</td>
<td>ORG$<em>{I} = 0.15 \times$ ORG$</em>{J}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ORG$<em>{J} = 0.85 \times$ ORG$</em>{J}$</td>
</tr>
<tr>
<td>Nitrate (NO$_3^{-1}$)</td>
<td>NO3J</td>
<td>NO$<em>{3I} = 0.15 \times$ NO$</em>{3J}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>NO$<em>{3J} = 0.85 \times$ NO$</em>{3J}$</td>
</tr>
<tr>
<td>PM of AD &lt; 10 µm (PM10)</td>
<td>PM10</td>
<td>PM$<em>{10} = 0.201 \times$ PM$</em>{10}$</td>
</tr>
<tr>
<td>HC3</td>
<td>HC5</td>
<td>HC$<em>{3} = 0.08084 \times$ HC$</em>{5}$</td>
</tr>
<tr>
<td>HC5</td>
<td>HC5</td>
<td>HC$<em>{5} = 0.05331 \times$ HC$</em>{5}$</td>
</tr>
<tr>
<td>HC8</td>
<td>HC5</td>
<td>HC$<em>{8} = 0.03802 \times$ HC$</em>{5}$</td>
</tr>
<tr>
<td>Ethane (C$_2$H$_6$)</td>
<td>C2H6</td>
<td>ETH = 0$\times$C2H6</td>
</tr>
</tbody>
</table>

Acronyms: AD – aerodynamic diameter; CBMZ – Carbon Bond Mechanism – version Z; MOSAIC - Model for Simulating Aerosol Interactions and Chemistry; RADM2 – Second Generation Regional Acid Deposition Model; MADE – Modal Aerosol Dynamics Model for Europe; SORGAM – Secondary Organic Aerosol Model; HC3 – Alkanes with HO rate constant between $2.3 \times 10^{-13}$ and $3.4 \times 10^{-12}$; HC5 – Alkanes with HO rate constant between $3.4 \times 10^{-12}$ and $6.8 \times 10^{-12}$; HC8 – Alkanes with HO rate constant greater than $6.8 \times 10^{-12}$
Figure 3.1. Map depicting the locations of ground observations sites used during the Texas Air Quality Study in 2000 (TexAQS-2000) (from University of Texas, http://uts.cc.utexas.edu/~gcarch/HoustonSuperSite/site_listmainpage1.htm).
Figure 3.2. The modeling domains at 12-km (d01) and 4-km (d02) over eastern Texas.
4.1 Baseline Simulation Evaluation

The baseline simulation pair of the Noah LSM coupled with the YSU PBL scheme (hereafter referred to as N_Y), is compared with observations of meteorological variables and chemical species. In terms of temporal analyses, the following sites were chosen as representative of the entire dataset for a variety of reasons: Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA). All these sites are in or around the Houston metropolitan area, with the exception of GALC, which is located in Galveston. Figure 3.1 shows the locations of these sites. The aforementioned sites were selected based on the abundance of observational data (meteorological and chemical), as well as site location (e.g., urban, coastal, etc.). Of the five sites, GALC and DRPA can be considered under coastal influences. As shown in Figure 3.1, GALC is under direct influence of the Gulf of Mexico, while DRPA sits within 6 miles of Galveston Bay. The other three locations (HALC, BAYP, and C35C) are at least 15 miles away from any major body of water, and are thus classified as urban sites. Though the complex geography of those locations does not allow for total dissociation from coastal influences, an analysis of relativity to coastline can be shown. It should also be noted that no measurements for PBL height are available at the aforementioned locations. A description of the sites used for temporal analyses of PBL height will be given in section 4.2. For consistency, the same set of locations is also used in analyzing results from simulations for studying the sensitivity of
model performance to physical parameterizations. However, for some chemical species (e.g., 
CO and PM$_{2.5}$), some of these sites were lacking observational data. For this reason, other 
sites were substituted in chemical analyses. The following sites were included in the 
analyses for CO: Houston Crawford (HCFA) and LaPorte (H08H). For the analyses of 
PM$_{2.5}$, the following sites were used: Houston East (HOEA), Conroe (CONR), and LaPorte 
(H08H).

4.1.1 Meteorological Variables

An analysis of meteorological variables for the N_Y simulation is presented. 
Temperature at 2 m (T2), relative humidity (RH) at 2 m, wind speed (WSP) and wind 
direction (WDR) at 10 m, U- and V-vector components, and PBL height (PBLH) are 
presented using temporal plots. For a better examination of WDR, time series of U- and V-
vector components are also shown. Temporal analyses are followed by a thorough statistical 
analysis and spatial distributions of selected variables and chemical species at specific times. 
Finally, an examination of the vertical distribution of meteorological variables and chemical 
species from model simulation and aircraft measurements is presented.

Figure 4.1 shows the temporal distribution of T2 at several selected sites. Simulated 
temperature values appear to correspond relatively well with observed values at all locations. 
The diurnal pattern of daily maximum and minimum values appears to be well captured 
within the simulation. One exception can be observed for C35C, where the nighttime 
minimums are under-predicted by nearly 3°C on all nights except day four, where the under-
prediction was only around 1.5°C. The model appears to simulate maximum temperatures on
day one very well at all locations. Daily maximum temperatures are generally too cool at all
sites for days two through four. A slight over-prediction of the daily maximum temperature
is observed at all sites for day five with the exception of GALC. It is interesting to note the
lack of a strong diurnal pattern in temperature at GALC. This is most likely due to the land-
sea interactions that occurred at this location, where variations in temperature during daytime
and nighttime are minimal.

Figure 4.2 shows the temporal distributions of RH. Overall, the diurnal variation at
all sites appears to be well represented within the simulation, though the magnitudes of the
simulated values are not well captured. N_Y appears to under-predict RH at all sites at most
times. It is interesting to note that daily minimum values of RH are better represented than
daily maximum values at most sites, in contrast to simulated T2. When examining simulated
values of RH at C35C, N_Y grossly under-predicts RH at all times, though the magnitude of
the under-prediction is lessened during days three through five. If atmospheric moisture is
significantly low, higher sensible heat fluxes to the PBL would be predicted. This could
result in a deeper, drier PBL to form.

In terms of wind speed, N_Y performed relatively well at all locations. Figure 4.3
displays temporal distributions of wind speed for the selected sites. It is clearly obvious the
model simulation performed better at GALC as compared with other locations in terms of
capturing the diurnal pattern. Speeds were generally over-predicted by N_Y at all locations
at most times, especially nighttime. There were, however, several periods during daytime
simulations at all locations except GALC where simulated wind speeds were smaller than
observed values. For example, on day two at C35C, an observed value of 4.5 m s\(^{-1}\) was 3.89
m s\(^{-1}\) stronger than the simulated value of .61 m s\(^{-1}\).
Figure 4.4 shows the temporal distribution of wind direction at the selected sites. Overall, simulated values of wind direction do not correspond well with observed values, with the exception being GALC. In general, large discrepancies between observed and simulated values occur during late afternoon into evening hours at all locations for all five days. Differences between observed and simulated values are largest on day three. When examining the variation between observed and simulated values for this day, differences range from 15.3° at GALC to 214.5° at C35C at 5:00 PM CDT. One caveat to note when using this method to analyze simulated wind direction is using a numerical value for a vector can cause large problems when numerical differences are significant. For example, on a wind rose plot, wind directions of 350° (NNW) and 10° (NNE) are actually only 20° apart. Numerically, the difference between the two is 340°, which makes numerical analysis difficult. For this reason, a temporal comparison of U- and V-vector components is made in Figures 4.5 and 4.6.

Temporal analysis of U- and V-vector components shows an overall better agreement of the model with observations than looking at wind direction (Figures 4.5 and 4.6). In general, it appears that the model simulates the east-west (U) component of the vector more accurately than the north-south (V) component, though only slightly. The timing of variations in wind shifts seems to be captured fairly well, though the model is off by a few hours at most locations for both species several times.

The deeper PBL heights are simulated throughout the domain. As mentioned previously, locations with PBL height observations do not correspond to the aforementioned sites. Five locations were equipped to take lidar measurements and obtain the depth of the boundary layer during TexAQS-2000. These five locations are: Wharton (WHAR),
Ellington Field (ELLF), Southwest Houston (HSWH), Liberty (LBTY), and LaMarque (LMRQ). As shown in Figure 4.7, simulated heights are generally higher than observed values at all locations for most times. In general, the growth of the boundary layer appears to be well represented, though initial growth appears to be too fast. Simulated heights at LBTY and LMRQ appear to be significantly over-predicted on days two and three as compared with other locations. There would seem to be some correlation with the under-prediction of RH and the over-prediction of PBL heights. Sites DRPA and ELLF are within 5 miles of one another, which makes a comparison between PBL heights and RH somewhat possible. For example, on day five, the difference between observed and simulated RH at DRPA is 36.37%. Similarly, the simulated PBL height at ELLF is larger by 1022.4 meters (51.8%) than the observed value. This may be attributed mostly to differences in heat fluxes between simulations. For example, higher surface heat fluxes could lead to decreased RH and higher PBL heights. Another issue, which was mentioned earlier, is that problems arise in using the bulk Richardson number as a determination of PBL height during nighttime conditions. For this reason, the YSU scheme arbitrarily sets an unrealistic value of 15 m for the nocturnal PBL height.

Table 4.1 shows performance statistics for several meteorological variables. These statistics include observations and simulated data at all sites within the domain. When examining these statistics, it can be seen the baseline simulation performed very well in terms of surface temperature, with an NMB of -0.3%. Comparatively, the under-predictions seen in temporal analyses for RH are in line with an NMB of -27.4%. Wind speed was moderately over-predicted by N_Y with an NMB of 12.6%. Statistically, N_Y simulated wind direction relatively well, with an NMB of 6.6%. However, this could be attributed to a
compensation of over-predictions to under-predictions. When examining the NMBs of U- and V-component vectors, the N_Y simulation shows an NMB of the U-component vector of 21.6%, while V-component vectors have an NMB of -34.6%. By looking at these NMBs, we can conclude that N_Y simulates a more southerly wind direction than observed values, which are more southwesterly. PBL heights were largely over-predicted by the baseline simulation with an NMB of 54.4%.

Next, an examination of the spatial distribution of several meteorological variables is presented. Figures 4.8 through 4.11 display the spatial distributions of T2, RH, wind speed and direction, and PBLH at 20 UTC (3PM CDT) throughout the simulation period.

The spatial distribution of surface temperature follows the observed pattern of increasing daily maximum temperatures throughout the time period. Coastal influences on simulated temperature values are apparent along the Gulf coast, where temperatures are significantly lower than inland temperatures (on the order of 5 to 10°C cooler). It is interesting to note the ability of the model to capture the lower surface temperatures which exist over large bodies of water located inland. Spots of lower surface temperature in eastern Texas correspond to several large lakes in that part of the state. In general, simulated maximum temperatures are much warmer (by nearly 4°C) to the east and north of Galveston Bay at most times.

Spatial distributions of RH also show the decreasing values throughout the simulation period. This is similar to the noted increasing daily maximum temperatures in previous analyses. In general, values inland appear to be slightly higher than those nearer the coast, but generally highest for areas immediately along the Gulf coast. Differences in simulated
RH could be attributed to surface sensible heat flux, which influences surface temperature and atmospheric moisture content.

The variations in the wind field over the simulation period appear to be minimal, and show a mostly moderating surface weather pattern. As discussed earlier, this period was typically dominated by a slow-moving surface high pressure system, which varied only slightly in east-west orientation over the time period. The model simulation appears to move the high pressure south and west during the time period, nearer the border of Mexico and Texas on days three through five. This could have significant implications on the surface concentrations of certain chemical species, by determining transport of emitted of species and their precursors.

An examination of the spatial distribution of PBL heights shows much larger simulated values on days three through five, especially over Houston-Galveston, Texas. For example, simulated heights on days four and five are nearly 1000 m higher north of Galveston Bay when compared with those on days one and two. This pattern of increasing maximum PBL height was also observed in temporal analyses of simulated values (e.g., 3251.3 m on day 5 at HSWH vs. 3613.0 at LBTY). However, N_Y does seem to capture the influence of coastal effects on PBL height. This is most apparent on days one through three when examining the heights located at the coast and several kilometers inland. Simulated values in these areas are generally one order of magnitude lower than areas located further inland.

Vertical profiles of simulated temperature and relative humidity are compared with measurements taken from NOAA’s Electra aircraft during takeoff in Figure 4.12. Three flights were made during our period of interest: 15 UTC (10AM CDT) 28 August, 17 UTC
(12PM CDT) 30 August and 17 UTC (12PM CDT) 1 September 2000. For this comparison, we are assuming the take-off trajectory of the aircraft to be similar to an atmospheric sounding. In terms of temperature, the simulated vertical distributions correspond relatively well with observations, especially on 28 August. Predictions on 30 August and 1 September are only slightly different from observations, though N_Y under-predicts at heights greater than 500 m. N_Y simulates variations in temperature with height decently, though it does simulate a lower (317 m to 562 m versus 578 m to 896 m) and shallower (245 m versus 318 m) stable layer on 1 September than observed.

Variations in RH with height are handled quite well by N_Y, as simulated values appear to increase and decrease with height at roughly the same altitudes as the observations. The general under-prediction noted in the temporal analysis is also seen here on 28 August and 1 September for most heights. An exception exists on 30 August at an altitude of 500 m and higher, where simulated values become larger than observations.

### 4.1.2 Chemical Species

Figure 4.13 shows temporal distributions of O\(_3\) at the sites selected for analysis. Overall, N_Y over-predicts hourly average values of O\(_3\) at all sites for most times. Exceptions occur for the maximum ozone values on days three and four when the highest maximum hourly average ozone values were recorded for TexAQS-2000. N_Y does seem to reproduce the temporal variability in simulated values, though it fails to reproduce the lack of a strong diurnal pattern at GALC during day two. However, the model does capture the lack of a diurnal pattern exhibited on day one at GALC.
Precursors to ozone formation (NO and NO₂, together NOₓ) are shown in Figures 4.14 and 4.15. For NO, one notes the extreme under-prediction of N_Y at all times at all locations. One exception is the simulation of NO on days two through four at GALC, where simulated values of NO are significantly higher than observations (10.2 to 14.5 ppb higher). Though the simulation misses the magnitude of the daily maximum values of NO, the observed diurnal pattern is reproduced relatively well.

Contrastingly, N_Y significantly over-predicts NO₂ at all sites for most times. The magnitude of the over-predictions greatly outweighs the magnitude of the under-prediction of simulated NO. One possible explanation for the large discrepancy between observed and simulated values for NOₓ is accuracy (or lack thereof) of the emissions data for NO and NO₂. Inaccuracies in emissions of NOₓ species could lead to gross misrepresentations of simulated values. Another uncertainty is the quasi steady state approximation used within the RADM2 mechanism could adversely affect nitrogen species if ambient conditions do not hold for this particular episode.

Temporal distributions of CO are shown in Figure 4.16. Overall, diurnal patterns of CO mixing ratios are reproduced relatively well, though the magnitudes of simulated values are not well captured. N_Y simulates values that are generally higher than observed mixing ratios at most sites for most times. The over-predictions become much more significant during nighttime hours versus daytime hours, especially on days three and four. There are periods during nighttime hours at some sites where N_Y greatly over-predicts mixing ratios of CO. For example, nighttime simulated values on days three and four at C35C range from 800 to roughly 1000 ppb higher than observed values. However, the period of interest was dominated mostly by the over-predictions at most other times. The inaccuracies in model
simulated CO concentrations could be explained by examining the PBL height biases for N_Y. During this period, N_Y demonstrated an over-prediction of PBL height, with an NMB of 54.4%. Though mostly only applicable during daytime, this over-prediction provides gaseous species with a greater effective mixing volume for the species to become diluted. Over-predictions of PBL heights for this time period by N_Y may have lead to decreased mixing ratios of CO at the surface.

Temporal distributions of fine particulate matter (PM\textsubscript{2.5}) are shown in Figure 4.17. Overall, N_Y performs reasonably well for PM\textsubscript{2.5}. An examination of the observations sites reveals that the model performs the best at GALC and Conroe (CONR) in terms of diurnal variations and simulated values. At the other sites (East Houston (HOEA), DRPA, and LaPorte (H08H)), simulated concentrations were not well represented. In particular, simulated values at DRPA were grossly over-predicted (by 37% to 1228%) at all times. Deviations between model simulations and observed values at DRPA appeared to grow larger after day two. N_Y seems to under-predict nighttime values of PM\textsubscript{2.5} at most sites, while a slight over-prediction can be observed during daytime hours at some sites. Possible reasons for the large discrepancy in model predictions and observed values could be uncertainties in other factors, such as emissions estimates of primary particulate species, such as BC and OM.

Table 4.2 shows performance statistics for chemical species for daytime and nighttime hours in addition to daily average. N_Y shows a slight over-prediction of 6.2% for daytime O\textsubscript{3} mixing ratios, with an NME of 27.6%. This over-prediction increases significantly during nighttime simulation, as the NMB increases to 83.1%. Overall, N_Y
performed moderately well when simulating O\textsubscript{3} in terms of NMB, with an overall value of 26.1%.

When examining NO and NO\textsubscript{2}, it clearly obvious that the poorest performance for both occurs during the nighttime hours. NO is under-predicted by N\_Y, with an NMB of -99.7%, while NO\textsubscript{2} is greatly over-predicted with an NMB of 111.0%. This may be attributable to the extremely low PBL height simulated during nighttime. The low mixing heights could lead to higher levels of O\textsubscript{3}, which would lead to lower values of NO due to the NO\textsubscript{x} titration process at night. This process would also lead to an over-prediction of nighttime NO\textsubscript{2} mixing ratios. Daytime simulations of both are greatly improved over nighttime simulations in terms of statistics. Both species are under-predicted, though NO\textsubscript{2} less so than NO (NMBs of -21.6% and -8.0%, respectively). Overall, the poor performance during nighttime hours for both species dominates the overall performance of N\_Y. The NMB of -80.2% for NO overall is only slightly better than the nighttime bias. NO\textsubscript{2} predictions were highly over-predicted overall with an NMB of 54.9%.

Statistically, N\_Y simulated CO mixing ratios rather poorly both during daytime and nighttime, as well as overall. Large under-predictions exist at all times, though nighttime simulations are slightly better than daytime (-32.3% versus -42.9%). Overall, the NMB over the entire time period is between that of daytime and nighttime, with a value of -37.3%.

In general, predictions of PM\textsubscript{2.5} were relatively good in terms of NMB. Daytime simulations showed a slight over-prediction of 5%. Nighttime simulations also slightly under-predicted, with an NMB of -9.1%. The compensation between the over-prediction during daytime and under-prediction during nighttime leads to an overall under-prediction of -1.0%. 

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Spatial distributions of the maximum hourly average ozone mixing ratios are shown in Figure 4.18. One obvious characteristic of these values is the ability of the model to simulate significant O$_3$ values in and downwind of major metropolitan areas. More specifically, N_Y simulates larger mixing ratios in areas near the cities of Houston, Dallas, San Antonio, as well as New Orleans. Offshore flow appears to be most evident on days two through four, as extremely high mixing ratios of O$_3$ are shown out over the Gulf of Mexico. The general trend of increasing mixing ratios seen in the temporal analysis is also observed in the spatial distributions. Days three and four have extremely high maximum O$_3$ values, which diminish significantly on day five.

Figures 4.19 and 4.20 show the spatial distributions of NO and NO$_2$ mixing ratios, respectively. Overall, N_Y simulates values which are very similar for both species for all days. However, NO$_2$ mixing ratios on days three and four are much higher just off the coast of southeastern Texas, nearly directly east of Galveston Bay. This is most likely due to regime shift in the meteorology around 30 August, where winds have a more westerly component, causing transport of species offshore. The impact of offshore flow is most apparent on days three and four for NO$_2$. However, mixing ratios of NO appear to be unaffected by offshore or onshore winds, as the spatial distribution at any day does not appear to vary considerably. Areas with the largest values for both NO and NO$_2$ that directly affect the Houston-Galveston region are just north of Galveston Bay. Simulated values of both mixing ratios do not appear to vary considerably just outside the immediate vicinity of Houston.

The effect of horizontal transport on simulated chemistry is best examined by analyzing simulated values of chemical species with a long atmospheric lifetime. Spatial
distributions of CO mixing ratios are shown in Figure 4.21. Though these plots do not represent the maximum daily values for CO, we can still examine the effect of horizontal transport. On days three and four, the offshore flow noted earlier is quite evident, as higher values are transported downwind of Galveston and over the Gulf of Mexico. Inland, there appears to be less discernible variations over most of the domain, with an exception being on day five in the southern region of Texas. Simulated mixing ratios on day one are overall lower than the rest of the time period. CO mixing ratios near the area of interest appear to be higher over the urban area of Houston as compared with coastal regions by roughly 100 ppb.

Simulated concentrations of fine particulate can also be affected by horizontal transport by the wind. Spatial distributions of PM$_{2.5}$ concentrations are shown in Figure 4.22. Areas with the highest concentration are located generally over Houston and Galveston Bay for all days. Surrounding concentrations are on the order of 12 µg m$^{-3}$ lower than those in and around Houston-Galveston. On days three through five, the effect of offshore winds can be seen as high concentrations of PM$_{2.5}$ are advected over the Gulf of Mexico. On days one and two, the largest concentrations typically remain inland, near Houston and just northwest of Galveston Bay. It is interesting to note the reversal in the trend of simulated values of chemical species to grow larger with time as seen with O$_3$. Simulated concentrations of PM$_{2.5}$ typically decreases with time, as largest values distributed over the domain are typically observed on days one and two.

An examination of the vertical distribution of chemical species will enable us to view how well the model simulates chemical species aloft. Vertical profiles of O$_3$ mixing ratios are shown in Figure 4.23 at three different times on three days. Overall, the model seems to simulate the overall vertical distribution of O$_3$ reasonably well, though the magnitude of the
simulated values may not correspond as well. The variation in mixing ratios aloft when comparing N_Y values with observations is interesting. The simulated concentration gradients (i.e., dc/dz) tend to be smaller than observed values. That is to say, when O_3 increases with height on 30 August and 1 September, the increase in mixing ratios is not as large as observed values. For instance, on 30 August, surface simulated mixing ratio of O_3 is 37.8 ppb, and the maximum simulated value aloft is 60.8 ppb, making a difference of about 23 ppb from surface to maximum value aloft at 3500 m. However, observed values for that same range from 26.9 ppb at the surface to a maximum value aloft of 70.8 ppb at 3500 m. The difference of 43.9 ppb is much larger than the simulated difference at 17 UTC (12PM CDT) on 30 August.

Vertical distributions of NO and NO_2 (Figures 4.24 and 4.25, respectively) are simulated quite well. Though N_Y simulations of mixing ratios for both at the surface are significantly over-predicted at this time, the simulated values quickly begin to correspond well with observed values as height increases. On 30 August and 1 September, simulated values go to or very near zero ppb just above 500 m, which is in direct correlation to what is observed. On 28 August, while the simulated values at and above 500 m are not as similar to the observations as the next days, the vertical pattern is similar to the observations, as NO and NO_2 decrease with height.

An examination of CO mixing ratios aloft reveals that N_Y is capable of simulating the variation in values aloft, although the magnitude of the simulated mixing ratios do not correspond well with observed values (Figure 4.26). For example, on 30 August and 1 September, observed values around 500 m decrease sharply. From this point on, mixing ratios of CO tend to vary only from 110-130 ppb vertically. Simulated mixing ratios for
these days follows a similar pattern, with marked decreases occurring near 500 m, after which mixing ratios become fairly constant in the vertical direction.

One possible explanation for the differences in magnitude of simulated species when compared with observed values is the uncertainty in boundary conditions. For this simulation, boundary conditions for CO were set at 70 ppb at the top layer and 80 ppb throughout the troposphere. This setting would affect the simulation of long-lived species throughout the upper layers. A sensitivity simulation was conducted where the BCs for CO were shifted to 120 ppb throughout the troposphere. This alteration managed to increase the accuracy of simulated mixing ratios aloft, though it also increased the mixing ratios of surface-level CO.

4.2 Sensitivity to Planetary Boundary Layer Schemes

4.2.1. Meteorological Variables

When analyzing the sensitivity of the model prediction to various PBL schemes, one must pay close attention to the quantities mostly affected by differences in handling turbulence closure. Such meteorological variables include wind speed, wind direction, and PBL height. Because surface layer processes also largely drive surface temperature and relative humidity, one would expect to see minimal changes when maintaining the same LSM while using a different PBL option.

Temporal analyses of observed surface temperatures and simulated values from N_Y and N_M are shown in Figure 4.27. Overall, simulated values for N_M are very similar to
those from N_Y, though N_M simulates slightly lower values at night when compared with N_Y. Under-predictions at night for the N_M simulation are significantly lower than N_Y at some sites, as shown at HALC and C35C. Simulated nighttime temperatures are 1.3° to 2.1° lower than values simulated by N_Y at the aforementioned sites. N_M simulates the same lack of a strong diurnal pattern at GALC as that simulated by N_Y. Deviations in simulated values between different simulations appear to grow with time, especially for days three through five. This phenomenon may be attributable to the lack of a data assimilation system used in this version of WRF/Chem.

Temporal distributions of RH show that both N_Y and N_M perform similarly for all times at all sites (Figure 4.28). Slight deviations are observed on days three through five. During these days, N_M simulates nighttime RH values which are slightly higher than those simulated by N_Y. However, those values still are under-predicted by nearly the same amounts when comparing values from both simulations to observations. The largest difference between simulated values from N_M and N_Y occurs at the peak value on 1 September at C35C, with N_M predicting an RH value that is 9.0% higher than that of N_Y. Overall, both simulations perform quite similarly at all times for all sites.

Larger differences are apparent in the simulation of wind speed at several sites when comparing N_Y to N_M (Figure 4.29). At sites HALC and BAYP, the largest differences between simulations occur. However, wind speed at BAYP by the N_M simulation shows much higher wind speeds than both observed and simulated N_Y values. Differences in simulated values at BAYP range from 0.59 m s\(^{-1}\) to as high as 5.68 m s\(^{-1}\).

Differences in wind direction are not quite as large as those for wind speed (Figure 4.30). Overall, both simulations perform similarly at all sites. Both simulations appear to
follow similar diurnal patterns with only minimal differences in wind speed at most locations for most times. The largest differences between both simulations appear to occur during late afternoon and evening hours at all sites.

Examining the temporal variations in the U- and V-vector components (Figures 4.31 and 4.32), there do not appear to be largely significant differences between either simulation in terms of U-vector components. It can be stated that N_Y simulates a slightly higher magnitude of the U-vector at most times for most sites, but. Moderate differences exist for some times when simulating V-vector components. N_M appears to better capture changes in the magnitude of the north-south component vector when compared with N_Y. This phenomenon is evident at several times (day 2 at BAYP and DRPA; days 4 and 5 at HALC).

The largest differences between the two PBL schemes are observed in terms of PBL height (Figure 4.33). An examination of the temporal distribution of the PBL heights from both simulations reveals that N_M generally simulates a more accurate representation of boundary layer depth. This could be due to inaccurate implementation of the bulk Richardson number as a method of determining the PBL heights within this region. Overall, N_M gives PBL heights that are lower than those simulated by N_Y, except on day five at WHAR. N_M also provides a more accurate representation of temporal variations when compared with observations of PBL depth. Additionally, N_M simulates a nocturnal boundary layer height that appears to be more accurate in terms of meteorological understanding. The N_Y simulation collapses the nighttime PBL down to an unrealistic value of 16 meters. However, N_M simulates nighttime values on the order of hundreds of meters, which is more consistent with meteorological dynamics. By simulating a
theoretically more representative boundary layer, it is possible that simulations of chemical species during nighttime would be more accurately represented in the N_M simulation.

Table 4.1 shows performance statistics for several meteorological variables from both N_Y and N_M simulations. In terms of surface temperature, N_M appeared to simulate values that were slightly less under-predicted in terms of NMB when compared with N_Y (-1.2% versus -2.4%). The higher bias in simulated wind speeds observed in the temporal analysis is reinforced when examining statistical parameters for wind speed. N_M simulates wind speeds which are 27.1% higher than observations overall (compared with 12.6% by N_Y). Statistically, both N_M and N_Y performed similarly in terms of wind direction as NMBs were 6.4% and 6.6%, respectively. The better overall representation of the PBL height in temporal distributions is also seen in statistical analysis. N_M simulations of PBL height show an NMB of 22.7%, compared with 54.4% from N_Y.

A comparison of spatial distributions of surface temperature between N_M and N_Y is shown in Figure 4.34. Similar to comparisons of temporal distributions, simulated values from both simulations are nearly identical. Minor differences exist over the entire domain. However, N_M simulated temperatures along the coastline appear to be slightly lower than those from the N_Y pair. This discrepancy could be due to different mechanisms responsible for simulating wind speed and direction along the coastline. Differences in wind speed and direction could cause differences in temperature advection, especially in areas affected by coastal fronts and land-sea breezes. Simulated surface temperatures from N_M appear to be less smooth in a spatial sense when compared with N_Y. Overall, however, no major differences can be observed between the two PBL schemes in terms of surface temperature.
Little differences are observed in terms of spatial variability of surface RH. N_M simulates RH values along the coast that are slightly (5-10%) higher than those simulated by N_Y. However, differences among the model simulations appear to decrease with time when examining the other plots. These minor variations were also noted in the temporal analysis of RH. These minor differences could be attributable to different vertical transport of meteorological variables.

The differences in spatial distribution of wind vectors show no major effects of various PBL parameterizations. The overall pattern of the wind field is simulated quite comparably among the two model simulations. The only differences exist in terms of magnitude of the vectors at some locations, though the differences appear to be slight (0-.5 m s\(^{-1}\)).

An examination of the spatial distributions of PBL heights between N_M and N_Y are shown in Figure 4.37. The overall lower PBL heights are immediately obvious in the N_M simulation as compared with N_Y. Also, N_M appears to provide more detail over the entire domain, while N_Y seems more spatially averaged. Along the coastline, N_M simulates much lower PBL heights at all times as compared with N_Y. Differences in heights along the coast are around 500 meters lower when using the N_M simulation versus N_Y. The largest differences between the two simulations appear to occur on day five west and northwest of Galveston Bay and Houston. N_Y simulates heights in the Houston-Galveston region which are at or near 3000 meters, while N_M gives values which are nearly 1000 meters lower.

Figure 4.38 shows the same data as Figure 4.9, with the addition of simulated vertical profiles from N_M. In terms of the vertical temperature profile, both simulations seem to
perform similarly. For all times, N_M appears to simulate lower temperatures at the surface than N_Y, but reverses as N_Y simulates slightly higher temperatures aloft. However, differences aloft are minor as they are on the order of tenths of a degree Celsius. Larger differences between the two simulations can be seen on 31 August and 1 September, as N_Y gives higher temperatures from the surface to 750 to 900 meters, where temperatures become nearly indistinguishable.

Larger differences for meteorological variables aloft can be seen when examining the vertical distribution of RH for both simulations. N_M simulates lower level (< 1500 m) RH more accurately than N_Y, though values are still under-predicted in general when compared with observed values. At altitudes greater than 1500 m, N_Y generally gives values that are more accurate when compared with observations. Both simulations tend to capture the vertical variability in RH with height.

### 4.2.2 Chemical Species

Temporal distributions of O₃ mixing ratios for N_M and N_Y are shown in Figure 4.39. Overall, the two simulations seem to perform fairly similarly in terms of diurnal variation, as both manage to reproduce daily variability in hourly average ozone mixing ratios. As mentioned previously, N_Y seems to over-predict daily maximum values at most sites for days one, two, and five. N_M shows a similar pattern of over-prediction, though to a slightly lower amount. One notable difference between the two simulations is the more accurate reproduction of nighttime O₃ mixing ratios by N_M. The discrepancies between simulated and observed values of ozone mixing ratios at night could be partially attributable
to the NO\textsubscript{x} titration process at night. Both simulations under-predict nighttime NO mixing ratios, which could lead to less titration of O\textsubscript{3} during nighttime hours. This is more clearly seen in the mixing ratios in the evening at GALC for NO (Figure 4.40) and O\textsubscript{3}. When simulated NO values more closely correlate with observations, a close correlation between observed and simulated O\textsubscript{3} mixing ratios by N\_M is also found.

NO and NO\textsubscript{2} (Figure 4.41) mixing ratios are generally comparable between N\_M and N\_Y. Mixing ratios of NO simulated by N\_M are on the average larger than those simulated by N\_Y, especially during daytime hours. N\_M does, however, simulate values for NO\textsubscript{2} which are, on the average, lower than those simulated by N\_Y. This is the opposite of what was expected in terms of treatment of PBL height and its relation to chemical species. Better treatment of the PBL depth does not necessarily indicate a more accurate representation of certain gaseous species. Other uncertainties that exist include emissions misrepresented vertical and horizontal transport within the model. It should also be noted that the equilibrium assumptions for nitrogen chemistry used in RADM2 may not hold well for this particular episode, as mentioned previously. The ambient conditions necessary in the assumption may not necessarily be observed during this time period over this domain.

The temporal distributions of CO mixing ratios for N\_M and N\_Y are depicted in Figure 4.42. Overall, both simulations perform similarly, though magnitudes of predictions are typically different. On average during periods of higher simulated mixing ratios, values simulated by N\_M are typically 70 – 900 ppb higher than those simulated by N\_Y. However, during periods of low CO concentration (generally from 11:00 AM to 6:00 PM CDT), simulated values from both simulations are quite similar. The largest differences between model simulations tend to occur during nighttime simulations (late evening), where
differences between N_M and N_Y are generally 100 – 500 ppb on average, with N_M simulating higher values.

A comparison of temporal distributions of PM$_{2.5}$ concentrations is shown in Figure 4.43. As seen with other chemical species, the temporal variability between both simulations is fairly similar. Both simulations seem to perform fairly well when simulating fine particulates at GALC and CONR, though simulated values from N_M tend to be slightly higher than those from N_Y, on average. However, the differences between model simulations when analyzing sensitivity to PBL schemes are relatively minor.

Performance statistics for N_M and N_Y when simulating daytime, nighttime, and daily values for chemical species are shown in Table 4.2. In terms of O$_3$, daytime biases between N_M and N_Y are relatively small (NMB of 4.4% versus 6.2%, respectively). Larger differences are seen for nighttime simulations, where N_M over-predicts nighttime mixing ratios of O$_3$ by 27.9% (compared with 83.1% with N_Y). The poor prediction of mixing ratios at night could be attributed to the large nighttime under-prediction of NO mixing ratios in N_M and N_Y (-99.5% and -99.7%, respectively). The large bias in nighttime predictions of O$_3$ tends to dominate the overall daily bias for both simulations. The daily NMB values for N_M and N_Y are 10.5% and 26.1%, respectively.

Biases for NO$_2$ mixing ratios are much higher when using N_M as opposed to N_Y for daytime, nighttime, and daily predictions. Daytime bias for N_M simulating NO$_2$ is 8.4% (versus -8.0% for N_Y). Nighttime biases are much worse for both simulations, though N_M simulates much higher values with an NMB of 150% (versus 111% for N_Y). Daily biases show the same phenomenon with an NMB for N_M of 83.2% compared with 54.9% when using N_Y.
Performance of both simulations for CO mixing ratios in terms of NMB is relatively similar. Daytime simulations from N_M give an NMB of -33.9% (versus -42.9% for N_Y). Nighttime biases for CO mixing ratios are better, as N_M has a bias of only -15.3% (versus -32.3% for N_Y). Overall, daily simulations of CO mixing ratios are better represented by N_M, in terms of NMB. The N_M simulation under-predicts daily mixing ratios of CO by 24.1%, compared with an under-prediction of 37.3% in N_Y. Temporal analysis showed that at some times, CO was grossly over-predicted by both simulations. However, the dominancy of the larger under-predictions leads to a mean negative bias.

In terms of fine particulate, N_M simulates nighttime particulates more accurately in terms of NMB (-5.3% versus -9.1%), while N_Y performs better for daytime simulation of PM$_{2.5}$ concentrations (5.0% versus 14.0%). The moderate under-prediction (nighttime: NMB of -9.1%) and slight over-prediction (daytime: NMB of 5.0%) for N_Y lead to an overall NMB of -1.0% for daily simulations, while N_M has an overall NMB of 6.1%.

Spatial distributions that highlight times of the largest difference between the simulated values of O$_3$ for both simulations are shown in Figure 4.44. Times shown were chosen based on the fact that they were times when the largest difference between model simulated values for each simulation existed. For nighttime values, it is clearly evident that N_M simulates much lower values over the entire domain, except over the Gulf of Mexico. This is consistent with both temporal and statistical analyses comparing the two simulations. Daytime spatial distributions of the two simulations are more similar than nighttime. Though the differences appear rather large at 18 UTC (1PM CDT) 31 August, the differences are still relatively small considering this was one of the times with the largest difference for daily maximum ozone mixing ratios. The lack of a significant difference between model...
simulations serves to reinforce the statistical finding of a slightly lower bias of N_M versus N_Y for daytime simulations of O_3 mixing ratio.

NO and NO_2 mixing values over the entire domain for N_M and N_Y are shown in Figures 4.45 and 4.46, respectively. Simulated NO mixing ratios in the N_M simulation are much higher for these times as compared with the N_Y simulation. Values along the coast are nearly 5 to 10 ppb larger. Also, values over major metropolitan areas such as Dallas and San Antonio are much larger in N_M when compared with N_Y. Similarly, N_Y simulates large values for mixing ratios of NO_2 as compared with N_M at more localized locations. N_M appears to simulate a more stratiform level of higher values over central Texas when compared with N_Y. However, simulated mixing ratios of NO_2 from N_Y are higher over the region of interest for this study. These findings are consistent with the results of temporal analyses.

Figure 4.47 shows spatial distributions of CO mixing ratios from N_M and N_Y. One characteristic to note is the similarity of the spatial distribution. While the magnitude of some localized mixing ratios are different, the overall spatial pattern of CO is consistent within both simulations. N_M simulates larger mixing ratios of CO over urban areas such as Dallas, San Antonio and Houston-Galveston. One possible explanation for this is the depth of the PBL simulated in N_M is much lower than that of N_Y, which could have effects on the surface mixing ratio of long-lived atmospheric species.

PM_{2.5} concentrations are simulated relatively similar between both N_M and N_Y in terms of spatial distribution (Figure 4.48). N_M simulates concentrations in Houston and north of Galveston which are slightly higher than N_Y. Relatively minor differences
between the simulations are observed on a spatial scale over the Houston-Galveston area, which is similar to the findings of the temporal analysis.

Figures 4.49 through 4.52 display the vertical distribution of chemical species simulated by N_M and N_Y for comparison of the PBL schemes. In examining the vertical distribution of O\textsubscript{3} mixing ratios simulated by N_M and comparing with simulations from N_Y, N_M values are less well-mixed throughout the atmosphere. That is to say, there is much more vertical variability in the magnitude of the mixing ratio gradient (i.e., \( dc/dz \)) relative to height in the N_M simulation when compared with N_Y. This is perhaps due to the effect of local closure used in MYJ as opposed to non-local closure employed by YSU. Vertical distribution of O\textsubscript{3} in N_Y may be more averaged over several layers as opposed to mixing layer-by-layer as the height increases (Alapaty and Mathur, 1998). The pattern demonstrated in the N_M simulation may appear to be a more realistic simulation of the atmosphere, as the vertical variations are more indicative of vertical variations seen in the observations, even though the magnitude of simulated values are inaccurate.

Both NO and NO\textsubscript{2} appear to perform very similarly, regardless of simulation. Minor differences (1 – 2.5 ppb) in simulated values of NO\textsubscript{2} at the surface are observed. These differences are consistent with findings from temporal analyses. One notable characteristic when examining the mixing ratios of CO is that N_M simulates mixing ratios which decrease less rapidly with height in the lower layers when compared with N_Y. Especially on 30 August and 1 September, mixing ratios of CO decrease slowly up to a height near 750 to 1000 m, then decrease rapidly, almost forming a discontinuity between layers. Above 1000 m, both simulations appear to simulate CO quite similarly. This could be partly attributed to the boundary conditions used for CO profile initialization.
4.3 Sensitivity to Land Surface Models

4.3.1 Meteorological Variables

This section provides temporal, statistical, spatial and vertical analyses of meteorological variables and how they vary when simulated using various types of LSMs. Typically, LSMs are responsible for sensible and latent heat (SH and LH, respectively) fluxes to the boundary layer, as well as initializing and simulating soil moisture content. Possible impacts could reach a broad list of meteorological variables, as surface fluxes could impact surface temperature, soil moisture could impact surface fluxes, which could alter temperature and PBL height, as well as relative humidity.

Figures 4.53 through 4.59 are similar to 4.1 through 4.7, with the addition of simulated values from two other simulations, slab/YSU (S_Y) and RUC/YSU (R_Y). Examining the temporal distribution of surface temperature shows that each simulation handles the diurnal variation in temperature very well at most sites. It is interesting to note that the S_Y simulation exhibits a strong cold bias when simulating maximum daily temperatures and afternoon into overnight temperatures. This cold bias for afternoon and evening temperatures is exhibited in the R_Y simulation as well. Simulations generally correspond well with the increasing temperature throughout the morning hours for S_Y, however. R_Y demonstrates a nighttime minimum temperature cold bias as well, though not as significant as that for S_Y. The cold bias for maximum temperatures when using the S_Y simulation is magnified for days three through five, as deviations from the maximum
continue to increase. Also, discrepancies among model simulations appear to grow larger after day three as well. This phenomenon was mentioned previously in section 4.2.1 and most likely has to deal with lack of data assimilation in this version of WRF/Chem.

One of the variables with the largest differences between the three simulations is surface relative humidity. All three simulations appear to capture the diurnal variation RH, increasing values throughout the night and decreasing values throughout the day. R_Y shows a strong negative bias, especially on days three through five, but even on days one and two at some sites. In this particular study, values for RH given by R_Y are less than half of the observed values at times. Comparatively, the S_Y simulation performs very well when simulating RH values. This was not an expected development, as S_Y is a simple thermal diffusion scheme, with less physically rigorous dynamics for soil moisture. One would assume that models using a more dynamically complex scheme would be better able to accurately simulate atmospheric moisture content. This was not the case for this particular episode, as all simulations except S_Y demonstrated a net negative bias for RH simulations. S_Y even begins to over-predict values for RH at some sites for days three through five. As noted previously, S_Y exhibits a much stronger cold bias when compared with N_Y and R_Y. This cold bias may help explain the better-simulated values for RH because of the dependency of saturation vapor pressure on surface temperature. In general understanding, saturation vapor pressure is analogous to saturation mixing ratio, and both may be used (with vapor pressure and mixing ratio, respectively) in determining RH. If a cold bias is found, it can be assumed that higher values for RH will be simulated, which is the case for S_Y when compared with the other two simulations.
Simulated wind speeds among the three simulations are quite similar for days one and two. Deviations in the magnitude of wind speed appear to grow among the models after days three. Of the simulations, S_Y shows a negative nighttime bias, with values at times nearing 0 m s\(^{-1}\). R_Y appears to simulate values that are on average larger than either N_Y or S_Y at days three through five, though times exist when its simulated wind speeds are at or below values given by those simulations. However, diurnal variations among the three simulations are very similar. It appears as though the major difference among the simulations is being able to reproduce an accurate magnitude for wind speed.

In terms of wind direction, S_Y and N_Y perform very similarly throughout the entire simulation period. All three simulations perform exceptionally well at GALC, where only minor differences are shown, which can be seen near noon on day four. It is interesting to note that R_Y differs significantly from the other two simulations on days three through five when simulating late afternoon shifts in wind direction. The magnitudes of the simulated shifts given by R_Y are not seen in observations. This phenomenon is seen most clearly at BAYP and C35C. Though the amount of wind shift may not be well-represented by R_Y, it is interesting to see that R_Y actually simulates a shifting wind direction which is more accurate in time to when a shift actually occurs in observations.

Examining the U- and V-vector components, each model simulation appears to perform relatively similarly for both variables. Some differences exist in terms of magnitude of vectors at certain times and locations, but overall, no significant differences are apparent when using various land-surface parameterizations.

All three simulations overestimate the height of the boundary layer on day one at all sites. However, S_Y appears to simulate depths that more closely correspond to observed
values. The early development of the boundary layer is handled relatively well by all simulations, though all three develop the height slightly fast on day one. Days two through four demonstrate better agreement with the observations in terms of daytime development of the PBL. Marked differences between simulated values occur on days three through five at all sites. Interestingly, neither N_Y nor R_Y is responsible for gross over-prediction at all sites. For example, N_Y simulates the greatest over-prediction of the PBL height at WHAR, ELLF, and LBTY. In contrast, R_Y provides the largest over-prediction at HSWH and LMRQ. Possible causes for discrepancy in the simulated boundary layer heights could be associated with varying surface sensible heat fluxes from each simulation. The more accurate predictions by the S_Y scheme compared with N_Y and R_Y may be attributed to lower sensible heat fluxes from the surface. This lower level of sensible heat flux could also be attributable to the cold bias exhibited in S_Y. One can assume that higher sensible heat fluxes at the surface in N_Y and R_Y would lead to higher surface temperatures, which lead to lower RH values. Similarly, these larger sensible heat fluxes can cause higher simulated PBL heights.

Statistically, the cold bias described earlier for the S_Y scheme is confirmed, as the NMB for T2 for this scheme is -4.1% (see Table 4.3). Comparatively, N_Y had a slightly smaller cold bias of -0.3% and R_Y performed the best statistically with an NMB of -0.3%. Overall, the strongest wind speeds were simulated using the R_Y coupling, with an NMB of 24.2%. This is in stark contrast to the prediction of wind speed by the S_Y simulation (NMB of 1.7%). N_Y over-predicted wind speeds by almost half as much as R_Y, with an NMB of 12.6%. NMBs in terms of wind direction for all three simulations were relatively similar. S_Y performed the worst among the three, with an NMB of 7.5% (versus 6.6% and 5.7% for
N_Y and R_Y, respectively). Examining the U- and V-vector components of the wind, both N_Y and R_Y simulated higher values for the U-component (NMBs of 21.6% and 25.4%, respectively), while S_Y simulated lower values (NMB of -11.7%). All three simulations gave lower values for V-components in terms of NMB. The lowest predictor was N_Y at -34.6%, followed by R_Y at -23% and finally S_Y at -14.4%. The temporal analysis that showed S_Y performing better than the other two simulations in terms of RH was confirmed through statistical analysis. S_Y slightly over-predicted RH overall with an NMB of 2.5%. Contrastingly, both N_Y and R_Y under-predicted RH, giving NMBs of -27.6% and -30.5%, respectively. All simulations over-predicted PBL heights, though to a lesser extent for S_Y. S_Y over-predicted the PBL height by 24.3%. N_Y and R_Y were nearly the same in terms of statistical analysis of PBL height simulations, with NMBs of 54.4% and 53.7%, respectively.

Spatial distributions of surface temperature, RH, wind vectors, and PBL height are shown in Figures 4.60 through 4.63, respectively. An examination of the spatial plots confirms the cold bias that was mentioned previously regarding the S_Y simulation. Temperature values across the domain appear to be mostly uniform over the eastern half of Texas, with an exception just northwest of Galveston Bay. By contrast, R_Y provides large spatial variability in surface temperature over the entire modeling domain. The highest simulated temperatures for this time are observed over the Mississippi River and near the Dallas area. The variations in the spatial variability among simulations are quite interesting. The range of values for the S_Y simulation for example varies from around 34°C to 40°C, while those for R_Y range from 36°C to 46°C.
The large variation in simulated RH values noted in the temporal analyses can be seen in the spatial plots as well. S_Y appears to simulate higher values than either N_Y or R_Y, which as noted previously is most likely due to differences in simulated sensible and latent heat fluxes upward from the surface. S_Y simulates higher heat flux away from the surface (not shown) when compared with N_Y and R_Y, which has large effects on T2 and PBL height as well.

Overall, the spatial distribution of the wind fields shows no major differences among the model simulations, as noted in the discussion of the temporal analyses. The areas of largest difference among the three model simulations are over the Gulf of Mexico and towards the eastern edge of the domain. Over the domain of interest (Houston-Galveston), the vector field appears to be captured similarly by all simulations. Transport of chemical species would seemingly be comparable among the three simulations.

The spatial distributions of PBL heights across the domain from all three simulations have the same pattern. However, large differences lay in the magnitude of the PBL height. S_Y shows much lower values when compared with N_Y and R_Y. This confirms the statistical biases and temporal analysis provided earlier. For this time, heights given by the S_Y simulation are typically 1000 – 1500 m lower than either N_Y or R_Y. All three simulations do, however, simulate PBL heights which are comparably lower in and around the Galveston Bay area, along the coast.

In terms of vertical distribution of temperature and relative humidity (Figure 4.64) all simulations appear to give similar vertical variability. While magnitudes of temperature predictions may not agree well, the overall pattern is fairly well represented by each scheme. The S_Y simulation tries to develop the stable layer at a lower level than N_Y or R_Y on 30
August and 1 September. The stable layer for S_Y begins 150 – 250 m lower than observed values. R_Y and N_Y are much more in agreement with the development of the stable layer, though they also simulate the start of the stable layer slightly lower than observed (around 50 m).

Overall, vertical distribution of RH is captured pretty well by all three simulations. Although the S_Y simulation performs better for surface level RH, there is no marked difference between results from the three runs. It is interesting to note on 1 September how S_Y simulates a layer of decreasing RH from 500 to 1200 m while the other two simulations and observations show increasing RH with height. It does not appear to show that one simulation performs better than the others in terms of simulating RH aloft.

4.3.2 Chemical Species

Temporal variations in O₃ mixing ratios are shown in Figure 4.65. Overall, the diurnal pattern is well captured by all three simulations. In terms of over-prediction and under-prediction, R_Y tends to over-predict nighttime mixing ratios of O₃ at most sites, as well as over-predict daytime maximum values at HALC on day one, BAYP, C35C, and DRPA on days one and two, as well as on days one, two, four and five at GALC. S_Y performs much the same way, though it appears to have a greater under-prediction of nighttime mixing ratios than either of the other two simulations. None of the simulations capture the extremely high values for O₃ observed on days three and four at HALC, BAYP, C35C, and DRPA. S_Y appears to greatly over-predict daily maximum mixing ratios of O₃.
at GALC on days four and five as compared with the other two simulations, though both N_Y and R_Y over-predict as well.

Part of the explanation for the low values of O_3 simulated by S_Y at night may be the large simulated mixing ratios for NO_x (Figures 4.66 and 4.67) during nighttime hours. Higher simulated mixing ratios of NO could lead to significant titration of O_3, which would explain the significant under-prediction of O_3 at night. The three simulations perform relatively similarly in terms of NO, though S_Y simulates higher mixing ratios on average. However, significant differences between model simulations occur for NO_2. S_Y simulates much higher mixing ratios of NO_2 at most times and sites than either N_Y or R_Y, at times being more than 60 ppb higher than the highest value of other simulations. However model simulated values are very similar at most sites for day one. Variations in model predictions appear to grow from day two onward.

Temporal distributions of CO mixing ratios are shown in Figure 4.68. In general, there appears to be an under-prediction of mixing ratios at all sites for most times. However, significant periods of over-prediction are also observed. Overnight predictions of CO at HALC, DRPA and C35C are clearly overestimated by all three simulations, though the greatest over-predictions appear to occur on days three and four. The lower simulated PBL heights by the S_Y simulation could explain the larger simulated mixing ratios during this time period.

Temporal distributions of PM_{2.5} for the three model simulations show that during days one through three, simulated concentrations are relatively similar (Figure 4.69). Deviations in model-simulated concentrations begin to emerge towards the beginning of day four. At this time, S_Y begins to simulate concentrations of fine particulate that are higher
than either N_Y or R_Y. These deviations are most obvious at HOEA, DRPA, and H08H beginning with day four. Simulated concentrations of PM$_{2.5}$ by S_Y are, on average, 13 to 16 µg m$^{-3}$ higher than maximum values simulated by N_Y or R_Y, and sometimes as high as 26 µg m$^{-3}$. Differences in the prediction of various components of PM$_{2.5}$ by each simulation may be the underlying cause of the differences in total PM$_{2.5}$. Other uncertainties include the emission of primary particulates such as BC and OM, and their role in the simulation of total fine particulate matter.

More information on the overall accuracy of the simulated values of chemical species may be gathered by examining performance statistics for nighttime and daytime hours, as well as daily totals (Table 4.4). All three simulations show an over-prediction of O$_3$ for daytime, nighttime, and overall daily totals. With an NMB of 1.5%, S_Y performs better when simulating daytime O$_3$ values than N_Y or R_Y (NMBs of 6.2% and 1.7%). Nighttime simulation of O$_3$ is also performed better by S_Y, though with a much higher bias of 33.2% (versus 83.1% and 46.9% for N_Y and R_Y). However, these large positive biases indicate that none of the simulations is very good for nighttime O$_3$ mixing ratios. Overall, S_Y performs slightly better than R_Y (9.7% versus 13.4%), and both perform much better than N_Y (NMB of 26.1%).

N_Y under-predicts NO and NO$_2$ during daytime simulations (NMB of -21.6% and -8.0%, respectively). Interestingly, S_Y has an NMB of 0.0% for daytime simulation of NO, which is likely due to the balancing of over-predictions with under-predictions, as the NME is 80%. NO$_2$ simulations from S_Y are over-predicted by 18.9% during daytime. Comparatively, R_Y shows relatively small biases for daytime simulation NO and NO$_2$ (-6.4% and 4.4%, respectively). All three simulations under-predict nighttime mixing ratios of
NO while over-predicting NO$_2$ mixing ratios during the same period. No particular simulation performs good for nighttime NO mixing ratios. NMBs of -99.7%, -99.6%, and -99.7% for N$_Y$, S$_Y$, and R$_Y$ indicate equally large under-prediction. This could possibly explain the higher nighttime mixing ratios of O$_3$. If abundant NO is unavailable for O$_3$ titration, this could lead to over-predicted mixing ratios. Nighttime NO$_2$ is more accurately simulated by R$_Y$ with an NMB of 110%, which is slightly better than 111% by N$_Y$, but much better than 190% by S$_Y$. Overall predictions of NO mixing ratios are generally bad for all simulations (NMBs of -80.2%, -74.7%, and -76.4% for N$_Y$, S$_Y$, and R$_Y$, respectively). Overall, NO$_2$ is better predicted by N$_Y$ (54.9%) as compared with R$_Y$ and S$_Y$ (60.4% and 110%, respectively).

CO mixing ratios are simulated better by S$_Y$ for both daytime and nighttime simulations (-28.0% and -3.2%). Simulations of daytime and nighttime CO are greatly under-predicted by N$_Y$ (-42.9% and -32.3%) and R$_Y$ (-35.6% and -31.0%). Overall predictions by S$_Y$ are moderately better than those simulated by N$_Y$ and R$_Y$ (-14.9% versus -37.3% and -33.2%). However, all models under-predict CO mixing ratios, regardless of the time of day.

Each simulation over-predicts concentrations of PM$_{2.5}$ during daytime simulations. N$_Y$ appears to have a more accurate representation of daytime fine particulates (5.0%) compared with S$_Y$ and R$_Y$ (20.4% and 7.7%, respectively). Performance for nighttime simulation of PM$_{2.5}$ is relatively similar between N$_Y$ and R$_Y$ simulations, as both under-predict by –9.1% and –11.4%. Contrastingly, S$_Y$ over-predicts nighttime simulated PM$_{2.5}$ concentrations by 6.8%. Overall, compensations of over-predictions during daytime and under-predictions during nighttime allow R$_Y$ to perform most accurately with an NMB of
0.5%. N_Y performed relatively similarly, though with a net negative bias of –1.0%. Finally, S_Y showed an overall over-prediction of PM$_{2.5}$ concentrations by 14.6%.

Spatial distributions of O$_3$ mixing ratios are shown in Figure 4.70. The nighttime biases observed in the statistical analysis are difficult to observe in terms of spatial distribution. However, one can see that compared with N_Y, S_Y and R_Y simulate slightly lower values over a larger area in the Houston-Galveston region. Likewise, the large bias that was seen in the prediction of daytime mixing ratios of O$_3$ in statistical analysis can be viewed. N_Y simulates much higher mixing ratios over the domain, though most of the values are confined to Louisiana. Spatial distributions of O$_3$ over the Gulf of Mexico seem to be simulated similarly by all three simulations. The relatively small differences in bias between S_Y and R_Y are clearly evident in the spatial distributions, as minor differences across the domain are observed.

NO and NO$_2$ over the entire domain are simulated rather similarly among all three simulations (Figures 4.71 and 4.72). Minor differences are visible in the spatial distribution of NO, for example. At 13 UTC (8AM CDT) on 30 August, mixing ratios of NO along the coast are relatively similar between N_Y and R_Y, while slightly lower values are observed in S_Y. Twenty-four hours later, simulated values along the coast have areas of larger mixing ratios simulated in the S_Y simulation as opposed the other two. However, differences at both times are of a very small magnitude. S_Y simulates much higher values of NO$_2$ over the Houston area as compared with spatial distributions from N_Y and R_Y at similar times. However, N_Y and R_Y simulate much higher mixing ratios of NO$_2$ over Dallas. Overall, differences between simulations of these two gaseous species are relatively minor.
When examining the spatial distribution of CO, one can see the lower values simulated over the Houston area by the N_Y coupling as opposed to S_Y and R_Y (Figure 4.73). Differences between S_Y and R_Y at 20 UTC (3PM CDT) are almost indistinguishable over the area where observations were taken. However, differences are more noticeable at earlier times (not shown), as higher values over the Houston-Galveston area are simulated by S_Y and cover a slightly larger area than those simulated by R_Y. This broad area of high mixing ratios may help to explain the lack of a stronger negative bias for S_Y in the statistical analysis.

Overall, spatial distributions of PM$_{2.5}$ concentrations are relatively similar over the domain. However, S_Y simulates larger concentrations, as was seen earlier in the statistical and temporal analyses. Differences between S_Y and the other two simulations are nearly 10 µg m$^{-3}$ higher for the times shown in Figure 4.72. All simulations seem to agree on the general pattern of spatial distribution of PM$_{2.5}$ over the entire domain.

Vertical distributions of O$_3$, CO, NO and NO$_2$ are shown in Figures 4.75 through 4.78, respectively. In terms of O$_3$, all three simulations perform similarly on 28 August. However, S_Y appears to simulate nearly constant values from the surface to near 1500 m before increasing, while both N_Y and R_Y show increasing mixing of ratios vertically with height around 1000 m. The areas of the largest variation with O$_3$ mixing ratio with height occur on 30 August and 1 September. On 30 August, S_Y simulates an increase in mixing ratios with height that appears to recreate more accurately what was observed in terms of increasing mixing ratio from the surface. The range in values for the observations from 500 – 750 m is about 40 ppb, which is similar to what is found by S_Y, though the magnitude of the mixing ratios is different. On 1 September, S_Y appears to simulate a rapid decrease in
O$_3$ that occurs at a much lower height than observed values. Both N\_Y and R\_Y appear to simulate vertical O$_3$ values quite similarly throughout the time period.

The largest difference among the simulations when examining the vertical distributions of NO and NO$_2$ appears to occur on 30 August. S\_Y simulates a much slower decrease in the mixing ratio of NO$_2$ up to a level of 1000 m as compared with simulations from N\_Y and R\_Y. Overall, the three simulations appear to simulate vertical profiles of NO$_x$ relatively well. The overall variation in vertical distribution of CO within the model simulations is relatively small for most times. It should be noted, however, that S\_Y simulates a slower decrease in CO mixing ratios with height than either N\_Y or R\_Y, while also showing the highest surface level concentrations of the three simulations. However, as previously observed in the PBL sensitivity study, all three simulations appear to perform similarly at a level above 1000 m, partially attributable to CO boundary conditions within the model.

4.4 Computational Cost

Table 4.5 shows the CPU cost for the baseline (N\_Y) and all three sensitivity simulations (N\_M, S\_Y, and R\_Y). Overall, the baseline simulation performed best in terms of computational efficiency, taking on average 12.4 minutes per simulation hour and 4.96 hrs. for one daily simulation. Interestingly, S\_Y performed the slowest (15.1 min. and 6.04 hrs., respectively) even though it utilized the least physically intensive land-surface parameterization among the three LSMs.
In terms of sensitivities to PBL parameterizations, there was no appreciable difference between the two schemes, as 30 seconds on average separated the two simulations for a simulation hour (12.4 min. for N_Y versus 12.9 min. for N_M). Overall, there appeared to be no significant differences in terms of time for any of the sensitivity simulations. It should also be noted that when using a shared-memory computing environment, CPU time is dependent upon the availability of both simulation processors and memory. An increased load on the systems could lead to increased CPU times for model simulations.
Table 4.1. Performance statistics for both baseline (N_Y) and sensitivity (N_M) simulations for temperature at two meters (T2), relative humidity (RH), wind speed (WSP) and direction (WDR), U- and V- vector components, and PBL height.

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Acronyms: N_Y – NOAH/YSU pair, N_M – NOAH/MYJ pair
Table 4.2. Performance statistics for \( \text{O}_3 \) (A), \( \text{NO} \) (B), \( \text{NO}_2 \) (C), \( \text{CO} \) (D), and \( \text{PM}_{2.5} \) (E) for the baseline (N_Y) and sensitivity (N_M) simulations.

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Acronyms: N_Y – NOAH/YSU pair, S_Y – slab/YSU pair; R_Y – RUC/YSU pair
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Table 4.4. Performance statistics for O\textsubscript{3} (A), NO (B), NO\textsubscript{2} (C), CO (D), and PM\textsubscript{2.5} (E) for N\textsubscript{Y}, S\textsubscript{Y}, and R\textsubscript{Y} simulations.

A. O\textsubscript{3}

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Table 4.5. Computational cost for the N_Y, N_M, S_Y, and R_Y simulations on a per hourly simulation and daily simulation basis.

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Acronyms: N_Y – NOAH/YSU pair; N_M – NOAH/MYJ pair; S_Y – slab/YSU pair; R_Y – RUC/YSU pair
Figure 4.1. Temporal distribution of temperature at two meters (T2) at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.2. Temporal distribution of relative humidity (RH) at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.3. Temporal distribution of wind speed (WSP) at 10 meters at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.4. Temporal distribution of wind direction (WDR) at 10 meters at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.5. Temporal distribution of U-vector component at 10 meters at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.6. Temporal distribution of V-vector component at 10 meters at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.7. Temporal distribution of PBL height at Wharton (WHAR), Ellington Field (ELLF), Southwest Houston (HSWH), Liberty (LBTY), and LaMarque (LMRQ).
Figure 4.8. Spatial distribution of T2 at 20 UTC (3PM CDT) on 28 - 31 August and 1 September, 2000.
Figure 4.9. Spatial distribution of RH at 20 UTC (3PM CDT) on 28 - 31 August and 1 September, 2000.
Figure 4.10. Spatial distribution of wind fields at 20 UTC (3PM CDT) on 28 - 31 August and 1 September, 2000.
Figure 4.11. Spatial distribution of PBL height at 20 UTC (3PM CDT) on 28 - 31 August and 1 September, 2000.
Figure 4.12. Vertical profiles of temperature (left) and RH (right) compared with observations from NOAA’s Electra aircraft instrumentation.
Figure 4.13. Temporal distribution of O$_3$ at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.14. Temporal distribution of NO for Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.15. Temporal distribution of NO$_2$ at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.16. Temporal distribution of CO at Aldine (HALC), Clinton (C35C), Deer Park (DRPA), Dallas Hinton Street (C401), and LaPorte (H08H).
Figure 4.17. Temporal distribution of PM$_{2.5}$ at Houston East (HOEA), Galveston Airport (GALC), Deer Park (DRPA), Conroe (CONR), and LaPorte (H08H).
Figure 4.18. Spatial distribution of O₃ mixing ratios and wind vectors at 20 UTC (3PM CDT) on 28 – 31 August and 1 September 2000.
Figure 4.19. Spatial distribution of NO mixing ratios (left) and NO emissions (right) at 20 UTC (3PM CDT) on 28 and 30 August and 1 September 2000.
Figure 4.20. Spatial distribution of NO$_2$ mixing ratios (left) and NO$_2$ emissions (right) at 20 UTC (3PM CDT) on 28 and 30 August and 1 September 2000.
Figure 4.21. Spatial distribution of CO mixing ratios (left) and CO emissions (right) at 20 UTC (3PM CDT) on 28 and 30 August and 1 September 2000.
Figure 4.22. Spatial distribution of PM$_{2.5}$ at 20 UTC (3PM CDT) on 28 – 31 August and 1 September 2000.
Figure 4.23. Vertical distribution of O$_3$ compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 4.24. Vertical distribution of NO compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 4.25. Vertical distribution of NO$_2$ compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 4.26. Vertical distribution of O$_3$ compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 4.27. Temporal distribution of temperature at two meters (T2) at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.28. Temporal distribution of relative humidity (RH) at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.29. Temporal distribution of wind speed at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC, and Deer Park (DRPA).
Figure 4.30. Temporal distribution of wind speed at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.31. Temporal distribution of U-component vectors at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.32. Temporal distribution of V-component vectors at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.33. Temporal distribution of PBL height at Wharton (WHAR), Ellington Field (ELLF), Houston Southwest (HSWH), Liberty (LBTY) and LaMarque (LMRQ).
Figure 4.34. A comparison of spatial distribution of T2 between N_Y (left) and N_M (right) at 22 UTC on 28 and 30 August and 1 September 2000.
Figure 4.35. A comparison of spatial distribution of RH between N_Y (left) and N_M (right) at 22 UTC on 28 and 30 August and 1 September 2000.
Figure 4.36. A comparison of spatial distribution of wind fields between N_Y (left) and N_M (right) at 22 UTC on 28 and 30 August and 1 September 2000.
Figure 4.37. A comparison of spatial distribution of PBL height between N_Y (left) and N_M (right) at 22 UTC on 28 and 30 August and 1 September 2000.
Figure 4.38. Vertical profiles of temperature (left) and RH (right) compared with observations from NOAA’s Electra aircraft instrumentation.
Figure 4.39. Temporal distribution of O$_3$ at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.40. Temporal distribution of NO at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.41. Temporal distribution of NO$_2$ at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 4.42. Temporal distribution of CO at Aldine (HALC), Clinton (C35C), Deer Park (DRPA), Dallas Hinton Street (C401), and La Porte (H08H).
Figure 4.43. Temporal distribution of PM$_{2.5}$ at Houston East (HOEA), Galveston Airport (GALC), Deer Park (DRPA), Conroe (CONR), and La Porte (H08H).
Figure 4.44. A comparison of spatial distribution of O$_3$ between N_Y (left) and N_M (right) at 20 UTC (3PM CDT) 28 and 30 August and 1 September 2000.
Figure 4.45. A comparison of spatial distribution of NO between N_Y (left) and N_M (right) at 20 UTC (3PM CDT) 28 and 30 August and 1 September 2000.
Figure 4.46. A comparison of spatial distribution of NO$_2$ between N_Y (left) and N_M (right) at 20 UTC (3PM CDT) 28 and 30 August and 1 September 2000.
Figure 4.47. A comparison of spatial distribution of CO between N_Y (left) and N_M (right) at 20 UTC (3PM CDT) 28 and 30 August and 1 September 2000.
Figure 4.48. A comparison of spatial distribution of PM$_{2.5}$ between N_Y (left) and N_M (right) at 20 UTC (3PM CDT) 28 and 30 August and 1 September 2000.
Figure 4.49. Vertical distribution of O$_3$ compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 4.50. Vertical distribution of NO compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
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In order to better understand the impact of horizontal grid resolution and nesting options on simulated meteorology and chemistry, several simulations were performed. These include: one-way nesting using 12-km horizontal grid spacing (1W12), one-way nesting using 4-km horizontal grid spacing (1W4), two-way nesting utilizing both 12- and 4-km horizontal grid spacing (2W12 and 2W4, respectively).

### 5.1 Meteorological Variables

A temporal analysis of surface temperature reveals that all four model simulations seem to give relatively similar performance (Figure 5.1). Diurnal variability seems to be well reproduced at all sites by all simulations. Major differences between simulations can be observed at C35C and DRPA, where 2W12 simulates higher afternoon and evening temperatures, while other simulations (especially 1W4 and 2W4) exhibit a cold bias during those times. There appears to be a general under-prediction of the daily maximum surface temperature by all simulations for most days, with largest differences on days two through four. It is noted that the 1W4 simulation has a tendency to decrease temperatures on days four and five after reaching the daily maximum. 1W4 begins to decrease surface temperature by up to 2 hours before any other model simulation does so. Overall, all model simulations appear to exhibit an overall cold bias, on average.

Temporal variations in relative humidity among the four model simulations were relatively negligible (Figure 5.2). However, it is worth noting that the 2W4 simulation
appears to simulate much lower values of RH at all times than other simulations. Comparatively, the 1W4 simulation does a better job of reproducing observed values. The most notable difference in RH between types of model simulations occurs mostly when variations in the type of nesting are used rather than different grid spacing. However, there was no standalone 4-km simulation to compare with one-way and two-way nesting of a finer domain.

Large variations in wind speed tend to occur at BAYP and GALC (Figure 5.3). For the other three locations, the model simulations of wind speed are relatively consistent with one another. However, at BAYP, 2W12 simulates wind speeds that are on average 1 to 3 m s\(^{-1}\) higher than other simulations. The same holds true for most times at GALC, although there is a relatively noticeable under-prediction of wind speeds at this location by the 1W4 simulation. In fact, wind speeds at GALC are better represented in the 2W12 simulation than others. Overall, it would appear as though wind speeds are generally well reproduced by most simulations, though there is a noticeable over-prediction by the 2W12 simulation at a few sites.

Overall, simulations of wind direction among the four simulations are relatively similar (Figure 5.4). No marked differences between using one-way or two-way nesting, nor when using finer grid-spacing occur. The only minor differences exist in the timing of wind shifts at certain locations. This timing issue is most clearly evident at GALC during daytime. This site may be prone to uncertainty in simulated changes in wind direction due to coastal influences. Moderate wind shifts occur throughout the day as land-sea breeze interactions occur. This interaction is the most likely cause for the discrepancy in shifts of simulated wind direction.
Figures 5.5 and 5.6 respectively show the temporal distribution of U- and V-vector components from all four simulations. As expected, only minor differences among model simulations occur, which is also consistent with temporal analyses discussed previously. Slight magnitude variations occur among all four simulations, but there appears to be no major impact when varying horizontal grid spacing or nesting options.

Temporal distributions of PBL height depicted in Figure 5.7 show that 1W4 simulates PBL heights which are more representative of observed values. Contrastingly, 1W12, 2W12 and 2W4 all simulate PBL heights that are generally much too high. This is quite an interesting result as one would expect if a one-way nested 4-km simulation produces a lower PBL height, so too would a two-way nested 4-km simulation if all other physical options remain the same. In this case, however, the feedback from the larger 12-km domain to the smaller 4-km domain may have had lingering effects when attempting to simulate PBL height, influencing the simulation into larger values. This influence may be feasible, as PBL heights for 2W4 are lower than those from 2W12, but not as low as those from 1W4.

Statistical analysis of the meteorological predictions confirms what we have seen in the temporal analysis (Table 5.1). In terms of surface temperature, 2W12 did a better job of reproducing observed values (NMB of -1.8%), though all simulations did an acceptable job. All simulations exhibited a cold bias with only minor differences in the strength of the under-predictions. The effects of nesting appear to have a stronger influence on the prediction of surface temperature than horizontal grid spacing. Differences between 1W4 and 2W4 were quite apparent in terms of the NMBs shown here (-7.4% versus -2.8%). The same finding is true to a lesser extent for the 12-km simulations, as 2W12 performed slightly better than 1W12 (-1.8% versus -2.7%).
The 1W4 simulation gave more accurate values of RH in terms of NMB (-9.3%). All other simulations under-predicted RH by almost 20%. The next most accurate simulation was that of the 2W12 (NMB of -18.4%). It would appear as though horizontal grid-spacing had a larger effect on the simulation of RH as opposed to nesting options. Differences in NMB between 1W12 and 1W4 were 12.8%, while differences between 1W4 and 2W4 were 12.3%. Similarly, differences between two-way and one-way nesting at 12-km were only 3.7%.

The biases noted earlier in terms of wind speed are evident in the statistical analysis. 1W4 simulated lower wind speeds than observed (-4.8%), while all other simulations overestimated. The largest over-prediction was seen when using the 2W12 simulation (22.8%), while 1W12 and 2W4 over-predicted to a lesser extent (3.0% and 6.4%, respectively).

There is no significant difference between model simulations in terms of wind direction. All simulations incorrectly simulated wind direction, though all the biases were within 4% of the others. 2W12 simulated more accurate wind directions (10.6%) while 1W12 performed worst of the four (14.8%). No large differences were observed for simulated wind directions between 1W4 and 2W4 (NMBs of 12.1% and 13.1%, respectively).

Only minor differences exist in the statistical analysis of U- and V-vector components. 1W4 and 2W12 (13%) appear to simulate the lowest value for U-vectors, while 2W12 simulates the lowest (-37%) values for V-vector components. Overall, differences among the simulations are within 3-4% for both variables, indicating only slight differences among variations of horizontal grid spacing and nesting options.
The large biases seen in the temporal analysis of PBL height is confirmed in the statistical analysis. 1W4 simulated much more accurate heights than any other simulation, with an NMB of -2.7%. All other simulations greatly overestimated the height of the boundary layer, though 2W12 performed the worst (NMB of 59.3%). 1W12 and 2W4 performed more similarly, though still grossly over-predicting (54.8% and 53.8%, respectively).

Spatial distributions of T2, RH, wind vectors, and PBL height are shown in Figures 5.8 through 5.11. Examining distributions of T2 over both 12- and 4-km domains, the 4-km resolution offers much more texture in terms of available information. For example, the lake to the north of Galveston is much more defined with greater detail, and the ability to discern a broader spectrum of simulated temperatures is possible, whereas at 12-km, the surface temperature over the lake would be represented by maybe fewer grid cells. The benefit of the feedback using two-way nesting at 4-km is evident when examining the distributions of surface temperature for both. Because all simulations in general simulate lower temperatures near the coast but warmer inland, 2W4 is able to integrate warmer temperatures near the western boundaries of the domain, as opposed to the 1W4 simulation. By allowing more information from the parent domain to be integrated, 2W4 is able to simulate more accurate temperatures over its domain when compared with 1W4. In general, temperatures for both 1W12 and 2W12 are remarkably similar, with minor differences occurring near Galveston Bay. These differences could be attributed to the information 2W12 receives as feedback from the 2W4 domain.

Examining the spatial distribution of RH among the four simulations, it is noted that when comparing 12-km grid spacing, no significant differences occur. The largest
differences are noted when varying the nesting option from one-way to two-way.  1W4 gives larger predictions of RH when compared with 2W4, as well as when compared with 1W12. Values in the Houston-Galveston area in the 1W4 simulation are nearly 5-15% higher than those given by other simulations.

In analyzing the spatial variability in the wind fields, the same phenomenon that was noted in RH is seen here. Generally, differences between the 12-km simulations are small, while differences among the 4-km simulations are more noticeable, especially in terms of magnitude. The overall spatial patterns in 1W4 and 2W4 appear to be captured similarly. However, 1W4 appears to simulate wind vectors that are almost 1 m s\(^{-1}\) lower than those given by 2W4.

As expected from temporal analysis of PBL heights, large differences are found in the spatial distribution of PBL heights between different simulations. Overall, 1W12 and 2W12 perform similarly, as expected. The largest differences are seen when comparing 1W4 with 1W12 and 2W4, as well as 2W12. Simulated PBL heights over the entire domain for 1WAY are several hundred of meters to sometimes more than 1000 meters lower than those simulated by any other setup. 2W4 does simulate lower PBL heights directly along the coast than does 1W4, but those quickly rise to much larger values. This discrepancy is most likely due to the integration of simulated PBL heights from the 2W12 simulation being incorporated simultaneously into the 2W4 simulation. This finding is interesting in that it appears as though errors simulated in the parent domain have quite a large impact on two-way nested domains. Two-way nested simulations from inner domains do not seem to be able to overcome erroneous boundary information.
Vertical distributions of temperature and relative humidity are shown in Figure 5.12. There is little difference between 1W12, 1W4, and 2W12 simulations at any time. 2W4 however, seems to struggle in terms of reproducing the vertical structure for temperature, as well as RH. While surface temperatures are well captured, vertical temperatures appear to be significantly different from 2W4, especially on 30 August and 1 September. While 2W4 does appear to reproduce the overall decrease of temperature with height throughout the boundary layer, it fails to accurately reconstruct stable layers, such as one depicted on 30 August. 1W12 and 2W12 are most accurate when simulating such layers, while 1W4 simulates a stable layer at a lower level than observed values.

In terms of RH, 1W12 and 2W12 do a fairly good job in reproducing the vertical variability in atmospheric moisture. Again, we see a difficulty to reproduce observed values from the 2W4 simulation. 1W4, while simulating more accurate surface RH, is not quite as accurate as either of the 12-km simulations aloft. It is interesting to note that the feedback between 2W12 and 2W4 seems to neither help 4-km simulations nor harm 12-km simulations. From earlier analysis of PBL height, one would expect to at least see similar performance for meteorological variables in two-way nested simulations. However, that is not the case as demonstrated here.

5.2 Chemical Species

Temporal variations of O₃ among the four simulations are shown in Figure 5.13. All four simulations appear to simulate the temporal distribution of O₃ similarly. Very few, if
any, differences exhibited among the simulations are best observed on days three through five. Overall, it does appear as though 1W4 does a better job of simulating nighttime mixing ratios than any of the other simulations. However, overall, all simulations seem to perform very similarly, with significant differences among simulated values occurring rarely.

Given a rather uniform $O_3$ performance similar uniform performance would be expected for $NO_x$ across the board. Temporal distributions of NO and $NO_2$ are shown in Figures 5.14 and 5.15. Overall, the simulations seem to capture the diurnal pattern of mixing ratios of NO fairly well, even if under-predicting occurs during nighttime simulations. Large deviations occur due to the fact that the simulations do not capture the early morning mixing ratios of NO at HALC and C35C. The 1W4 simulation simulates the highest values at most sites, except at GALC, where both 12-km simulations give similar maximum values. None of the simulations appear to capture the very large mixing ratios observed on days one and two at HALC and C35C, perhaps due to uncertainty in emissions from petrochemical plants in the region. Simulations of $NO_2$ mixing ratios are greatly over-predicted by all simulations during nighttime. Daytime simulations are more in agreement with observations, though under-predictions occur most days at most sites. The magnitude of the under-prediction is much lower than the over-prediction of mixing ratios at night. 1W4 simulates much higher values of $NO_2$ than all other simulations at most sites and times, except at GALC, where 2W12 simulates higher mixing ratios.

One variable where there are large discrepancies for model simulated values is CO (Figure 5.16). 1W4 simulates much higher mixing ratios over the entire simulation period than other simulations. These high mixing ratios could be attributable to the very low PBL heights that were simulated over this period. Lower effective mixing volume with the same
concentration of pollutants would lead to much higher mixing ratios. At some times, the mixing ratios are grossly over simulated (> 3000 ppb). On the other hand, all simulations predict lower nighttime values of CO mixing ratios than observations. 2W4 gives values that are more closely associated with observations, though it does over-predict greatly at times, as seen on days four and five at several sites. On the average, there is a net under-prediction of temporal distributions of CO for the 12-km simulations as opposed to the 4-km. However, it would seem as though incorporating two-way nesting for this particular episode is beneficial for CO mixing ratios.

In general, nesting options have less of an impact than horizontal grid spacing on the simulation of PM$_{2.5}$ (Figure 5.17). Simulated values for PM$_{2.5}$ are quite similar at all times and locations for the 12- and 4-km simulations. Irrespective of nesting options, choosing finer or coarser resolutions has larger impacts than that of nesting. This could be attributable to different emissions datasets available at varying resolutions. At times (e.g., day four at GALC), 1W4 simulates concentrations of particulates that more closely associated with observed values. In general, 1W4 simulates only slightly higher concentrations of PM$_{2.5}$ than the other simulations.

Performance statistics outlining the sensitivity to horizontal grid spacing and nesting are shown in Table 5.2. For nighttime simulation of O$_3$, all three simulations significantly over-predict mixing ratios. Of the four simulations, 1W4 performed the best in terms of NMB (42.6%). 1W12 (59.0%), 2W12 (56.7%), and 2W4 (54.4%) all over-predict nighttime mixing ratios of O$_3$ by more than 50%. Daytime simulation is much better among all simulations. The highest value for daytime over-prediction in terms of NMB was 10.5% by 1W12. Comparatively, 2W12 performed slightly better with an NMB of 8.2%. Between
1W4 and 2W4, 1W4 performed moderately better, with an NMB of 3.0% (versus 7.9% for 2W4). Overall, 1W4 simulated more accurate mixing ratios in terms of NMB (18.5%). The other three simulations performed similarly, with NMBs in the mid to upper 20s.

All four simulations exhibit a strong negative bias for nighttime predictions of NO. No simulation performed better than any of the others, as NMBs ranged from -99.7% to -99.8%. Daytime simulation of NO was better simulated using the 2W4 simulation (NMB of 15.5%). Comparatively, 1W4 simulated much higher mixing ratios than other simulations, with a bias nearly four times as high as that of 2W4 (62.7%). 1W12 and 2W12 performed relatively similarly for daytime mixing ratios of NO. Both biases were just under 21%. The dominancy of the nighttime under-predictions resulted in a net negative bias for all simulations. 1W12 and 2W12 performed exactly the same in terms of NMB (-80.0%). 1W4 was most accurate, with an NMB of -59.0%. Also, 2W4 performed on par with the 12-km simulations, with an NMB of -70.8%.

Simulation of nighttime predictions of NO\textsubscript{2} mixing ratios was particularly poor, with each simulation obtaining an NMB of well over 100%. Daytime simulations were much better in terms of NMB. While 1W4 still over-predicted greatly (NMB of 154%), 1W12 and 2W12 simulated values that most represented the observations (NMBs of 18.5% and 13.8%, respectively). While over-predicting significantly, 2W4 still outperformed the 1W4 simulation, with a daytime bias of 75.7%. Overall, biases were dominated by the severe over-prediction of NO\textsubscript{2} at night by all simulations. No bias was less than 100%.

Daytime simulations of CO were over-predicted by 4-km simulations and under-predicted by the 12-km simulations. 2W4 performed the best during daytime with an NMB of 7.6%. Comparatively, 1W4 over-predicted CO values by 64.2%. Biases between the two
12-km simulations were comparable (-47.8% for 1W12 and -45.2% for 2W12). Nighttime simulations showed the same pattern as during the day, with both 4-km simulations over-predicting while 12-km simulations under-predict. The magnitudes of the over-prediction by the 4-km simulations grew larger, while the under-prediction by 12-km simulations decreased. However, 2W4 still performed better than other simulations with a moderate over-prediction of 14.4%. 1W4 greatly over-predicts daytime mixing ratios of CO (71.6%). NMBs for the 12-km simulations were once again quite comparable (-28.6% and -22.1% for 1W12 and 2W12). Overall, 2W4 performs better at simulating daily CO, while both 12-km simulations perform nearly equally at under-predicting daytime mixing ratios. A large over-prediction in the 1W4 simulation could be caused by the low PBL heights simulated during daytime.

1W4 performs the best for both daytime and nighttime simulation of PM$_{2.5}$, though it under-predicts moderately during both time periods (-38.1% and -23.1%, respectively). All simulations under-predict daytime and nighttime concentrations of particulate matter. 1W12, 2W12, and 1W4 all perform comparably for daytime and nighttime predictions, with biases nearly -40% during the day and larger than -22% during the night. Overall, 1W4 over-predicts less than the other three simulations (-21.5%). Interestingly, no significant differences are observed for different horizontal grid spacings using two-way nesting. Nor are there any major differences between using a two-way nesting option and a non-nested 12-km (1W12) simulation (-33.1% vs. -31.6%, respectively).

The spatial distributions of O$_3$, NO, NO$_2$, CO, and PM$_{2.5}$ are shown in Figures 5.18 through 5.22, respectively. Examining the spatial distribution of O$_3$ mixing ratios, one can see that the four simulations perform relatively similarly in terms of magnitude and
horizontal transport. Major differences can be seen between 1W4 and 2W4 in the magnitudes of the mixing ratios west of Galveston Bay. 2W4 simulates values that are generally near 18 to 24 ppb higher on average near the west edge of the 4-km domain. This may be attributable to the feedback between 2W12 and 2W4, as opposed to 1W4 being driven entirely by output from 1W12. Spatially, it could be claimed that two-way nesting has more of an impact on the simulations of the finer domain than simply running a finer-scale simulation driven by coarse simulation output.

All simulations give rather uniform distributions of NO mixing ratios across all domains. If we examine closer the differences between 2W4 and 1W4 for separate days, we notice that simulated mixing ratios vary significantly on one day (30 August) and not quite as much on the second (31 August, not shown). If we then examine the simulated values from both 12-km simulations, we see that both have exceptionally similar distributions on both days. It is possible that simulated values along the border between Louisiana and Texas have a stronger impact when factoring in the feedback mechanism for two-way nesting, rather than using such values for boundary conditions in a one-way nesting simulation. Regarding NO2, 1W4 simulates mixing ratios that are much higher than those given by any other simulation. Overall transport seems to be treated similarly, regardless of nesting option or grid spacing.

When examining distributions of CO, it is interesting to note the similarity between 1W12 and 2W12 in the simulation of chemical species. Though we would expect simulated values to be relatively similar due to consistent model physics and chemistry, the impact of feedback from the nested grid appears to be mostly negligible at most places within the area of interest. Simulated values from 1W4 are much higher than those simulated in other simulations. It is most likely that this is the case due to significantly different predictions of
the boundary layer height in this area. If we compare the simulated PBL depths (see Figure 5.11) as we look at CO (see Figure 5.21) mixing ratios, we see that while both 1W4 and 2W4 seem to handle well the point of origin for CO, the transport and dispersion are different. The most likely cause for this would be the significant differences in simulated PBL depth and wind vectors in and around the Houston-Galveston area.

The distribution of simulated concentrations of fine particulates are handled relatively similarly among all four simulations. The effect of horizontal transport is quite clear, though greater information is inferred when examining the 4-km simulations. Differences between the two 12-km simulations are relatively negligible, but observable differences exist between the two 4-km simulations. Spatially, 1W4 simulates higher concentrations of PM$_{2.5}$ than does 2W4, especially in localized areas surrounding Houston.

The vertical distributions of O$_3$, CO, NO, and NO$_2$ from each model simulation are examined (Figures 5.23 through 5.26, respectively). For O$_3$, there are significant discrepancies between simulations at 4-km and those at 12-km. Simulations at 4-km tend to show a less uniform decrease in mixing ratios with height than those at 12-km. However, 2W4 is significantly different in terms of lower level mixing ratios when compared with 1W4. 2W4 gives significantly larger mixing ratios up to 250 m than any other simulation. Differences at that level from other simulations range from 25 to near 70 ppb.

The overall distributions of NO and NO$_2$ appear to be well reproduced by the one-way nesting simulations (1W12 and 1W4). The simulations utilizing two-way nesting do not appear to capture vertical mixing ratios as well as the one-way simulations. The vertical variation of the simulated mixing ratios is similar to that observed, even if magnitudes of NO and NO$_2$ are not simulated as well. Although 2W12 and 2W4 have much higher surface
values, but they decrease rapidly with height; signifying that vertical processes are well-handled for both. 2W4 is a little faster when decreasing mixing ratios of both NO and NO₂ to their upper-level values of near zero. The difference, however, is not exceptionally significant.

Vertical distributions of CO are mostly similar among the four simulations, though both 1W4 and 2W4 have to overcome the larger values simulated at the surface. These higher surface values are consistent with what was observed in temporal analyses and their associated statistical biases. Distributions of CO are simulated to be uniform at any level above 500 meters at each time for each simulation. This value is near 80 ppb lower than the observed values aloft from aircraft. However, the uniform distribution of CO in the atmosphere is mostly due to the model initialization, setting CO mixing ratios aloft equal to near 70 ppb.

5.3 Computational Cost

Table 5.3 shows the CPU cost for the four simulations when analyzing the sensitivity to grid spacing and nesting options. It should be noted that differences exist in the execution of the simulations. More specifically, when performing a one-way nesting sensitivity study, it was necessary to perform two separate simulations; one for the coarse 12-km simulation and another for the one-way nested 4-km simulation. However, when performing the two-way sensitivity, both the 12-km and 4-km simulations are occurring simultaneously, making
it a little more difficult to compare. For this reason, we will present the times for the one-way nesting as a sum of both simulations when comparing to two-way nesting.

The one-way simulations were faster than two-way simulations by 6.8 minutes per simulation hour on average. Using one-way nesting, a 1-hour simulation was completed in 25.4 minutes and a daily simulation in 10.16 hours, while two-way simulations took 32.2 minutes and 12.88 hours, respectively. For a five-day simulation as presented here, the extra time in running a two-way nested simulation would result in an increase of 13.6 CPU hours (26.8%). While utilizing two-way nesting could be beneficial to atmospheric modeling, the increased CPU cost for this particular episode does not appear to be worth the minor differences seen in simulated values for meteorological variables and chemical species.
Table 5.1. Performance statistics for: (A) T2, RH, and PBL height, (B) WSP and WDR, and (C) U- and V-vector components for the 1W12, 1W4, 2W12, and 2W4 simulations.

A.

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Acronyms: 1W12 – one-way 12 km; 1W4 – one-way 4 km; 2W12 – two-way 12 km; 2W4 – two-way 4 km
Table 5.1 (continued). B.

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Table 5.3. Computational cost for the 1W12, 1W4, 2W12, and 2W4 simulations on a per hourly simulation and daily simulation basis.

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*Acronyms:* 1W12 – one-way 12 km; 1W4 – one-way 4 km; 2W12 – two-way 12 km; 2W4 – two-way 4 km
Figure 5.1. Temporal distributions of temperature at two meters (T2) at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.2. Temporal distributions of relative humidity (RH) at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.3. Temporal distributions of wind speed at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.4. Temporal distributions of wind direction at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.5. Temporal distributions of U-component vectors at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.6. Temporal distributions of V-component vectors at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.7. Temporal distributions of PBL height at Wharton (WHAR), Ellington Field (ELLF), Houston Southwest (HSWH), Liberty (LBTY), and LaMarque (LMRQ).
Figure 5.8. A comparison of spatial distribution of $T_2$ between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 22 UTC (3PM CDT) 30 August 2000.
Figure 5.9. A comparison of spatial distribution of relative humidity (RH) between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.10. A comparison of spatial distribution of the wind fields between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.11. A comparison of spatial distribution of PBL height between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.12. Vertical profiles of temperature (left) and RH (right) compared with observations from NOAA’s Electra aircraft instrumentation.
Figure 5.13. Temporal distributions of O$_3$ at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.14. Temporal distributions of NO at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.15. Temporal distributions of NO$_2$ at Aldine (HALC), Bayland Park (BAYP), Clinton (C35C), Galveston Airport (GALC), and Deer Park (DRPA).
Figure 5.16. Temporal distributions of CO at Aldine (HALC), Clinton (C35C), Deer Park (DRPA), Crawford (HCFA), and LaPorte (H08H).
Figure 5.17. Temporal distributions of PM$_{2.5}$ at Houston East (HOEA), Galveston Airport (GALC), Deer Park (DRPA), Conroe (CONR), and LaPorte (H08H).
Figure 5.18. A comparison of spatial distribution of O$_3$ between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.19. A comparison of spatial distribution of NO between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.20. A comparison of spatial distribution of NO$_2$ between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.21. A comparison of spatial distribution of CO between (from left to right) 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.22. A comparison of spatial distribution of PM$_{2.5}$ between (from left to right), 1W12, 1W4, 2W12, and 2W4 at 20 UTC (3PM CDT) 30 August 2000.
Figure 5.23. Vertical distribution of O$_3$ compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 5.24. Vertical distribution of NO compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 5.25. Vertical distribution of NO$_2$ compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
Figure 5.26. Vertical distribution of CO compared with observations from NOAA’s Electra aircraft measurements on 28 and 30 August and 1 September 2000.
6.1 Summary

The Weather Research and Forecast model with Chemistry was successfully applied for the TexAQS-2000 episode for 28 August – 2 September. An analysis was performed of model simulations with various planetary boundary layer (PBL) parameterizations and land surface modeling (LSM) schemes available in a recent version of WRF (v. 2.1.1). Simulations with two PBL schemes, Yonsei University (YSU) and Mellor-Yamada-Janjic (MYJ) TKE closure, were conducted to study the sensitivity to PBL schemes. Simulations with three LSM schemes, NOAH, slab, and RUC were conducted to study the sensitivity to land surface models. Additional simulations were conducted to analyze the capability of the model to accurately simulate predictions using various grid resolutions and nesting options. In this study, two horizontal grid spacings, 12- and 4-km, both with one- and two-way nesting options were used. One-way nesting involves using output from a coarse simulation to serve as input for a finer-resolution simulation, while two-way nesting involves feedback from one domain to the other and vice versa.

In terms of PBL sensitivity, the N_Y pairing using the NOAH LSM and YSU PBL scheme performed better in terms of surface temperature (T2) and wind speed, while the N_M pairing using the NOAH and MYJ schemes performs better at simulating surface RH, as well as PBL height. Temporally, N_Y simulates higher values for T2 when compared with N_M, though N_M simulates slightly higher values for surface RH. Both simulations comparably capture wind speed and direction, as well as U- and V-vector components. The
largest difference in temporal meteorology among the two simulations is that of PBL depth. N_M simulates a much more accurate depiction of the PBL in terms of height, while N_Y simulates values which are much higher than those observed.

In terms of chemical predictions, N_M simulates O_3 and CO more accurately than N_Y, which reproduces PM_{2.5} better. Temporally, N_M over-predicts daytime maximum O_3 to a lesser extent than N_Y. Neither simulation is found to capture the chemistry of nitrogen species very well, as N_M simulates higher values for NO, while N_Y simulates higher values for NO_2. One explanation for this is that the emissions of nitrogen species are too coarse for these simulations and may not be represented accurately. In terms of temporal variation of fine particulate (PM_{2.5}) between simulations, there appears to be only minor differences.

Spatially, the schemes performed quite similarly in terms of meteorological variables and chemical species. The largest difference was in the simulation of PBL depth, as N_M simulated values that were generally much lower over the Houston-Galveston area when compared with N_Y. In general, the chemical species were captured quite similarly on a spatial scale by both simulations.

Vertically, the largest differences were noted in the vertical variability of chemical species. Differences in the amount of mixing in the PBL schemes may be the cause of differences. Greater mixing in the vertical would lead to more uniform mixing ratios and concentrations.

LSM options within WRF allow for a little broader study of the sensitivity to such schemes. In terms of meteorological variables, the S_Y pairing using the slab LSM and YSU PBL simulates PBL height, RH, and wind speeds more accurately than either of the other
schemes. Both R_Y (RUC and YSU pairing) and N_Y simulate surface temperature equally well, as S_Y shows a significant cold bias over the simulation period of -4.1%. Temporally, S_Y exhibits a significant cold bias when compared with the other two simulations. This is most likely due to differences in simulated surface sensible heat flux among the three simulations. Differences in T2 could also be associated with those for RH, where S_Y gave much higher and more accurate values. Heat fluxes also seemingly played a role in differences for PBL depth. Lower sensible heat fluxes allowed for the decreased growth of the boundary layer in the S_Y simulation as compared with the others.

Spatial examinations also revealed the differences among the model simulations for T2, RH, and PBL height, as S_Y simulated lower values over the entire domain for T2 and PBL height, while giving higher values for RH as compared to N_Y. Differences in the simulated wind fields were minimal.

For chemistry, S_Y simulates O_3 and CO more accurately than either N_Y or R_Y. It should be noted that temporal analyses revealed that R_Y and N_Y over-predicted nighttime mixing ratios of O_3, while S_Y under-predicted. The more accurate representation of the nocturnal boundary layer is partly attributable for better nighttime representation of O_3 mixing ratios. CO mixing ratios appear to have been mostly overestimated by all three simulations. PM_{2.5} concentrations are predicted fairly similarly in all simulations until day four at most locations, when S_Y appears to give much higher values. However, PM_{2.5} concentrations are more accurately captured by R_Y, in terms of normalized mean bias (NMB). Again, the errors are obvious surrounding nitrogen-chemistry for this particular episode.
Spatially, the largest differences in terms of chemical species are seen in simulated O$_3$ and CO. N_Y simulates much higher mixing ratios of O$_3$ over the entire domain than the other two simulations, while CO mixing ratios are generally simulated higher over the domain by the S_Y simulation.

The most noticeable difference in terms of vertical mixing ratios of chemical species is in terms of their vertical variability. All three simulations yield similar values, with only minor differences occurring in their vertical profiles. There is a tendency for one simulation (none in particular) to differ slightly in terms of height at which values begin to vary.

Temporal variations for nesting (1- or 2-way) and grid-spacing sensitivity revealed that in general, all simulations appeared to perform similarly, though 4-km simulations appear to simulate temperatures which are slightly cooler than the 12-km simulations. Surface RH was more accurately represented in the 1W4 simulation, while 2W4 simulated values which were the lowest of the four simulations. Differences in wind fields were relatively minor. It is interesting to note that the 1W4 simulation gave much more accurate values of PBL depth when compared with other simulations. Neither the 12-km simulation nor the 4-km two-way nesting simulation gave accurate representations of PBL depth when compared with 1W4. When examining the effects of nesting and horizontal grid spacing on meteorological variables, it was found that the effects of nesting are more apparent on some variables than others. For example, the effects of nesting were more noticeable in examining 1W4 and 2W4, as the simulation with two-way nesting gives a more accurate prediction of surface temperature.

Spatially, differences among the simulations are most noticeable when examining RH and PBL height. 1W4 gives much higher values of surface RH and lower values for PBL
height when compared with other simulations. Possibly, the feedback between 12-km and 4-km using two-way nesting has some impact on simulated values. Seemingly, surface sensible heat flux among the four simulations would be similar when utilizing the same LSM. However, this has not been examined yet.

Vertical variations of meteorological parameters are mostly similar for 1W12, 1W4, and 2W12. However, 2W4 appears to have some issues with simulating values in the vertical. Typically, 2W4 follows a pattern that is, at times, opposite from the other three simulations. No significant explanation for this phenomenon has been determined at this time.

Chemically, noticeable differences were seen when using two-way nesting and one-way nesting. \( \text{O}_3 \) was better represented by the one-way nested simulation at 4-km, while \( \text{CO} \) was better simulated using 2W4. 1W4 also simulated \( \text{PM}_{2.5} \) more accurately when compared with 2W4. This indicates that the more computationally rigorous method of simulating with two-way nesting does not always lead to more accurate simulated values.

The spatial distribution of chemical species reveals that 2W4 simulates higher values over the domain as compared to the other three simulations. In general, spatial distributions of nitrogen species are typically handled similarly among all four simulations, with only minor differences seen, which could be attributable to minor differences in horizontal transport. 12-km simulations of \( \text{CO} \) appear to be quite similar between one- and two-way nesting, with more noticeable differences occurring between the 4-km simulations. 1W4 seems to simulate slightly higher values over a broader spatial scale when compared with 2W4. Because \( \text{CO} \) is a long-lived species, these differences could be attributed to differences in simulated transport. Spatial distributions of fine particulates show that once again, the
largest differences appear to occur between one- and two-way nesting at 4-km. 12-km simulations show that no appreciable differences exist, but 1W4 simulates higher concentrations when compared with 2W4.

The aforementioned issues with 2W4 and vertical simulations are also noted in the vertical distributions of chemical species. In general, there appears to be greater issues with two-way nesting and chemical species in the vertical, as neither 2W12 nor 2W4 appeared to perform similarly to the one-way nested simulations. Further investigation of differences between one- and two-way nesting simulations is required.

Computationally, there appears to be no great benefit in choosing between different physical parameterizations. More or less, the decision to choose a certain parameterization remains a personal or episode-specific preference. No large differences were found between any of the simulations in terms of CPU time, with the largest differences being a matter of minutes.

However, differences were more apparent when utilizing one- or two-way nesting. Generally, the 4-km simulations were similar with 12-km in terms of CPU efficiency. Two-way nesting took nearly 7 minutes longer (26.8%) per simulation hour, which is equivalent to more than a total of 13 hours extra for this particular 5-day episode. Because of the relatively minor differences in terms of simulated meteorology and chemistry, with no appreciable benefit, two-way nesting was not computationally efficient for this particular episode.
6.2 Conclusions

A summary of the statistics for this episode are shown in tables 6.1 and 6.2. For this particular episode, in terms of meteorological variables, the simulation pairing the slab LSM with the YSU PBL scheme performed with the lowest level of overall bias in terms of statistical parameters. This is best illustrated in Table 6.3. It can be noted that S_Y slightly under-predicted temperature while slightly over-predicting wind speed and RH and moderately over-predicting PBL height.

Similarly, the 1W4 simulation performed better than the others in terms of overall statistical bias for meteorological variables. The 1W4 slightly under-predicted temperature, RH, wind speed, and PBL height. The other three simulations all seemed to perform similarly.

In terms of chemical species, the S_Y was the best in terms of overall statistical bias (see Table 6.4). Though all simulations have problems simulating NO\textsubscript{x} chemistry, S_Y did an overall better job with other species (O\textsubscript{3}, CO, and PM\textsubscript{2.5}).

For the sensitivity to grid spacing and nesting options, the 12-km simulations performed better than both 4-km simulations overall. The differences among the four simulations exist in the simulation of CO. Both 12-km simulations moderately under-predict CO mixing ratios, while both 4-km simulations greatly over-predict. In terms of other chemical species, all simulations performed similarly overall.

In general, the use of more physically complex meteorological schemes did not give more accurate results. The simple slab scheme paired with the YSU scheme performed more
accurately than either the NOAH or RUC LSMs. However, CPU time for the less physically complex simulation was slightly higher than others.

Overall, the use of nesting and finer horizontal grid spacing showed no appreciable benefit for this episode. Finer horizontal grid spacing served to increase CPU time (likewise for nesting options) rather than improve model performance. At this time, it cannot be recommended to implement nesting for use in simulating more accurate atmospheric chemistry. More research is needed into the effects and benefits of nesting before accurate implementation can commence.

6.3 Limitations

There are several limitations associated when performing sensitivity studies of meteorological and chemical species using the WRF/Chem modeling system. First, this is a region-specific analysis, giving results that may or may not be indicative in other areas of the United States. The Houston-Galveston region in Texas is an extremely geographically-complex area. The Gulf of Mexico provides warm, moist onshore flow on a daily basis. Galveston is also one of the busiest areas in terms of oil refinery services. This allows larger values of O$_3$ precursors to be emitted into the air of an already populous and polluted city.

Secondly, the emissions data used to simulate the sensitivities to horizontal grid spacing and nesting were not originally derived for use with the RADM2 + MADE/SORGAM chemistry pair. Calculations were used to convert particulates and the necessary gaseous species over to be more compatible with the chemistry modules used in
this study. For this reason, simulations of chemical species for the third analysis may not be entirely accurate.

A third limitation for this particular work is the use of an older version of the WRF/Chem code. Theoretically, updates from version 2.1.1 to the most recent version (2.2) would provide upgrades in terms of simulated meteorological variables and chemical species.

The limitations of using the aircraft observations to compare with grid-averaged simulated data should also be noted. The time-scale on which the measurements were obtained differs significantly from the time-resolution of the model output. Also, we are comparing a mobile measurement to a point-specific location using a rudimentary averaging method. The implementation of a more accurate method of comparing aircraft observations to model data may lead to better results.

Another limitation that should be discussed is the comparison of point-specific data to grid-averaged simulated values. For example, the simulations derive a value representative of a 12-km by 12-km grid box. The model assumes this value to be the average over the entire area. However, observational data is representative of a specific point within that grid cell. Some implications of grid averaging could be seen if a specific point observation is lower than the grid. This could be attributable to areas within the grid box that bias the grid average higher.

Lastly, we should take into account limited observational data, especially in terms of co-located meteorological and chemical measurements. For instance, PBL height observations were made at locations where no measurements were made for meteorological variables or chemical species. The lack of co-located information makes it difficult to come
to accurate conclusions based on PBL height data in terms of meteorological variables and chemical species.

### 6.4 Future Work

The processes that govern the surface and boundary layers are still not totally understood. Likewise, the simulation of atmospheric chemistry is quite an arduous task that is still under development. The abundance of chemical reactions that occur in the lower atmosphere makes accurate simulation of chemistry difficult. Further studies should incorporate more upper-level data to allow for better understanding of vertical processes that affect transport and distribution of chemical species.

The schemes used in this study are still in wide use today, though they are slightly aged. The development of more physically-intensive schemes with more accurate atmospheric dynamics may lead to more accurate simulations of meteorological variables. The accurate implementation of physical parameterizations in coupled meteorological-chemistry models is imperative to achieve accurate predictions of chemical species.
Table 6.1. Statistical summary (in terms of NMB) of meteorological variables for all simulations.

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Table 6.2. Statistical summary (in terms of NMB) of chemical species for all simulations.

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Table 6.3. Graphical summary of meteorological variables for all simulations.

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Table 6.4. Graphical summary of chemical species for all simulations.

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