Review of the manuscript titled “The impact of observation nudging on simulated meteorology and ozone concentrations during DISCOVER-AQ 2013 Texas campaign” By Xiangshang Li et al. Submitted to the ACP

Recommendation: minor revision

General response:

Thanks for the very helpful comments. We think the reviewer's comments are based on an earlier version (v1) of the manuscript. The version in discussion (ACPD) has added several missing references pointed out by the reviewer. It also has several new plots which we think are better than old version (please refer to uploaded updated manuscript according to the first reviewer’s comments too). Also there are enough differences from v1 such that the line number changed substantially. In this response, we will refer to the version in ACPD regarding to line number through keeping the original line number in item title.

1. Comments Line 11-12, it is confusing to say observational nudging is objective analysis and to use “OA” representing observational nudging for the rest of the paper. In the WRF modeling community, objective analysis usually refers to “OBSGRID” which is an extra package in the WRF model system to take observations to improve the first guess fields (WPS output files) through an objective analysis method. Observational nudging is the Newtonian relaxation method implemented in WRF code to use observations to minimize model error during the simulation. It is known as “four-dimensional data assimilation (FDDA)” introduced by Stauffer and Seaman (1990). The observational nudging is not necessary to be run with objective analysis package even though the OBSGRID provides the observational data written in required by WRF for nudging. Stauffer, D., Seaman, N.L., 1990. Use of four-dimensional data assimilation in a limited area mesoscale model. Part I: Experiments with synoptic-scale data. Month. Weather Rev. 110, 1250-1277.

Reply: Thanks for pointing out the issue. We understand the differences between "objective analysis" and "observation nudging". In WRF, to perform obs-nudging, one has to use OBSGRID (Objective Analysis) to generate necessary input. As seen in the flow chart of OBSGRID (usually on page 7-2 of WRF-ARW User's Guide), after OBSGRID is run, three types of output files (metoa_em for OA, wrfsfdda for surface analysis nudging and OBS_DOMAIN for
obs-nudging) are generated and all of them are to be used. This is because performing three tasks (OA+sfdda+obs-nudging) can maximize the benefit of assimilating observations. Therefore, running OBSGRID tends to imply performing all three tasks. Although one can do obs-nudging without performing OA (i.e., discard "metoa_em"), this should not be considered normal since it is likely degrade WRF performance.

To address the issue, we made two changes. We

1) included an explanation on objective analysis and obs-nudging in introduction (line 65-75) and clarified the case names in section 2.2

2) changed all the OA in paper to “obs-nudging” except for case names. Using “OA” and “No-OA” as case name seems easier.

2. Line 70-71, what does this mean?? There are detailed statistics about the nudging impacts shown in those studies (Deng 2009, Gilliam and Pleim 2010, Otte 2008 and Ngan et al 2012).

Reply: The sentence is about the studies by Ngan et al. (2012), Deng (2009), Gilliam and Pleim (2010), which only have statistics for meteorological variables, none for chemical variables. Only Otte (2008) includes the chemical statistics in her paper.

It should be rewritten as:

“However, the statistics from their study cannot be used for interpreting the sensitivity of obs-nudging since its base WRF case is a forecast run which used a different analysis input “ – line 90-91

3. Line 91, Daum et al., 2004

Reply: Thanks. typo, corrected

4. Line 96, missing reference for Lefer and Rappengluck 2010. Olaguer et al., 2009

Reply: Thanks. missing in v1, already corrected in online ACPD version
5. Line 103, it is good to have a citation for DISCOVER-AQ.

*Reply: we added a link to the DISCOVER-AQ website (from which all the data were collected)*

6. Line 141-143, suggesting not to use “OA” to refer observational nudging. Instead, just use “no-FDDA” vs. “FDDA”

*Reply: Because the base case performed the “standard” grid nudging, so it did use “FDDA”. Hence it seems “no-FDDA” is not proper for base case. Please see our revisions outlined in item 1 reply.*

7. Line 171, give citation for those prior modeling studies.

*Reply: added citations.*

8. Line 202-224, these three paragraphs should be shortened since this is not project report and technical note. Please summarize what are the data frequency for analysis nudging, surface nudging and observational nudging, what variables to be nudged, and for what vertical layers.

*Reply: Thanks for the suggestions. Modified (shortened) as suggested.*

9. Line 242, missing reference for Willmott 1981

*Reply: Thanks. Added.*

10. Line 306, it is more desirable to see time-series of hourly temperature and ozone instead of daily average since both variables have strong diurnal variation. What did the authors choose to show the daily average plots?

*Reply: In the past we usually use daily average plots to check some important meteorological and chemical features during the simulated period, but we agree with reviewer’s point and replaced the daily time series with hourly time series.*
As a result, all the texts related to the two plots are modified. Updated figure 3 and 4 are shown below.

11. Line 378, Figure 7 is hardly to read due to poor figure quality and small text.

Reply: Thanks. Already changed in ACPD online version, should be OK now.

12. Line 394, it should be showing hourly ozone plot instead of daily average. There are a lot variations for ozone through a day.

Reply: Thanks. We replaced the plot as the reviewer suggested.
13. Line 484, Did the nudged met. data provide better ozone results than the base case in the comparison with aircraft measurements?

Reply: Yes, the nudge case is better. In the two plots (Fig 11 and 12), we showed spatial ozone for base case as background. Fig.11 is intended to show the high ozone aloft in early morning, which contributed to later model’s underprediction. The comparison of model vs aircraft ozone is given in Figure 13 and 14.

14. Line 487, missing reference for Li and Rappengluck 2014

Reply: Thanks. added in ACPD online version

15. Line 500, the model under-predicted ozone both at the surface and aloft on Sep 25th. Even with nudged meteorology, there was not much improvement. Is that because the met data are still wrong or emission data may have problem?

Reply: We think that the missed high ozone on Sep 25th is a combination of transport (high observed ozone aloft in early morning), not-so-good meteorology even after nudging (even though we show some improvements in this study), and possibly unreported emission upsets.

We already identified a problem in current WRF OA process and developed new processes to correct the problem and results are surprisingly good. In the paper, the ongoing study is briefly mentioned in the last section.

16. Line 543-548, the discussion about the impact of nudging on cloud/precipitation prediction is ambiguous. There is no comparison on these two variables shown. Did the nudging configuration help to prevent the inaccuracy of the prediction or make it worse?

Reply: We felt compelled to mention cloud/precipitation since they heavily impact ozone and performing obs-nudging certainly altered the two variables (despite that nudging coefficient is set to zero for moisture). Yet we do not have good observations to quantitatively analyze the changes brought by obs-nudging. It entails another study to analyze the impact of nudging on cloud/precipitation and how ozone might be ultimately affected.
17. Line 555, what does this “small-scale meteorological events” refer to? In what sense it is relevant to the high ozone events? Is this something for future works? The conclusion section is not clear. Suggest to revise and include future works.

Reply: Thanks for your suggestions. Small-scale events are discussed briefly in first paragraph of page 5(27361) of ACPD online version, with a few references. The conclusion section has been substantially modified in the online version. We value the comment and added future works.

The last section of Discussion now reads:

“Small-scale meteorological events are frequently cited for their contributions to high ozone events. Model’s capability in reproducing these events is critical in simulating such high ozone episodes. The base case did not recreate the 25 September small-scale events likely due to the complex winds and a lack of local information which can be used to steer model state closer to reality. On the other hand, the inability of the sensitivity case to replicate the local winds is likely a result of the imperfection of the nudging process pending further investigation. An ongoing study by the current authors suggests that errors in the metrological fields from the default grid nudging files are important sources. Methods are being tested to improve the quality of grid nudging files. Early results showed that the bay breeze which caused the wind reversal around La Porte was well captured through improved grid nudging files. In addition, more observational data (e.g., more sites and higher data frequency) and more testing on the combination of nudging setting should help improve the obs-nudging performance. Also, the impact of obs-nudging on precipitation and clouds should be further investigated to understand their chain effect on chemistry.”
Reviewer 2

Original comments by reviewer 2:

Specifically, the sentences are ambiguous, incomplete, and awkward throughout the text. One has to go over several times for many sentences to guess what the authors are trying to say. The amount of corrections needed is beyond what a reviewer can suggest in details. I am listening a few typical issues below.

***

It should have been clearly stated early on what exactly the study is trying to accomplish; what variables they “nudged” exactly, and what results they examined. A reader should not have to read through all the details of the model setups to find out what variables they actually “nudged”. Statements such as “. . .the impact of OA on the simulated meteorology and ozone concentrations. . .” or “. . . indicated that OA improved the timing of wind transition . . .”, are throughout the paper without indicating OA on what, or nudging what.

Another issue is that this manuscript was not written for more general readers, terminologies were used without providing background. They never explicitly explain the connection between WRF and CMAQ before using WRF-CMAQ. The terms nudging and OA were used interchangeably without explaining the differences.

***************

General response:

*We thank the reviewer for his/her input. As for scientific significance, we think the paper has several findings not seen before in the previous studies (regarding more detailed impact of objective analysis on meteorology including temperature, winds and PBL height and chemical concentrations of ozone). And these findings are important for later works in their effort to improve the WRF’s nudging process. In the revised manuscript, we worked to clearly explain about how the objective analysis improved the performance of WRF and WRF-CMAQ simulations. For example, we showed how the nudging process improved the meteorology and chemical concentrations on the 25 September (Our group worked as air quality*
forecasting group for DISCOVER-AQ project performed in Houston in September of 2013. As we authors acknowledged, none of the previous forecasting/modeling exercises from a few modeling groups couldn’t make a reasonable simulation of ozone on September 25).

In this study, we showed that objective analysis approach significantly improved meteorology for September and it also improved chemical concentrations of ozone, but the order being improved is smaller than that of meteorology. Further, we discussed what would be another cause for the uncertainty in the ozone simulation.

On the language issue, we acknowledge the paper was heavy and occasionally hard to follow. As the reviewer suggested, we, authors did proofread all the text again and rewrote/modified the significant amounts of the contents from the beginning to the end and we believe now that the English issue the second reviewer suggested was resolved. For example, over a hundred changes have been made from abstract to conclusion of the revised manuscript.

Itemized response:

Since the reviewer’s comments are not with line numbers, we try to respond as best as we can.

1. One of the major concerns is the contribution of the paper to science. Here we elaborate a few points.
   a. Meteorology is the foundation for emission and chemistry studies. Without a good set meteorology when studying real-world air quality, one can hardly draw conclusions with. As we addressed above, a good example is the 09/25 episode discussed in the paper, we still cannot say whether an emission event or unknown large-scale transport played major roles because meteorology is not well simulated. It was our motivation for this study in the beginning.
   b. FDDA is a critical tool in improving model performance in meteorology modeling. A large portion of performance gain in the last 30 years came from FDDA. Objective analysis (OA) and observation nudging are critical methods in FDDA.
   c. We have not found any paper providing a quantitative sensitivity study on the possible performance gain from OA and observation nudging on both meteorology and chemistry. Ngan et al. (2012) is the closest in
it evaluating both meteorology and chemistry yet it is not a sensitivity study on obs-nudging.

d. We have not found any other air quality study performing 1-hr observation nudging.

e. More importantly, the paper provided an example showing the failure of model to replicate the high ozone even after OA and observation nudging are performed. Implicitly, this means that trying different physical schemes is unlikely to solve the issue (we did test a few cases although this statement largely came from our years experience in air quality modeling). This begs for the question: what can we do to recreate the right meteorology so that we can produce high ozone in chemistry model? As we addressed in the discussion of the revised version, we have been working to develop a novel technology (a new nudging process) to address the issue (preliminary results are surprisingly encouraging).

f. We evaluated model PBL and ozone aloft to study the model sensitivity to obs-nudging and OA – which we have not seen before.

2. About nudging technique and related terminology.

a. The authors expected the readers to have basic knowledge on FDDA and nudging, i.e., what is nudging, what it for is, etc. We didn’t provide further explanations on certain details due to the large size of the revised manuscript. However, we added some explanation in the revised version, e.g., FDDA in line 49-50, Objective Analysis in line 70-72.

b. We have updated the manuscript to clarify the terminology, especially what we did in addition to standard grid nudging. We assimilated observations from various sources into the simulation. WRF has a separate program “OBSGRID” to perform objective analysis (OA) and create input for observation nudging. Therefore, performing OA generally means doing observation nudging simultaneously to make the most use of observations. However, the term “OA and observation nudging” is too cumbersome. Therefore, in revised manuscript, we used “observation nudging” and explained that it means the combined “OA and observation nudging” – line 72-75.

The changes on obs-nudging and OA are reflected throughout the text.
c. OA is to improve first guess meteorology analysis by incorporating observations – we included this statement in the revised version, line 70-72.

d. WRF observation nudging is performed on 4 variables, U, V, T, Q (water vapor mixing ratio), line 228-229. The default is nudging all. For grid nudging, there are two extra variables (geopotential and dry column mass) inside a grid nudging file, although there is no explicit control on the two variables in the namelist. There are concerns with nudging T and Q in some occasions that they may be turned off.

In original manuscript, we already stated we did not perform grid nudging on mass fields (T and Q) inside PBL, line 199-200. Also there is no observation nudging for “Q”, line 229-231.

3. WRF-CMAQ and OA/observation nudging
   a. We changed “WRF-CMAQ” to “WRF and CMAQ”, line 21.
   b. We explained the difference between OA and observation nudging. OA is to improve first guess meteorology analysis by assimilating observations, which is to improve the quality of analysis nudging. Observation nudging is to nudge model state toward observations at measurement locations – line 65-72.

4. The language issue

   We have done a major overhaul on the language part to improve the readability, with input from several co-authors. As one can see from the track-change version, many changes were made. This is in addition to the modification suggested by the handling editor, reflected in the ACPD version.

   We also made better plots to assist readability.

   We agree that the paper is not a light read and it has much information, especially on the 25 September, the high ozone day. We think most of them are quite relevant but did trim some contents, such as the ozone description on the 26th.
The impact of observation nudging on simulated meteorology and ozone concentrations during DISCOVER-AQ 2013 Texas campaign

Xiangshang Li¹, Yunsoo Choi¹, Beata Czader¹, Anirban Roy¹, Hyuncheol Kim²,³, Barry Lefer¹, Shuai Pan¹

¹Department of Earth and Atmospheric Sciences, University of Houston, Houston, TX 77204, USA
²NOAA Air Resources Laboratory, College Park, MD 20740, USA
³University of Maryland, Cooperative Institute for Climate and Satellite, College Park, MD 20740, USA

Corresponding author: Xiangshang Li: xli@central.uh.edu

Abstract

Air quality modeling demands accurate meteorological simulations; fields are imperative for correct chemical transport modeling. Observation nudging, also known as objective analysis (OA), is generally considered as a low-cost and effective technique to improve meteorological simulations. However, the meteorological impact of OA observation nudging on chemistry has not been well characterized. This study involved two simulations (with/without OA) to analyze the impact of OA observation nudging on the simulated meteorology and ozone concentrations during the 2013 Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) Texas campaign period in September 2013, using Weather Research and Forecasting (WRF) and Community Multiscale Air Quality (CMAQ) models. The results showed improved correlations between observed and simulated parameters from the OA sensitivity case. The index of agreement (IOA) improved by about 9% for surface temperature and 6-11% for surface zonal (U-WIND) and meridional (V-WIND) winds when
OA observation nudging was employed. Analysis of a cold front event indicated that OA improved the timing of wind transition during the front passage. Employing OA observation nudging also reduced the model biases for the planetary boundary height predictions. For CMAQ simulated simulations, the IOA improved by 6% in the sensitivity case for surface ozone during the whole simulation period, IOA improved by 6% in the OA case. The high ozone episode on September 25th was a typical post-front ozone event in Houston. The small-scale morning wind-shifts near the Houston Ship Channel combined with higher aloft ozone from recirculation early morning likely caused the day’s ozone exceedance. While OA observation nudging did not recreate the wind shifts on that day and failed to reproduce the observed surface and aloft-high ozone, analyses of surface and aircraft data found that OA results matched better with observation observation nudging helped model to yield improved ozone predictions. In a two-hour period during the event, substantially better winds in OA the sensitivity case noticeably improved the ozone. Further work on improving OA’s the capability of nudging to reproduce local meteorological events could enhance a chemical transport model’s ability to predict high ozone events.

Keywords: WRF, CMAQ, air quality model, DISCOVER-AQ, observation nudging

1. Introduction

Accurate meteorological simulations are essential to photochemical modeling since meteorological variables, such as cloud fraction, winds, planetary boundary layer (PBL) heights and precipitation, significantly impact air quality. They influence the production, transport, and deposition of various chemical species (e.g., Pour-Biazar et al. 2007; Banta et al. 2005; Cuchiara et al. 2014). Hence accurate meteorological inputs are imperative for air quality modeling. Common approaches of improving meteorological simulations include the selection of updated and high quality terrain and input data (e.g., Cheng and Byun 2008), the optimization of physics and dynamics options (e.g., Zhong et al. 2007) and the implementation of four dimensional data assimilation (FDDA). The air quality modeling group at the University of Houston (UH) had performed several sensitivity studies on the various parameterization schemes in the recent past (e.g., Zhong et al. 2007; Ngan et al. 2012; Cuchiara et al. 2014).
FDDA continuously merges new observational data into model simulation such that the model’s predictions do not drift away from observations. There are several FDDA methods including nudging (e.g., Stauffer and Seaman 2004) and Variational Methods (3D-VAR or 4D-VAR) (e.g., Le Dimet and Talagrand 1986; Huang et al. 2009). 4D-VAR obtains optimal states of the atmosphere using multi-time-level observations by globally adjusting a model solution to all available observations over an interval of time. Nudging is a simple yet flexible FDDA method originally developed by Stauffer and Seaman (1990, 1994), and implemented in the Fifth-Generation PSU/NCAR Mesoscale Model (MM5). Not intended for optimal adjustment, nudging is less computationally intensive and needs special care for the nudging coefficients. Nudging involves adding an artificial tendency term to one or more model prognostic equations that reflect the difference between the best estimate of the observed state and the model state at a given location and time. In short, the goal is to “nudge” model state towards observed state.

There are several types of nudging such as 3D analysis nudging, surface analysis nudging, and observation nudging. In the case of analysis nudging, the model state is nudged toward gridded analysis. The difference between 3D and surface analysis nudging is that 3D analysis (at all model levels except for surface) data are used to improve 3D fields while surface analysis data are used to improve surface fields. In observation nudging, the model is perturbed such that its predictions are nudged to match better with observations at individual locations, both on-surface and aloft. The MM5 nudging codes were later improved and incorporated into the Weather Research and Forecasting (WRF) model by Liu et al. (2005, 2006). The enhancements enable observation nudging to assimilate a large variety of direct or derived observations. In WRF, the inputs for obs-nudging are generated by WRF OBSGRID program. This program also performs Objective Analysis (OA) to improve the quality of analysis nudging files. Objective Analysis updates first guess meteorology analysis by incorporating observational data. Since obs-nudging is usually performed along with OA (as in this study) to maximize the benefits of assimilating observations, we also use OA to denote the combined Objective Analysis and obs-nudging processes in case names.

The benefit of applying nudging to improve meteorological simulations has been demonstrated in many studies (e.g., Deng 2009; Gilliam and Pleim 2010). However, only a few have extended the investigation into chemistry impact of the improved fields on air quality simulations.
investigated by relatively fewer studies. Otte (2008) showed that analysis nudging is able to improve MM5 meteorology, as well as the Community Multiscale Air Quality (CMAQ) model with improved MM5 meteorology using analysis nudging was able to better simulate ozone chemistry as reflected in ozone-model-measurement statistics. Better results indicated that better “model skill” scores were achieved for daily maximum 1-hr ozone mixing ratios after analysis nudging over a 35-day period. Byun et al. (2008) performed over a dozen tests on observation-nudging (with analysis nudging turned on) and showed observation-obs-nudging improved both winds and temperature in MM5 simulations. The study also gave an example in which improved wind fields on a given day helped the CMAQ model better capture the high ozone area hotspot southwest of Houston. Ngan et al. (2012) compared results from several MM5-CMAQ simulations and showed coupled to the MM5 model which included nudging. Their results indicated that fully nudged (with both analysis nudging and observation-obs-nudging implemented) simulations outperformed a forecast run in performed better with respect to both meteorology and ozone chemistry. Their study location was Houston Texas, the same as in this study. No detailed results were presented on the quantitative improvements from the nudging. Their study cannot be used for interpreting the sensitivity of obs-nudging since its base WRF case is a forecast run which used a different analysis input. Previous work studies by the current authors (e.g., Rappenglueck et al. 2011; Czader et al. 2013) showed that observation-obs-nudging helped correct errors in model wind fields, which are critical to the transport process of air pollutants, as well as the production of secondary pollutants. To the best of the authors’ knowledge, there is no comprehensive existing-study on the impact of observation-obs-nudging on chemistry, especially when air quality simulation using the meteorological WRF model is WRF.. This study intends to fill up the gap in the studies mentioned above by investigating the sensitivity of WRF- and subsequently, CMAQ simulations to the use of observation nudging. Although not elaborated here, the WRF-CMAQ sensitivity to different observation nudging frequencies was also explored. In theory, higher frequency of observation-obs-nudging input should have a higher probability to capture small scale events, such as local wind shifts. These events may only slightly impact local weather, yet they can have a large marked effect on chemistry since it. This is well-known that because local stagnation and wind
convergence/reversals can contribute to the pollutant build-up (e.g., as indicated by Banta et al. (1998); Cheung and Wang (2001) and Tucker et al. (2010).

There is a significant presence of petrochemical facilities, power plants and motor vehicles in the Houston-Galveston-Brazoria (HGB) region located in southeastern Texas (SETX). The major pollutant in the region is ozone due to the abundant emissions of precursors like nitrogen oxide (NOx) and Volatile Organic Compounds (VOCs). During the long and hot summer, ozone concentrations often rise above the threshold level as stipulated in the National Ambient Air Quality Standards (NAAQS). Consequently, HGB has been designated as an ozone non-attainment region by the US Environmental Protection Agency (USEPA) (http://www3.epa.gov/airquality/greenbook/hncs.html#TEXAS). The petrochemical plants are largely concentrated in the Houston Ship Channel (HSC) area just north of the Galveston Bay. The VOCs emitted from the HSC area are highly reactive and have been shown to contribute greatly to the high regional ozone episodes in HGB (e.g., Kleinman et al. 2002; Daum et al. 2003). Depending on the local meteorology, the plumes from HSC may be carried to different locations in HGB and trigger high ozone events on its path.

Metro Houston has a high level of NOx emissions partly due to heavy vehicular traffic in the city. As a result of the large amount of precursor emissions and favorable weather, relatively frequent high ozone events occur in the area. Ngan and Byun (2011) gave an analysis on the relationships between the high ozone frequency and underlying weather patterns. They derived the weather patterns from a classification scheme using large-scale 850-hPa synoptic flow as input.

The due to the reasons listed above, the Houston-Galveston-Brazoria region has been the focus of interest of many several air quality studies in the recent past (e.g., Banta et al. 2005; Parrish et al. 2009; Lefer and Rappengluck 2010; Olaugier et al. 2013; Czader et al. 2013, Choi et al. 2012; Choi 2014; Choi and Souri, 2015; Pan et al. 2015). It is a good place for studying ozone production and transport due to the existence of a dense surface monitoring network, as well as several intensive measurement field campaigns which provide ample observational data. For example, in September 2013, the National Aeronautics and Space Administration (NASA), joined by a number of agencies and universities, conducted a field measurement campaign in SETX as part of its the Deriving Information on Surface conditions
from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) program—The NASA (http://www-air.larc.nasa.gov/missions/discover-aq/discover-aq.html).

This program has conducted several air quality and meteorology measurements at several different locations in the U.S. The availability of dense surface observations is important in OA’s capability for obs-nudging to correct erroneous local winds in the model. Without a rich set of observations, the performance of OAobs-nudging will be handicapped without a rich set of observations.

This study involved performing two sets of WRF- and CMAQ model simulations for the 2013 DISCOVER-AQ Texas time period in order to understand the impact of observation obs-nudging using comprehensive. The data for nudging included multiple sets of observation data from both in-situ surface and aircraft aloft measurements. We evaluated model measurement performance and calculated statistics for both WRF and CMAQ. Meteorological fields critical to ozone chemistry were examined to explore the model sensitivity to OA. The paper is structured as following: Section 1 is introduction; Section 2 describes the measurement data and the modeling system; Section 3 covers the evaluation protocols; Section 4 discusses the general meteorological conditions that occurred during the campaign period; Section 5 presents the modeling results, and Section 6 provides discussions and conclusions output.

2. Observational Data and Model Configurations

For evaluation of the results, this study used regular measurements from the Continuous Ambient Monitoring Station (CAMS), operated by the Texas Commission on Environmental Quality (TCEQ), as well as PBL and aloft ozone measurements from DISCOVER-AQ campaign. For observation nudging, in addition to the CAMS data sets, several data streams from the Meteorological Assimilation Data Ingest System (MADIS) were also used.

2.1 Observational Data

This study used regular measurements from the Continuous Ambient Monitoring Stations (CAMS) operated by the Texas Commission on Environmental Quality (TCEQ). Additionally, PBL and aloft ozone measurement data were obtained from the DISCOVER-AQ campaign. For
observation nudging, CAMS data and several data streams from the Meteorological Assimilation Data Ingest System (MADIS) were used. The CAMS measurement network collected real-time meteorology and chemistry pollutant data. The measured parameters differ from station to station. The station density at South East Texas (SETX) is relatively high. There were 63 sites having meteorological measurements and 52 sites having ozone measurements in the 4-km domain. The network is represented in Figure 1 during DISCOVER-AQ time period. The stations are represented by dots, with the La Porte (C556) site labeled. All CAMS observations are accessible at TCEQ website: http://www.tceq.state.tx.us/cgi-bin/compliance/monops/daily_summary.pl.

Additionally, PBL height measurements for September were obtained from a team recorded at a site at the University of Houston, which employed LIDAR. The PBL height was measured using the Light Detection and Ranging system to detect the PBL height. Presently, only one site is currently available.

Figure 1. Locations of CAMS sites (dots) in CMAQ 4-km modeling domain during September 2013. Metro Houston, Houston Ship Channel, Galveston Bay and Gulf of Mexico are labeled.
only at this site. For analysis of ozone aloft on September 25, we also used measurements from aircraft P-3B, part of the rich datasets collected during DISCOVER-AQ campaign (http://www-air.larc.nasa.gov/missions/discover-aq/discover-aq.html). The P-3B data had over 100 parameters and which are accessible from the website online.

2.2 Model Configurations

The modeling system consists of the WRF- meteorological model (Skamarock et al., 2008), the Sparse Matrix Operator Kernel Emissions (SMOKE-) model for emissions modeling (Houyoux et al., 2000) and the CMAQ models as described model (Byun and Schere, 2006) for chemical transport modeling. The details about model configurations are presented in the following three subsections. Two sets of simulations were conducted, one set with the only difference in whether obs-nudging and OA was adopted, were performed and the other without. The base case, referred as “No-OA”, did not employ observation obs-nudging or OA. The second case, “1Hr-OA”, performed observation obs-nudging and OA using hourly observation nudging input.

2.2.1. WRF Configurations Setup

Both WRF simulations used the same nested domain and NARR (North American Regional Reanalysis) as input, with grid nudging turned on.

2.2.1.1. Domain Setup

Figure 2 depicts the horizontal domain setup. There were two nested domains were used with 12-km and 4-km resolution respectively. The 4-km domain covered SETX and a small portion of Louisiana. The 12-km domain (red box) encompassed Texas and parts of a few neighboring states (or parts). The number of grid sizes cells for the 12-km and 4-km domains were 161×145 (E-W by N-S), and 95×77 respectively. The projection type was Lambert conic conformal (LCC). Three projection parameters were considered: namely first latitude, the (33°N), second latitude (45°N) and the standard longitude, are 33°N, 45°N and 197°W degrees respectively. The USEPA used the same projection parameters to develop emission inventories for air quality modeling. Vertically both (Mason et al. 2010). Both domains had a vertical resolution of 27 eta layers based on dry hydrostatic pressures. The model top is set to be 100 hPa, corresponding to top layer pressure of the input NARR data.
Figure 2. Horizontal domains of WRF and CMAQ simulation at 4km and 12km grid resolution (the bigger domains are for 12km WRF and CMAQ and the smaller domains for 4km WRF and CMAQ).

2.2.1.2.1. Input Data
The NARR data used for WRF simulations were retrospective runs using NARR analysis as input. The data were based on an Eta 221 grid at 29 pressure levels. Its horizontal resolution was 32-km and the frequency was 3-hourly. The initial and boundary conditions were generated from the NARR analysis by WRF. An alternative to NARR was the Eta-NAM analysis data. However, the data temporal frequency was lowered from 3-hourly to 6-hourly starting 2013. Our tests showed that it was not as good as NARR for WRF input, likely because of lower temporal resolution.

### 2.2.1.32. Physics and FDDA Options

Major physics options were used in the model are listed in Table 1. These options are consistent with the WRF options in our daily air quality forecasting system (http://spock.geosc.uh.edu/). Among them, the PBL and cumulus cloud schemes are especially critical. Our past modeling experiences demonstrated that the Yonsei University (YSU) scheme is the best PBL scheme in Houston case study while the Kain-Fritsch (K-F) is the preferable cumulus scheme. The choice of YSU scheme gave the best results for the Houston area. YSU scheme was also corroborated recently by Cuchiara et al. (2014). The K-F scheme is “drier” than others and produces less bogus number of “false” convectional thunderstorms. The numbers in parentheses represent the value of corresponding namelist variable in WRF’s namelist file. For example, the “1” after YSU is the value of the namelist variable “bl_pbl_physics” in WRF’s namelist file. For both of the simulations, we performed standard grid nudging for both of the cases using NARR analysis. For grid nudging options, we generally followed the recommendations in the WRF’s User Guide. For example, the mass fields (temperature and moisture) were nudged only at layers above the PBL while wind fields were adjusted at all layers including the surface layer.

### 2.2.1.43. Observation Nudging with MADIS and CAMS data in WRF

As mentioned in the introduction, observation nudging is regarded as a low-cost and effective method for improving meteorological model performance, but it requires additional observational data. In this study, we acquired are required to implement obs-nudging and OA. To generate the input files for the OBSGRID program, we processed the observation data
generating files in “little_r” format using similar procedures found in the approach of Ngan et al. (2012) and Czader et al. (2013). Observational data came from the MADIS and TCEQ CAMS. MADIS (https://madis.ncep.noaa.gov/) is a National Oceanic and Atmospheric Administration (NOAA) program, which collects, integrates, quality-controls, and distributes observations from NOAA and other organizations. Additional information is available online, https://madis.ncep.noaa.gov/. The four MADIS datasets used for observation obs-nudging were NOAA Profiler Network (NPN), Cooperative Agency Profilers (CAP), Meteorological Terminal Aviation Routine (METAR) weather report and NOAA Radiosonde (RAOB). The METAR dataset was collected by mostly first-order, METAR reporting, surface monitoring stations.

The “little_r” files from previous step processed input observation data were fed into WRF OBSGRID module to update the domain analyses (“met_em” files), and generate additional surface analyses (“sffdda”) and text nudging files (“OBS_DOMAIN”). Actual observation obs-nudging was performed by the main WRF program by properly setting observation after obs-nudging was performed by the main WRF program by properly setting observation after obs-nudging namelist variables are properly set. The namelist for OBSGRID and relevant WRF section settings came largely from recommended values of WRF User’s Guide and a previous study by Ngan et al. (2012).

Theoretically, observation obs-nudging updating at a higher frequency should enhance the model’s performance. A typical frequency of input analysis data is 3-hourly while the frequency for observational data is hourly. The 3-hourly frequency of input analyses may be the reason for the default 3-hour time-interval in WRF’s OBSGRID settings for generating the observation obs-nudging files. Since there were few existing OAobs-nudging studies related to air quality and we are not aware of any reference to the adoption of 1-hour input frequency, we assume that all the existing studies used the default 3-hour interval. As the WRF model allows the interval to be set to 1-hour or smaller when corresponding observational data were available, we tested both 1-hour and 3-hour scenarios. The results indicated that 1-hour OAobs-nudging had slightly better performance than the 3-hour one. As a result, this study adopted 1-hour temporal frequency for observation nudging. The quantities that were nudged were temperature, moisture, and the two wind components (U-WIND and V-WIND). Obs-nudging for moisture was not performed in
This study. This was based on our past experiences since performing moisture nudging sometimes trigger excessive artificial thunderstorms which disrupted model flow fields.

It should be noted that the default time interval for modified gridded analyses, i.e., the “metoa-em” and “sgfdda” files have to match input analysis data in OBSGRID. The namelist variable was called “interval”, with a default value of “10800” seconds. The time interval for output nudging files was set by namelist variable “int4d”, with the same default value of “10800” seconds. To output the observation nudging files hourly, “int4d” should be set to “3600” seconds. This means that the OBSGRID output files, “metoa_em” and “OBS_DOMAIN”, did not have the same interval in our study.

In WRF, there were a few namelist variables controlling the frequency of grid nudging and observation nudging. The first one was “interval_seconds”, which should match the interval of input-grid nudging files (“met_em”). The second one was “sgfdda_interval_m”, matching the interval of surface grid nudging files (“sgfdda”). In our simulation, both intervals were equal to 3-hours. The third one was “auxinput11_interval”, controlling the updating interval for observation nudging files (“OBS_DOMAIN”). The last one, “obs_ionf”, determined the nudging frequency relative to internal integration time step. For example, if the integration time step for the coarse domain is 30 seconds, setting “obs_ionf” to 1 means performing OA every 30 seconds, while setting “obs_ionf” to 3 means performing OA every 90 seconds. In our simulation, “obs_ionf” is set to 1.

One departure from the default OA setting in WRF was that the moisture OA was turned off with “obs_nudge_mois” set to 0. This was based on our past experiences since performing moisture OA sometimes trigger excessive artificial thunderstorms which disrupted model flow fields.

2.2.2. Emission Processing

For anthropogenic sources we utilized the National Emission Inventory of 2008 (NEI2008) generated by the USEPA. The mobile (USEPA, 2011) Motor vehicle emissions for this inventory were processed with EPA’s Motor Vehicle Emission Simulator (MOVES) (USEPA, 2015). The inventory was processed using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System v3.1 the inventory was converted to obtain gridded emission rates as well as to emission species as listed in...
speciated for the Carbon Bond 05 (CB05) chemical mechanism that is used for use in the CMAQ modeling model. The biogenic emissions were estimated modeled using the Biogenic Emissions Inventory System (BEIS) v3.14. Although NEI2008 might have overestimated NOx emissions in Houston (e.g., Choi 2012; Czader et al. 2015) which could have impacted on ozone formation in the region (2015), we used base NEI2008 without adjustment because the adjustment of the NOx emission also has large uncertainty. Pan et al. (2015) showed that the CMAQ ozone performance using NEI2008 appears reasonable.

### 2.2.3. CMAQ Configurations

The USEPA’s CMAQ (Byun and Schere 2006) version 5.0.1 was adopted for this study, following the choice of several other Houston. Several air quality modeling studies focusing on the Houston area have used this model (e.g., Foley et al. 2010; Czader et al. 2013, 2015; Choi 2014; Pan et al. 2015). CMAQ horizontal domains were slightly smaller than the WRF counterpart in order to avoid the discontinuity near the domain boundary. The domains were shown in Figure 2 as green and brown boxes. The chemical boundary conditions for all the species in the 4-km domain were derived from 12-km domain air quality forecasting results (http://spock.geosc.uh.edu). Vertically, CMAQ inherited (http://spock.geosc.uh.edu). The model used the same layers from vertical structure as WRF without layer collapsing. Major CMAQ configurations were described are listed in Table 2. The texts in the parentheses were the values in the CMAQ build script.

Chemical processes were simulated with the available in CMAQ CB05 chemical mechanism with cloud/aqueous chemistry, active chlorine chemistry and updated toluene mechanism. For aerosol modeling, the fifth-generation CMAQ aerosol mechanism (AE5) with which includes sea salt is modeling was selected. Cloud/aqueous chemistry is included. The total number of included species is 132, with 70 reactive gas-phase, 49 aerosol and 13 non-reactive species.

### 3. Evaluation Metrics

To assess model performance against observations, we computed a set of five statistics including Pearson correlation, index of agreement (IOA, Willmott 1981), mean bias (MB), root mean
square error (RMSE), and Mean Absolute Error (MAE). This list is similar to one used by Li et al. (2008) for model performance evaluation. The goal is to have a comprehensive comparison between model and observation time series. The set of five statistics have been frequently used for performance evaluation in modeling community was divided into three groups:

1) Measuring the direct departure magnitude of model results from observation, vis-a-vis in measurement units-situ data

- Mean Bias (MB)
- Mean Absolute Error (MAE)
- Root Mean Square Error (RMSE)

2) Measuring how close the model values follow changes in the observations, unitless

- Correlation

3) A composite performance index, index of agreement (IOA or d) suggested by Willmott (1981), unitless

IOA is considered a better performance index than correlation as it takes into account the difference in the means and standard deviation. For example, when correlations are similar, lower model biases would yield higher IOA values. Additionally, the mean and the standard deviation of model values and observations were included as a reference. Additionally, the mean and the standard deviation (Std. Dev.) of model values and observations were included as a reference.

4. General Meteorological and Ozone Conditions in September 2013

The weather during the September 2013 simulation period was relatively dry with mostly southerly, easterly or southeasterly winds. From 09/05 to 09/19 (all dates are in MM/DD format), September, there was a lack of influence of strong synoptic weather systems. Shifting
wind patterns were observed during the period: light northeasterly in the early morning gradually turned clockwise to southeasterly in the afternoon and evening hours. In this period, winds shifted from southeast to near east and there were more clouds after 09/10 September. The only cold front arrived on the early morning of 09/21 September. Figure 3 shows the daily-regional average temperatures and periods marked with for the period and it can be seen that 21 September has the lowest daily high temperature drop. Although not very significant to photochemistry, temperature drop is usually a good proxy for the critical factors affecting ozone production or transport such as cloudiness, wind. The influences of the cold air intrusion lasted till early 25 September. Winds turned into southerly in the afternoon of the 25th and precipitation warming continued in the next few days until the 28th.

Figure 3. Regional daily/hourly temperature averaged over all available (typically around 1200) hourly CAMS observations, two model cases also included for September of 2013.
Rain events occurred on 09/02, 09/10, 09/16, 09/19 to 09/21 and 09/28 to 09/30. None of them was heavy. The 09/20 and 09/21 events consisted of widespread light to medium showers. Besides the above-mentioned dates, there were a few other days with sporadic drizzles. A majority of the days between 09/01 and 09/20 were mostly either sunny or cloudy. The periods from 09/08 to 09/10 and 09/18 to 09/20 had more clouds than other days. The period from 09/21 to 09/30 was influenced by a cold front passage. The days between 09/22 and 09/24 were sunny and cool. Then the cold. The surface wind reversed direction during midday of 09/25 and brought clouds back from 09/26 to 09/30.

In SETX, high ozone events in SETX during fall season were typically associated with a passage of cold front (e.g., Rappenglueck et al. 2008). The only ozone event with hourly surface ozone exceeding 120 ppb (parts per billion) in September, which occurred on the 25th, fell in this category.

Figure 4 shows plots the daily regional averaged ozone. On most days, the observed averaged ozone fell concentrations were below 3070 ppb. Since the winds after dawn consistently pushed the precursors from the industrial area to the southwest of the city, the wind pattern did not favor the local ozone production. The daytime winds also contained a persistent easterly component which moved the pollutants away from the Houston metropolitan area. In the first 10-day period, low background ozone originating from the Gulf of Mexico contributed to the low-ozone days. With overcast skies on the 19th and the 20th, hourly high ozone values dipped below 2430 ppb. The two highest ozone days, characterized by post-frontal ozone events, were the 25th and the 26th.
The daily hourly regional averaged ozone for the two cases (No-OA and 1hr-OA) at the stations which include observation surface O₃ over the 4km domain for September of 2013.

5. Evaluation of Simulation Results

To evaluate the WRF simulation, we calculated statistics for surface temperature and winds in the 4-km domain. For PBL heights, we chose to plot out the time-series for the one site we had observations due to significant amount of missing data (data coverage is about 50%). For CMAQ evaluation, we calculated the surface ozone statistics for the whole month. Also, we plotted vertical ozone profile and calculated biases for aloft ozone aloft on 09/25 the 25th.

5.1. Meteorology

5.1.1. Temperature

The comparison of regional averaged daily temperatures, average hourly temperature for the analyzed time simulation period is shown in Figure 3. The regional observed averaged daily surface temperature was calculated by averaging the hourly temperature from ~60 CAMS sites in the 4-km model domain. Despite the differences in the base case temperature was too high compared to the in-situ measurements. For example, the days with more clouds/precipitation, No-OA maximum temperature for the simulated averaged temperatures tracked 21st was 30°C compared to 25°C for the in-situ data very well. It was also evident that...
The high biases in the base case are sharply reduced in the “1Hr-OA” case and temperature matched better with the observations for several time periods, especially for September 20-23. The statistics of hourly surface temperature are listed in Table 3. With higher IOA and lower mean biases (MB), the “1Hr-OA” case was clearly better than the base case “No-OA”. The IOA of “1Hr-OA” was about 9% higher than the base case.

5.1.2. Winds

Wind fields are known to significantly affect chemistry (e.g., Banta et al. 2005, 2011; Darby 2005). In ozone chemistry, winds affect the accumulation of precursors and hence the resulting ozone production. Winds (e.g., Banta et al. 2005, 2011; Darby 2005). They are also responsible for dispersing high ozone and bringing in background ozone. In HGB, prevailing southerly to southeasterly winds in the summer HGB region significantly lower the ozone level concentrations in the metropolitan area. Therefore, high ozone events usually occur when such wind patterns change. Cold front intrusions coming as early as late August, blow pollutants to the south. As a result, an area of high ozone develops in the Gulf. A few days later, following cold fronts weakening and the weather warming up, reversing winds can bring high ozone back to land. High ozone may also occur during intra-day pollutant recirculation events when pollutants previously blown away from industrial zone are brought back by reversing winds. The high ozone event caused by post-front conditions. The ozone event in the HSC area on 09/25 was likely due to a combination of local recirculation caused by onset of the bay breeze and increased background ozone brought in by the much larger scale southerly flow from the Gulf transport. Due to the land-water thermal contrast and the different size of the Galveston Bay and the Gulf of Mexico, the western shore of the Galveston Bay often experiences a successive onset of bay breeze and sea breeze in the summer. The bay breeze is typically a weaker easterly while sea breeze is a stronger southeasterly. Sea breeze usually comes one to a few hours later after the bay breeze. The bay breeze and the subsequent sea breeze phenomena in Houston were described by Banta et al. (2005).
The statistics of zonal (U-WIND) and meridional (V-WIND) wind components are listed in Table 3. The purpose of choosing U and V over wind speed and direction is to avoid the anomalies in the wind direction statistics. For example, although wind direction of 5 and 355 degrees are close, the statistics suggest that they are distinctively different.

For both U and V components of wind, “1Hr-OA” had higher correlation and IOA than “No-OA”. The model performance on U and V are similar, with the correlation in a range of 0.76 to 0.81 for all the cases. As a reference for comparison, the performance of the OA case (“M1”) in Ngan et al. (2012) is very close to that in this study, with a correlation of 0.75 for U and 0.82 for V. In terms of IOA, the OA case had a larger lead over the base case, ahead by 5-6% in U and 10-11% in V over the base case. This can be explained by the much reduced wind biases in the OA case.

The base case had consistently stronger winds, especially the southerly component, than the observation. This was reflected in the mean bias “MB”, as well as the model mean “M_M”. Winds were reduced significantly after OA was performed. Interestingly, the high southerly bias in “No-OA” turned slightly negative after OA. Winds originating from the Gulf were also stronger in base case, which played a role in raising the ozone level in comparing to the area-sensitivity case. Figure 5 illustrated the slowing down of southerly winds after observation nudging. As a result, winds of nudging, the wind vectors matched better to the observations.
Figure 5. Model and observed winds at 09/01_00 CST: No-OA (top) and 1Hr-OA (bottom).

Model winds are blue arrows and the observations are orange arrows. Stronger southerly winds, especially along coastal region, were reduced in the OA case.

5.1.3. PBL height

Atmospheric pollutants are largely confined in the PBL as most of the emissions sources are close to the ground level. Hence the PBL height plays a critical role in mixing and spreading the pollutants. Haman et al. (2014) studied the relationship between ozone level and PBL height at a Houston CAMS site and found that nighttime and early morning PBL heights were consistently lower on high ozone days than on low ozone days. Czader et al. (2013) pointed out that the
model underprediction of PBL during nighttime may have caused the CO overprediction at the same site. CO is a good proxy for understanding model’s transport since it has low reactivity and a relatively long life time in the troposphere.

Cuchiara et al. (2014) conducted four WRF/Chem sensitivity tests on the using different PBL schemes over southeast Texas. While no preferred PBL scheme was identified for WRF simulations, the Yonsei University (YSU) scheme outperformed others in terms of ozone prediction. As a note, we used YSU in this study as it had been tested in the past and the study by Cuchiara et al. (2014).

The PBL height data were taken at an urban site very close to CAMS site C695, located on University of Houston campus. A study by Haman et al. (2012) showed that Houston’s daily maximum PBL height at the University of Houston site indicated previously reached its highest values of slightly over 2000 m in August. In September, typical daily maximum PBL height was 1500 m at 15 CST while daily minimum was just below 200 m between 00 CST and 06 CST. The comparison of observed and model PBL height is shown at Figure 6. Our results indicated that the model tended to overpredict the daily maximum and OA PBL height; obs-nudging helped to reduce the overpredictions. For the daily minimum PBL height, “No-OA” case had slightly high biases while the OA case matched quite well with observations. The observed minimum PBL height was lower than that reported by Haman et al. (2012), likely due to the cloudy conditions prevailing in September 2013. There was no apparent explanation on the reduced daytime PBL biases in the OA case than the base case, but it is likely the results of improved winds and temperatures in PBL.
Figure 6. Planetary Boundary Layer (PBL) height time series at CAMS C695 for September 2013.

5.1.4. Cold Front Passage

The surface winds on 09/20 were overwhelmingly southerly in the region and reversed on 09/21 September due to the arrival of a cold front. The hour-by-hour wind shifts for 11 sites in HGB on 09/21 September are plotted in Figure 7. The sites are sorted by latitude with the southernmost site, Galveston C1034, located at the bottom row. There was only one site, Deer Park C35, showing weak southerly at 00 CST while all the others had mostly weak northerly. Starting from 01 CST, winds in the entire HGB area turned northerly to northeasterly and continued gaining strength in the next few hours, indicating cold air had taken over the region.

Both cases performed reasonably well on 09/21 and the timing of wind shift was captured quite accurately; although “No-OA” lagged about an hour behind by ~ 1 hr. The winds turned weak northerly at 00 CST for most sites and but the “No-OA” case still showed the wind direction to be all southerly. Besides the timing, OA also helped moderate the winds as the northeasterly winds in “No-OA” case sometimes were too strong; obs-nudging helped moderate the winds. The reduced V-wind bias in “1Hr-OA” was also evident in the wind model-measurement statistics on 09/21 is reduced from -2.5 m/s to -0.6 m/s after OA was performed. The performance of the OA case during cold front passage was consistent with our past simulations September.
Figure 7. Hourly model (blue) and CAMS (orange) winds at 11 sites on 09/21 September: No-OA (top) and 1hr-OA (bottom). The 1hr-OA case is better in 00 CST to 02 CST and 17 CST to 20 CST.
5.2. Ozone

5.2.1. Regional Daily-Average Hourly Ozone

Figure 4 showed plots of the regional average daily hourly ozone, which was defined similarly to averaged daily temperature. Regional averaged daily ozone provides a global view on model’s performance. Model failure of daily averaged ozone (such as wrong trend or too high bias) was often a sign of model flaws. For example, a consistently high ozone bias could mean either the model background ozone or the emission of the precursors are too high. On the other hand, if the high biases are present only at certain days, then it is likely a meteorological problem than issues in model background or emission inventory. Overall, observed ozone level was lower and the model did well on the daily trend although positive biases were seen for some days.

Although model had high biases for majority of the days, biases were consistently lower for the OA case during two periods: 09/07 to 09/09. During the model high bias period, the OA case usually did better in reaching the daily low although it overpredicted the high a bit more than the base case. The night time biases were reduced likely because the lower southerly winds in the OA case since model had higher background transported ozone originated from the Gulf. In Figure 4, the first three orange circles showed the days with high model biases. The first two circles consisted of days with lower ozone concentrations were likely higher in the Gulf than “normal” background ozone actual. However during the 2nd – 4th and 7th–8th of September, the incoming ozone from the Gulf was markedly lower. Since the model ozone had fixed boundary values, the model was unable to capture the daily ozone variation at the boundary. The third circle consisted of days with model showed the highest biases during period of the 19th–20th likely due to overcast skies. The high model biases were likely the result of problems and uncertainties in model’s cloud fields and high background ozone values. Despite the overprediction, the biases in OA case are notably lower during the
nights of 19th and 20th. A future study to upgrade the accuracy of cloud fraction using remote sensing data (e.g., MODIS) should be helpful in explaining the biases.

There were a few days with elevated ozone due to post-front meteorology conditions. The only exceedance happened on 09/25, which was likely caused by meteorological events in Houston and the Galveston Bay. The overall ozone on 09/26 September was slightly higher after southerly winds transported back the ozone from the Gulf, raising the ozone level in the entire region. A more detailed analysis of model predictions on 09/25 and 09/26 will be presented in following subsection of 5.2.3.

5.2.2. Performance Statistics

The ozone statistics were displayed in Table 4. Both cases had very close correlation of 0.72 and 0.73. However, the mean biases in the OA case were lower by 3.2 ppb, which helped raise the IOA from 0.78 to 0.83. The model standard deviation increased in the OA case and matched better with observation that of the in-situ data. The improvement in IOA was slightly less compared to that for temperature and winds.

5.2.3. High ozone episode after the passage of a front

In SETX, high ozone events during the fall season usually occurred after the passage of a cold front (e.g., Rappenglück et al. 2008; Ngan and Byun, 2011; Ngan et al. 2012; Haman et al. 2014). Two factors may have contributed to the post-front ozone events: 1) following a cold spell; winds reverse direction and subsequent light winds and sunny skies create an ideal condition for ozone production and accumulation, 2) wind reversal transports back the pollutants that were previously blown into the Gulf, a phenomenon commonly known as recirculation.

During the DISCOVER-AQ period, the two days with highest ozone concentrations were 09/25 the 25th and the day 09/26 26th of September as indicated in Figure 4, but the two days exhibited different patterns. The 1-hour maximum ozone on 09/25 the 25th was localized and higher by about 40 ppb than the 26th. In addition to heightened background ozone on the 25th, the major contributor was the production resulting from favorable weather conditions: sunny, overall light winds and shifting winds over the industrial area. The light morning land breeze
carried pollutants from ship channel area to the Galveston Bay. As the day warmed up, the bay breeze started to develop and carry pollutants back to the land. This localized circulation was described by Banta et al. (2005). Ngan et al. (2012) reported the same phenomenon in their Texas Air Quality Study-II 2006 study. 09/26 is characterized by elevated background ozone from early morning to late night.

Figure 8 shows the ozone time series for the La Porte (C556) site located in the HSC area (Figure 1). In September, the highest hourly ozone occurred at C556 at 13 CST on 09/25. From 9 CST to 12 CST, ozone rose from 10 ppb to 150 ppb. The large increase in ozone was likely the result of increased photochemical activity under favorable meteorological conditions in an area with accumulated precursors. Figures 9 and 10 depict the wind and ozone concentrations at 08 CST and 13 CST.

From the wind plots of Figure 9, we can see that the winds in the HGB region at 8 CST were light northerly for sites located on the north side while they were mostly westerly for the sites in the middle and south. The base case winds were all northerly while the OA case had northwest winds for north side and west winds for the middle and south. The model winds in OA case were much more realistic than the winds in base case. The winds were similar to those of 08 CST. As a result, the ozone statistics in Table 5 showed that the OA case had much better correlation and IOA than the base case during 8-09 CST. This example demonstrated the ability of obs-nudging to correct erroneous winds. However, later events showed it may not always be able to perform consistently.

The bay breeze started to develop at 10 CST near the C556 site. The early onset was likely to be related to the warming up on the previous afternoon on 09/24 as indicated in Figure 3. At 10 CST most other sites to the west of HSC experienced light northwest winds while those at HSC were originated from the northeast. Combined with the easterly bay breeze, a convergence zone was formed just below C556, where emissions from the HSC area stalled and accumulated. At 13 CST, the whole region had light winds and the bay breeze was well developed. The highest ozone indeed appeared in C556 and its vicinity. The rapid increase of ozone concentration for C556 between 09-13 CST is shown in Figure 8.
Figure 8. Ozone time series of La Porte (C556) between 09/24_00 to 09/28_00 CST of 2013.

It is important to note that both modeled cases missed the wind shifts in the HSC area, and the resulting convergence zone near C556. This could explain the model’s inability to recreate the sharp ozone increase at C556. Figure 9 shows that the ozone level concentrations around HSC area are quite low (~10 ppb) at 08 CST. A further examination showed that while both model cases missed the wind shift and convergence, though the patterns were different. The base case had flawed winds for most of the morning: instead of a weak northerly westerly, it had stronger northwesterly to northerly. By 08 CST, winds were almost uniformly northerly in the base case while they were weak west-northwesterly in the OA case (Figure 9).

The oval in Figure 9’s top-left panel shows the mismatch of winds around C556 in the base case. As a result, the NOx produced in the city was carried further to the southeast in the model in the base case. Until 13 CST, base case winds did not shift directions by much. The OA case got the early hour weak northwesterly right, but missed the bay breeze onset between 10 and 13 CST (oval in Figure 10). The OA case could not reproduce the small-scale wind reversal near C556, suggesting there is a limitation in the current WRF OA’s capability. On the other hand, the OA case did improve the spatial ozone pattern, as the high ozone area was closer to HSC after OA (Figure 10).
Figure 9. Zoom-in ozone concentrations (right) and wind plots (left) at 09/25_08 CST of 2013 for “No-OA” (top) and “1Hr-OA” (bottom). Ozone observation is in small circle; wind observation is indicated by an orange arrow. La Porte site C556 is labeled. The value range of right-side colour scale is 0 to 200 ppb. Higher value than 200 ppb has the same colour as 200 ppb.
Figure 10. Zoom-in ozone concentrations (right) and wind plots (left) at 09/25 13 CST of 2013 September for “No-OA” (top) and “1Hr-OA” (bottom). Ozone observation is in small circle; wind observation is indicated by an orange arrow. La Porte site C556 is labeled. Bay breeze is shown in the orange oval.

The ozone measurements from aircraft P3-B provided a more complete picture for 09/25’s ozone evolution on 09/25. During the day, P-3B the aircraft flew around the industrial area, Galveston Bay, and Galveston Island for about 9 hours. Figures 11 and 12 showed the ozone concentrations along aircraft tracks at 08 and 13 CST with surface layer ozone from the
“No-OA” case is provided as background. The background was only intended as a for reference.

At 08 CST, ozone level of 60-80 ppb aloft was already observed at three locations (three loops in Fig.11): Galveston Island, Smith Point and inner city. Another high of ~90 ppb could be seen above the HSC area. Ozonesonde observations over HGB showed the aloft ozone concentrations were normally ~40-50 ppb (e. g., Li and Rappengluck 2014.) at the height level. The higher-than normal ozone aloft suggested a post-front ozone recirculation condition. Such high ozone aloft might raise surface ozone level as a growing PBL downwardly mixed the air aloft with near surface air. At 13 CST, high ozone over 100 ppb was observed at multiple locations. The highest aloft ozone aloft of ~ 160 ppb, occurred southwest of Smith Point in the Galveston Bay. Such high level of ozone increase in ozone concentrations was likely the result of active production photochemistry in the industrial zone and around Galveston Bay; indicating a high level of precursor accumulation in the area.

**Figure 11.** Ozone along aircraft tracks at 08 CST of September 25th, overlaid upon model No-OA surface ozone.
Figure 12. Ozone along aircraft tracks at 09/25_13 CST of September 25th, overlaid upon model “No-OA” surface ozone. Plumes can be seen as dark purple circles in Galveston Bay.

Figure 13 shows hourly ozone vertical profiles from 08 CST to 16 CST of September 25th, with ozone being displayed on the x-axis and height on the y-axis. One observation dot was averaged over all the grid cells in the same model layer. For example, during 08-09 CST, aircraft flew passing 30 cells at model’s 5th layer. The 5th layer had a mid-layer height of 287.5 m. The averaged ozone of the 30 cells was 56 ppb. It should be noted that the observed ozone was averaged over multiple measurements in the same model cell, such so that they could be properly compared to model output. Next, both model and observed ozone values were averaged over all the grid cells in the same model layer, such that one dot represents the average ozone of all the cells in the same layer. The 08 and 09 CST profiles showed there was a high ozone layer with average ozone of ~65 ppb, stretching from 450 m to 1200 m height. In comparison, all model runs had lower ozone in this layer. The model biases, as shown in Figure 14, were about -10 ppb at 08 CST and grew to -20 ppb at 09 CST. The discrepancies, large discrepancy between low surface ozone and ozone aloft was unusual and may be explained by the earlier reversal of winds, high ozone air mass aloft. Winds at surface layer still showed a light northwesterly in the
early morning while winds aloft already changed to southerly. The observed ozone rose continuously in following hours yet model simulated ozone stagnated around 60 ppb from surface up to 2000 m until 15 CST. At 16 CST, the ozone of OA case in the lowermost (0-1 km) layer rose 20 ppb over the previous hours yet the base case ozone increased only a few ppb. Although different in magnitude, ozone aloft ozone had a few similar features to the surface ozone. Firstly, the model missed the observed high ozone in the afternoon by a large margin. For example, the base case underpredicted the 0-1 km level ozone by up to 50 ppb. The primary cause for the lower ozone production was likely model’s wind fields as both model and observations had a clear sky in industrial area and Galveston Bay. Secondly, nudging clearly helped reducing the ozone biases aloft. In most plots of Figure 14, the OA case had lower biases than the base case. The largest difference was at 16 CST; when nudging reduced biases from ~45 ppb to ~30 ppb in the 300 – 1000 m layer.

While it is easy to understand the improvements in temperature and winds after obs-nudging was applied, it is more difficult to explain how other variables such as precipitation and clouds reacted to obs-nudging. The indirect impact of these meteorological variables on ozone was harder to assess. In our study, we did not evaluate clouds quantitatively as there were no digitized cloud fraction data available for our modeling domains. A preliminary analysis on convection showed that there were occasions in which model missed the convection or precipitation and there were other occasions in which model created artificial convection. The convection cells were usually visible as “star-burst” from surface wind vector plots – arrows going out to different directions from a center. However, the mismatch in convection appeared to be not a serious issue since only a few occurrences were observed in the month of September.
Figure 13. Vertical ozone profiles from 09/25_08 CST to 09/25_16 CST of 2013 for two cases of No-OA and 1Hr-OA compared with corresponding observations.
Figure 14. Model vertical ozone biases from 09/25_08 CST to 09/25_16 CST of 2013 for two cases of No-OA and 1Hr-OA.
6. Conclusions and Discussions

In this study, we performed two Weather Research and Forecasting (WRF) and Community Multiscale Air Quality (CMAQ) model simulations to explore model sensitivity to observation nudging. In evaluating meteorological and ozone conditions, we found that objective analysis (OA) improved the meteorology and ozone performance as shown in the index of agreement (IOA) of temperature, winds, and ozone. While the base case winds were overall well simulated, observation obs-nudging significantly reduced the high wind biases (especially the meridional wind) shown in the base case. For planetary boundary layer height, OAobs-nudging reduced high biases in both daily maximum and daily minimum values. In the end, the combined changes in meteorology lowered the ozone biases by about 3 ppb, a 35% reduction. There were short time periods (such as between 07 and 09 CST on 09/25) when the simulated base case model winds differed significantly from observation observational data and OAobs-nudging significantly corrected the meteorological simulation problems, leading to much better ozone simulation. It should be noted that the However, model ozone biases are also impacted by the emissions and model lateral boundary conditions.

While it is easy to understand the improvements in temperature and winds after OA was applied, it is more difficult to explain how other variables such as PBL and clouds reacted to OA. The indirect impact of these meteorological variables on ozone was harder to assess. In our study, we did not evaluate clouds quantitatively as there were no digitized cloud fraction data available for our modeling domains. A preliminary analysis on convection showed that there were occasions in which model missed the convection or precipitation and there were other occasions in which model created artificial convection. The convection cells were usually visible as “star-burst” from surface wind vector plots—arrows going out to different directions from a center. However, the mismatch in convection appeared to be not a serious issue since only a few occurrences were observed in the month of September.

The only high ozone episode in the simulation period was related to the cold front passage. The small-scale winds and high aloft ozone aloft-concentrations on 09/25, likely contributed to the ozone exceedance in the area. It is also possible that an unreported emission event played a role. Since the maximum surface ozone at La Porte was much higher than the morning-time aloft ozone, the active local ozone production was likely the dominant factor. Analyses of aloft...
ozone aloft on 09/25 showed while there was high aloft ozone aloft and large negative model biases, the OA case tended to have smaller biases, especially in late hours.

Small-scale meteorological events are frequently cited for their contributions to high ozone events. Model’s capability in reproducing these events is critical in simulating such high ozone episodes. The base case did not recreate the 09/25 September small-scale events likely due to the complex winds and a lack of local information which can be used to steer model state closer to reality. On the other hand, the inability of the OA sensitivity case to replicate the local winds is likely a result of the imperfection of the nudging process which requires further investigation. An ongoing study by the current authors suggests that errors in the metrological fields from the default grid nudging files are important sources. Methods are being tested to improve the quality of grid nudging files. Early results showed that the bay breeze which caused the wind reversal around La Porte was well captured through improved grid nudging files. In addition, more observational data (e.g., more sites and higher data frequency) and more testing on the combination of OA nudging setting should help improve the OA obs-nudging performance. Also, the impact of obs-nudging on precipitation and clouds should be further investigated to understand their chain effect on chemistry.

Acknowledgement

The authors thank Texas Air Research Center (TARC) for its support through grant number 413UHH0144A and Air Quality Research Program (AQRP) through 14-014, the DISCOVER-AQ team for the aircraft data, Vanessa Caicedo for LIDAR data, and the TCEQ CAMS site team for the in-situ ozone and meteorological data.
References

Banta, R. M., Senff, C. J., White, A. B., Trainer, M., McNider, R. T., Valente, R. J., Mayor, S., D., Alvarez, R. J., Hardesty, R. M., and Parrish, D.: Daytime buildup and nighttime transport of urban ozone in the boundary layer during a stagnation episode, Journal of Geophysical Research: Atmospheres (1984 – 2012), J. Geophys. Res.-Atmos., 103, 22519-22544, 1998.

Banta, R. M., Senff, C. J., Nielsen-Gammon, J., Darby, L. S., Ryerson, T. B., Alvarez, R. J., Sandberg, S. R., Williams, E. J., and Trainer, M.: A bad air day in Houston, Bulletin of the American Meteorological Society, B. Am. Meteorol. Soc., 86, 657-669, doi:10.1175/bams-86-5-657, 2005.

Banta, R. M., Senff, C. J., Alvarez, R. J., Langford, A. O., Parrish, D. D., Trainer, M. K., Darby, L. S., Hardesty, R. M., Lambeth, B., Neuman, J. A., Angevine, W. M., Nielsen-Gammon, J., Sandberg, S. P., and White, A. B.: Dependence of daily peak O_3 concentrations near Houston, Texas on environmental factors: Wind speed, temperature, and boundary-layer depth, Atmos. Environ., 45, 162-173, doi:10.1016/j.atmosenv.2010.09.030, 2011.

Byun, D., and Schere, K. L.: Review of the governing equations, computational algorithms, and other components of the models-3 Community Multiscale Air Quality (CMAQ) modeling system, Applied Mechanics Reviews, Appl. Mech. Rev., 59, 51-77, doi:10.1115/1.2128636, 2006.

Byun, D., Ngan, F., Li, X., Lee, D., Kim, S.: “Analysis of Air Pollution Events in Summer 2006 and Preparation of Model Input Data for the Assessment Study”, Grant No. 582-5-64594- FY07-02, Final Report: Evaluation of Retrospective MM5 and CMAQ Simulations of TexAQS-II Period with CAMS Measurements, Texas Commission on Environmental Quality, February, 2008, 25 pp

Cheung, V. T., and Byun, D.: Application of high resolution land use and land cover data for atmospheric modeling in the Houston-Galveston metropolitan area, Part I: Meteorological simulation results, Atmos. Env., 42, 7795-7811, doi:10.1016/j.atmosenv.2008.04.055, 2008.

Cheung, V. T., and Wang, T.: Observational study of ozone pollution at a rural site in the Yangtze Delta of China, Atmos. Env., 35, 4947-4958, 2001.
Choi, Y.: The impact of satellite-adjusted NOx emissions on simulated NOx and O3 discrepancies in the urban and outflow areas of the Pacific and Lower Middle US, Atmos. Chem. Phys., 14, 675-690, doi:10.5194/acp-14-675-2014, 2014.

Choi, Y., and Souri, A.: Chemical condition and surface ozone in large cities of Texas during the last decade: observational evidence from OMI, CAMS, and Model Analyses, Remote Sensing of Environment, 168:90-101, doi:10.1016/j.rse.2015.06.026, 2015.

Choi, Y., Kim, H., Tong, D., and Lee, P.: Summertime weekly cycles of observed and modeled NOx and O3 concentrations as a function of satellite-derived ozone production sensitivity and land use types over the Continental United States, Atmos. Chem. Phys., 12, 6291-6307, doi:10.5194/acp-12-6291-2012, 2012.

Cuchiara, G. C., Li, X., Carvalho, J., and Rappenglück, B.: Intercomparison of planetary boundary layer parameterization and its impacts on surface ozone concentration in the WRF/chem model for a case study in Houston, Texas, Atmos. Environ., 96, 175-185, doi:10.1016/j.atmosenv.2014.07.013, 2014.

Czader, B. H., Li, X. S., and Rappenglueck, B.: CMAQ modeling and analysis of radicals, radical precursors, and chemical transformations, J. Geophys. Res.-Atmos., 118, 11376-11387, doi:10.1002/Jgrd.50807, 2013.

Czader, B. H., Choi, Y., Li, X., Alvarez, S., Lefer, B.: Impact of updated traffic emissions on HONO mixing ratios simulated for urban site in Houston, Texas. Atmos. Chem. Phys., 15(3), 1253-1263, doi:10.5194/acp-15-1253-2015, 2015.
Darby, L. S.: Cluster analysis of surface winds in Houston, Texas, and the impact of wind patterns on ozone, *Journal of Applied Meteorology*, J. Appl. Meteorol., 44, 1788-1806, doi: 10.1175/jam2320.1, 2005.

Daum, P. H., Kleinman, L. I., Springston, S. R., Nunnermacker, L. J., Lee, Y. N., Weinstein-Lloyd, J., Zheng, J., and Berkowitz, C. M.: Origin and properties of plumes of high ozone observed during the Texas 2000 Air Quality Study (TexAQS 2000), *J. Geophys. Res.-Atmos.*, 109, A04D17, doi:10.1029/2003jd004311, 2004.

Deng, A., Stauffer, D., Gaudet, B., Dudhia, J., Hacker, J., Bruyere, C., Wu, W., Vandenberghe, F., Liu, Y., Bourgeois, A.: Update on WRF-ARW End-to-end Multi-scale FDDA System. 10th WRF Users’ Workshop, Boulder, CO, June 23, 2009. [Available online at, http://www2.mmm.ucar.edu/wrf/users/workshops/WS2009/abstracts/1-09.pdf] NCAR, 2009.

Foley, K. M., Roselle, S. J., Appel, K. W., Bhave, P. V., Pleim, J. E., Otte, T. L., Mathur, R., Sarwar, G., Young, J. O., Gilliam, R. C., Nolte, C. G., Kelly, J. T., Gilliland, A. B., and Bash, J. O.: Incremental testing of the Community Multiscale Air Quality (CMAQ) modeling system version 4.7, *Geoscientific Model Development*, 3, 205-226, doi:10.5194/gmd-3-205-2010, 2010.

Gilliam, R. C., and Pleim, J. E.: Performance Assessment of New Land Surface and Planetary Boundary Layer Physics in the WRF-ARW, *Journal of Applied Meteorology and Climatology*, J. Appl. Meteorol. Climatol., 49, 760-774, doi:10.1175/2009jamc2126.1, 2010.

Haman, C.L., Lefer, B., Morris, G.A.: Seasonal Variability in the Diurnal Evolution of the Boundary Layer in a Near-Coastal Urban Environment. *J. Atmos. Ocean Tech.*, 29, 697-710, 2012.

Haman, C.L., Couzo, E., Flynn, J.H., Vizuete, W., Heffron, B., Lefer, B.L.: Relationship between boundary layer heights and growth rates with ground-level ozone in Houston, Texas. J Geophys Res-Atmos, 119, 6230-6245, 2014.

Houyoux, M., Vukovich, J., Brandmeyer, J., 2000. Sparse Matrix Kernel Emissions Modeling System: SMOKE User Manual. MCNC-North Carolina Supercomputing Center. Available at: https://cmascen.org/smoke/.
Haman, C.L., Lefer, B., Morris, G.A.: Seasonal Variability in the Diurnal Evolution of the Boundary Layer in a Near-Coastal Urban Environment. J. Atmos. Ocean Tech. 29, 697-710, 2012.

Huang, X.-Y., Xiao, Q., Barker, D. M., Zhang, X., Michalakes, J., Huang, W., Henderson, T., Bray, J., Chen, Y., and Ma, Z.: Four-dimensional variational data assimilation for WRF: Formulation and preliminary results. Monthly Weather Review, 137, 299-314, 2009.

Kleinman, L. I., Daum, P. H., Lee, Y. N., Nunnermacker, L. J., Springston, S. R., Weinstein-Lloyd, J., and Rudolph, J.: Ozone production efficiency in an urban area. J. Geophys. Res.-Atmos. 107, Art. 4733, doi:10.1029/2002jd002529, 2002.

Li, X., and Rappenglück, B.: A WRF–CMAQ study on spring time vertical ozone structure in Southeast Texas. Atmospheric Environment, 97, 363-385, doi:10.1016/j.atmosenv.2014.08.036, 2014.

Li, X., Lee, D., Kim, S.-T., Kim, H., Ngan, F., Cheng, F., and Byun, D.: Performance Evaluation of a Year-long Run of an Air Quality Forecasting System for Southeast Texas, 10th Conference on Atmospheric Chemistry, New Orleans, January 2008, 2008. [Available online at, http://ams.confex.com/ams/pdfpapers/134453.pdf]

Liu, Y., Bourgeois, A., Warner, T., Swerdlin, S., and Hacker, J.: An implementation of observation nudging-based FDDA into WRF for supporting ATEC test operations, 2005 WRF user workshop, Boulder, CO, 2005. [Available online at, http://www2.mmm.ucar.edu/wrf/users/workshops/WS2005/abstracts/Session10/7-Liu.pdf]
Liu, Y., Bourgeois, A., Warner, T., Swerdlin, S., and Yu, W.: An update on "observation nudging"-based FDDA for WRF-ARW: Verification using OSSE and performance of real-time forecasts, 2006 WRF user workshop, Boulder, CO, 2006. [Available online at, http://www2.mmm.ucar.edu/wrf/users/workshops/WS2006/abstracts/Session04/1_7_Liu.pdf]

Ngan, F., and Byun, D.: Classification of Weather Patterns and Associated Trajectories of High-Ozone Episodes in the Houston-Galveston-Brazoria Area during the 2005/06 TexAQS-II, Journal of Applied Meteorology and Climatology, 50, 485-499, DOI: 10.1175/2010jamc2483.1, 2011.

Ngan, F., Byun, D., Kim, H., Lee, D., Rappengluck, B., and Pour-Biazar, A.: Performance assessment of retrospective meteorological inputs for use in air quality modeling during TexAQS 2006, Atmos. Environ., 54, 86-96, DOI:doi:10.1016/j.atmosenv.2012.01.035, 2012.

Mason, R.; Strum, M.; Houyoux, M. Technical Support Document (TSD) Preparation of Emissions Inventories for the Version 4, 2005-based Platform; U.S. Environmental Protection Agency, Office of Air and Radiation, Office of Air Quality Planning and Standards, Air Quality Assessment Division, 2010

Olaguer, E. P., Rappengluck, B., Lefer, B., Stutz, J., Dibb, J., Griffin, R., Brune, W. H., Shauck, M., Buhr, M., Jeffries, H., Vizuete, W., and Pinto, J. P.: Deciphering the Role of Radical Precursors during the Second Texas Air Quality Study, Journal of the Air & Waste Management Association, Manag. Assoc., 59, 1258-1277, doi:10.3155/1047-3289.59.11.1258, 2009.

Otte, T. L.: The impact of nudging in the meteorological model for retrospective air quality simulations. Part I: Evaluation against national observation networks, Journal of Applied Meteorology and Climatology, Meteorol. Climatol., 47, 1853-1867, doi:10.1175/2007jamc1790.1, 2008.

Pan, S., Choi, Y., Roy, A., Li, X., Jeon, W., and Souri, A.: Modeling the uncertainty of several VOC and its impact on simulated VOC and ozone in Houston, Texas, Atmos. Environ., 120, 404-416, 2015
Parrish, D. D., Allen, D. T., Bates, T. S., Estes, M., Fehsenfeld, F. C., Feingold, G., Ferrare, R., Hardesty, R. M., Meagher, J. F., Nielsen-Gammon, J. W., Pierce, R. B., Ryerson, T. B., Seinfeld, J. H., and Williams, E. J.: Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS), J. Geophys. Res.-Atmos. 114, D00F13, doi:10.1029/2009jd011842, 2009.

Pour-Biazar, A., McNider, R. T., Roselle, S. J., Suggs, R., Jedlovec, G., Byun, D. W., Kim, S., Lin, C. J., Ho, T. C., Haines, S., Dornblaser, B., and Cameron, R.: Correcting photolysis rates on the basis of satellite observed clouds, J. Geophys. Res.-Atmos. 112, D10302, doi:10.1029/2006jd007422, 2007.

Rappenglück, B., Perna, R., Zhong, S. Y., and Morris, G. A.: An analysis of the vertical structure of the atmosphere and the upper-level meteorology and their impact on surface ozone levels in Houston, Texas, J. Geophys. Res.-Atmos. 113, D17315, doi:10.1029/2007jd009745, 2008.

Rappenglück, B., Lefer, B., Mellqvist, J., Czader, B., Golovko, J., Li, X., Alvarez, S., Haman, C., and Johansson, J., 2011: University of Houston Study of Houston Atmospheric Radical Precursors (SHARP), Report to the Texas Commission on Environmental Quality, August 2011, 145 pp.

Skamarock, W. C., Klemp, J. B., Dudhia, J., Gill, D. O., Barker, M., Duda, K. G., Huang, Y., Wang, W., and Powers, J. G.: A description of the Advanced Research WRF Version 3, 1-113, 2008.

Stauffer, D. R., and Seaman, N. L.: Use of 4-dimensional data assimilation in a limited-area mesoscale model .1. Experiments with synoptic-scale data, Monthly Mon. Weather Review, Rev., 118, 1250-1277, 1990.

Stauffer, D. R., and Seaman, N. L.: Multiscale 4-dimensional data assimilation, Journal of Applied Meteorology-J. Appl. Meteorol., 33, 416-434, 1994.

Tucker, S. C., R. M. Banta, A. O. Langford, C. J. Senff, W. A. Brewer, EJ. Williams, B. M. Lerner, H. D. Osthoft, and R. M. Hardesty: Relationships of coastal nocturnal boundary layer winds and turbulence to Houston ozone concentrations during TexAQS 2006. Journal of Geophysical Research: Atmospheres, 115, D10301, doi: 10.1029/2009JD013169 no. D10 (2010).
Willmott, C. J.: On the Validation of Models, Physical Geography, 2, 184-194, doi:10.1080/02723646.1981.10642213, 1981.

Zhong, S. Y., In, H. J., and Clements, C.: Impact of turbulence, land surface, and radiation parameterizations on simulated boundary layer properties in a coastal environment, J. Geophys. Res.-Atmos., 112, D13110, doi:10.1029/2006jd008274, 2007.
Table 1. Major WRF physics and FDDA Options, the numbers in the parentheses are the related settings in WRF namelist file.

| WRF Version | V3.5.1 |
|-------------|--------|
| Microphysics | Lin et al Scheme (2) |
| Long-wave Radiation | RRTMG (4) |
| Short-wave Radiation | New Goddard scheme (3) |
| Surface Layer Option | Monin-Obukhov with CB viscous sublayer scheme (4) |
| Land-Surface Option | Unified Noah LSM (2) |
| Urban Physics | None |
| Boundary Layer Scheme | YSU (4) |
| Cumulus Cloud Option | Kain-Fritsch (4) |
| FDDA | Grid nudging on for all; Observation-nudging on for the OA case |

Table 2. Major CMAQ Options, the text in the parentheses are the related settings in CMAQ build script.

| CMAQ version | V5.0.1 |
|--------------|--------|
| Chemical Mechanism | cb05tucl_ae5_aq; CB05 gas-phase mechanism with active chlorine chemistry, updated toluene mechanism, fifth-generation CMAQ aerosol mechanism with sea salt, aqueous/cloud chemistry |
| Lightning NOx emission | Included by using inline code |
| Horizontal advection | YAMO (Yamartino) (hyamo) |
| Vertical advection | WRF omega formula (vwrf) |
| Horizontal mixing/diffusion | Multiscale (multiscale) |
| Vertical mixing/diffusion | Asymmetric Convective Model (ACM) version 2 (acm2) |
| Chemistry solver | EBI (Euler Backward Iterative) (ebi_cb05tucl) |
| Aerosol | AEROS5 for sea salt and thermodynamics (aeros5) |
| Cloud Option | ACM cloud processor for AEROS5 (cloud_acm_ae5) |
| Boundary conditions | Default static profiles |
Table 3 Statistics of surface T, U-wind and V-wind for three WRF simulations: N – data points; Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M – Model Mean; SD – Standard Deviation; Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD: degree C

| Case  | N    | Corr | IOA | RMSE | MAE | MB  | O_M | M_M | O_SD | M_SD |
|-------|------|------|-----|------|-----|-----|-----|-----|------|------|
| No-OA | 41058| 0.83 | 0.89| 2.0  | 1.5 | 0.9 | 27.4| 28.3| 3.1  | 2.8  |
| 1Hr-OA| 41058| 0.94 | 0.97| 1.0  | 0.8 | 0.0 | 27.4| 27.4| 3.1  | 3.1  |

Surface U wind

| Case  | N    | Corr | IOA | RMSE | MAE | MB  | O_M | M_M | O_SD | M_SD |
|-------|------|------|-----|------|-----|-----|-----|-----|------|------|
| No-OA | 43246| 0.76 | 0.84| 1.4  | 1.1 | -0.6| -1.3| -1.9| 1.6  | 1.9  |
| 1Hr-OA| 43246| 0.81 | 0.89| 1.0  | 0.8 | -0.3| -1.3| -1.6| 1.6  | 1.6  |

Surface V wind

| Case  | N    | Corr | IOA | RMSE | MAE | MB  | O_M | M_M | O_SD | M_SD |
|-------|------|------|-----|------|-----|-----|-----|-----|------|------|
| No-OA | 43246| 0.76 | 0.8 | 2.1  | 1.7 | 1.2 | 0.4 | 1.7 | 2.0  | 2.6  |
| 1Hr-OA| 43246| 0.80 | 0.89| 1.2  | 0.9 | -0.1| 0.4 | 0.4 | 2.0  | 2.0  |

Table 4 Statistics of ozone for CMAQ simulations, see table 3 for column header information

| Case  | N    | Corr | IOA | RMSE | MAE | MB  | O_M | M_M | O_SD | M_SD |
|-------|------|------|-----|------|-----|-----|-----|-----|------|------|
| No-OA | 33308| 0.72 | 0.78| 14.9 | 12.3| 9.3 | 24.4| 33.7| 16.5 | 14.1 |
| 1Hr-OA| 33308| 0.73 | 0.83| 13.8 | 11.0| 6.1 | 24.4| 30.6| 16.5 | 17.4 |
Table 5 Statistics of ozone on 09/25/2013, all day and hour 0 to 13. Both correlation and index of agreement are unitless. The red numbers indicate the three hours (07 CST to 09 CST) when the ozone in 1Hr-OA case is significantly better than the No-OA case due to much improved winds.

| Hr | All | No-OA | 1Hr-OA |
|----|-----|-------|--------|
|    |     | Corr  | IOA    | Corr  | IOA    |
|    | 1150| 0.79  | 0.86   | 0.81  | 0.88   |
| 0  | 48  | 0.04  | 0.30   | 0.40  | 0.46   |
| 1  | 43  | 0.20  | 0.24   | 0.36  | 0.30   |
| 2  | 48  | 0.14  | 0.25   | 0.35  | 0.35   |
| 3  | 48  | 0.19  | 0.30   | 0.32  | 0.35   |
| 4  | 48  | 0.27  | 0.36   | 0.31  | 0.35   |
| 5  | 47  | 0.24  | 0.36   | 0.28  | 0.37   |
| 6  | 47  | 0.33  | 0.38   | 0.35  | 0.37   |
| 7  | 48  | 0.06  | 0.39   | 0.29  | 0.47   |
| 8  | 48  | 0.09  | 0.43   | 0.53  | 0.63   |
| 9  | 47  | 0.05  | 0.41   | 0.55  | 0.74   |
| 10 | 47  | -0.10 | 0.29   | 0.30  | 0.51   |
| 11 | 47  | 0.13  | 0.39   | -0.07 | 0.36   |
| 12 | 49  | 0.09  | 0.38   | 0.25  | 0.40   |
| 13 | 49  | -0.09 | 0.37   | 0.36  | 0.46   |