

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, 1250e1277.

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.

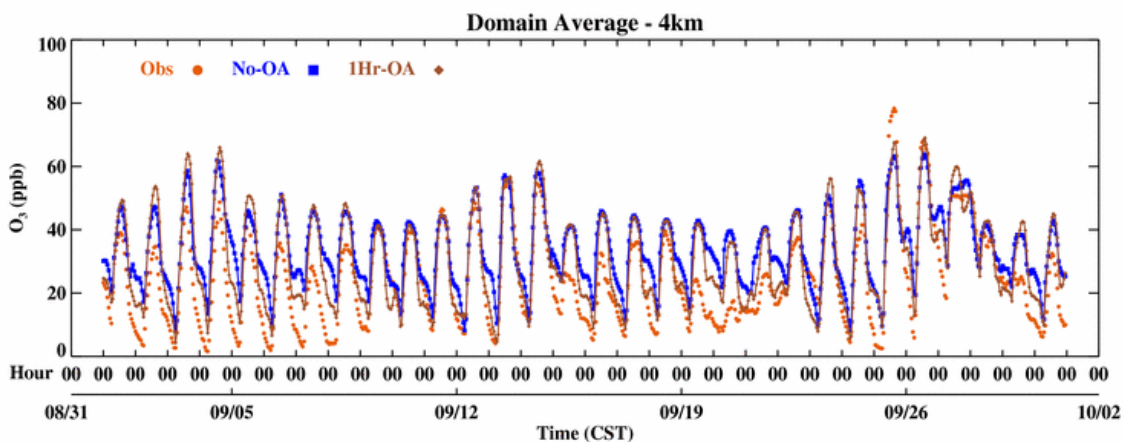
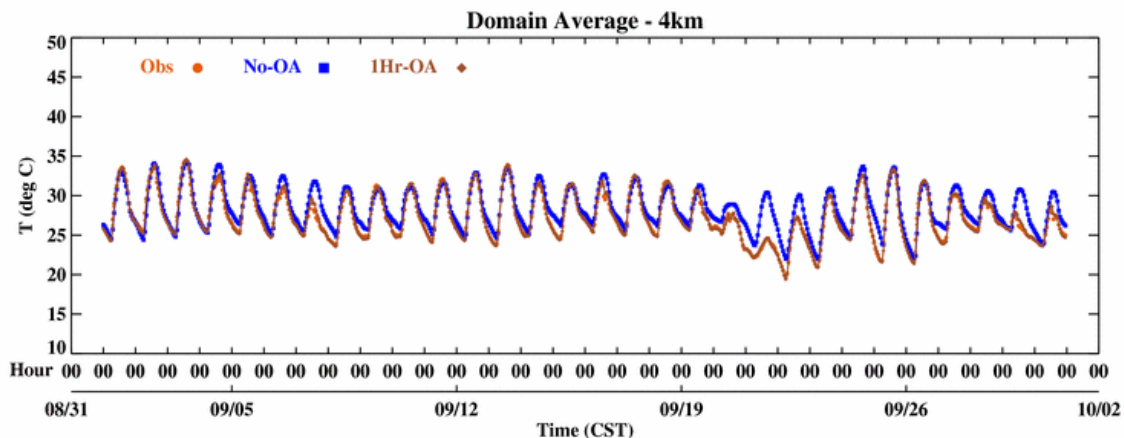
9. Line 242, missing reference for Willmott 1981

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.

1 **The impact of observation nudging on simulated meteorology and**
2 **ozone concentrations during DISCOVER-AQ 2013 Texas campaign**

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13 **Abstract**

14 ~~Air quality modeling demands accurate~~[Accurate](#) meteorological ~~simulations~~[fields are imperative](#)
15 [for correct chemical transport modeling](#). Observation nudging, ~~also known as~~[along with](#)
16 objective analysis ~~(OA)~~, is generally considered [as](#) a low-cost and effective technique to
17 improve meteorological simulations. However, the meteorological impact of ~~OA~~[observation](#)
18 [nudging](#) on chemistry has not been well characterized. This study involved ~~two~~ simulations
19 ~~(with/without OA)~~ to analyze the impact of ~~OA~~[observation nudging](#) on the simulated
20 meteorology and ozone concentrations during the [2013](#) Deriving Information on Surface
21 conditions from Column and Vertically Resolved Observations Relevant to Air Quality
22 (DISCOVER-AQ) Texas campaign period ~~in September 2013~~, using Weather Research and
23 Forecasting (WRF) and Community Multiscale Air Quality (CMAQ) models. The results
24 showed improved correlations between observed and simulated parameters from the
25 ~~OA~~[sensitivity](#) case. The index of agreement (IOA) improved by about 9% for surface
26 temperature and 6-11% for surface zonal (U-WIND) and meridional (V-WIND) winds when

27 ~~OA~~observation nudging was employed. Analysis of a cold front event indicated that ~~OA~~it
28 improved the timing of wind transition during the front passage. Employing ~~OA~~observation
29 nudging also reduced the model biases ~~infor~~ the planetary boundary height predictions. For
30 CMAQ ~~simulated~~simulations, the IOA improved by 6% in the sensitivity case for surface ozone
31 during the ~~whole simulated~~entire simulation period, ~~IOA improved by 6% in the OA case~~. The
32 high ozone episode on September 25th was a ~~typical~~post-front ozone event in Houston. The
33 small-scale morning wind ~~shifts~~near the Houston Ship Channel combined with higher aloft
34 ozone ~~from recirculation~~early morning likely caused the day's ozone exceedance. While
35 ~~OA~~observation nudging did not ~~reproduce~~recreate the wind shifts on that day and failed to
36 reproduce the observed ~~surface and aloft~~high ozone, analyses of surface and aircraft data found
37 that ~~OA results matched better with observations~~observation nudging helped model to yield
38 improved ozone predictions. In a two-hour period during the event, substantially better winds in
39 ~~OA~~the sensitivity case noticeably improved the ozone. Further work on improving ~~OA's~~the
40 capability of nudging to reproduce local meteorological events could enhance a
41 ~~chemistry~~chemical transport model's abilitycapability to predict high ozone events.

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

43

44 1. Introduction

45 ~~Accurate meteorological simulations are essential to photochemical modeling since~~
46 ~~meteorological~~Meteorological variables, such as cloud fraction, winds, planetary boundary layer
47 (PBL) heights and precipitation, significantly impact air quality. They influence the production,
48 transport, and deposition of various chemical species (e.g., Pour-Biazar et al. 2007; Banta et al.
49 2005; Cuchiara et al. 2014). Hence accurate meteorological inputs are imperative for air quality
50 modeling. Common approaches of improving meteorological simulations include the selection of
51 updated and high qualityresolution terrain ~~and input~~data (e.g., Cheng and Byun 2008), ~~the~~
52 optimization of physics and dynamics options (e.g., Zhong et al. 2007); ~~and~~ the implementation
53 of four dimensional data assimilation (FDDA). ~~The air quality modeling group at the University~~
54 ~~of Houston (UH) had performed several sensitivity studies on the various parameterization~~
55 ~~schemes in the recent past (e.g. Zhong et al. 2007; Ngan et al. 2012; Cuchiara et al. 2014).~~

56 FDDA continuously merges new observational data into model simulation such that the model's
57 predictions do not drift away from observations. There are several FDDA methods including
58 nudging (e.g., Stauffer and Seaman 2004) and Variational Methods (3D-VAR or 4D-VAR)~~);~~
59 e.g., Le Dimet and Talagrand 1986; Huang et al. 2009). 4D-VAR obtains optimal states of the
60 atmosphere using multi-time-level observations by globally adjusting a model solution to all
61 available observations over an interval of time. Nudging is a simple yet flexible FDDA method
62 originally developed by Stauffer and Seaman (1990, 1994), and implemented in the Fifth-
63 Generation PSU/NCAR Mesoscale Model (MM5). Not intended for optimal adjustment, nudging
64 is less computationally intensive ~~and~~but needs special care for the nudging coefficients. Nudging
65 involves adding an artificial tendency term to one or more model prognostic equations that
66 reflect the difference between the best estimate of the observed state and the model state at a
67 given location and time. In short, the goal is to “nudge” model state towards observed state.
68 There are several types of nudging such as 3D analysis nudging, surface analysis nudging, and
69 observation nudging- (obs-nudging). In the case of analysis nudging, the model state is nudged
70 toward gridded analysis. The difference between 3D and surface analysis nudging is that 3D
71 analysis (at all model levels except for surface) data are used to improve 3D fields while surface
72 analysis data are used to improve surface fields. In observation nudging, the model ~~is perturbed~~
73 ~~such that its~~ predictions are nudged to match better with observations at individual locations,
74 both ~~on~~ surface and aloft. The MM5 nudging codes were later improved and incorporated into
75 the Weather Research and Forecasting (WRF) model by Liu et al. (2005, 2006). The
76 enhancements enable ~~observation nudging to assimilate a large variety of direct or derived~~
77 ~~observations-~~obs-nudging to assimilate a large variety of direct or derived observations. In
78 WRF, the inputs for obs-nudging are generated by WRF OBSGRID program. This program also
79 performs Objective Analysis (OA) to improve the quality of analysis nudging files. Objective
80 Analysis updates first guess meteorology analysis by incorporating observational data. Since
81 obs-nudging is usually performed along with OA (as in this study) to maximize the benefits of
82 assimilating observations, we also use OA to denote the combined Objective Analysis and obs-
83 nudging processes in case names.

84 The benefit of applying nudging to improve meteorological simulations has been demonstrated
85 in many studies (e.g., Deng 2009; Gilliam and Pleim 2010). However, ~~only a few have extended~~
86 the ~~investigation into chemistry~~impact of the improved fields on air quality simulations-~~has been~~

87 ~~investigated by relatively fewer studies.~~ Otte (2008) showed that ~~analysis nudging is able to~~
88 ~~improve MM5 meteorology, as well as the~~ Community Multiscale Air Quality (CMAQ) ~~model~~
89 ~~with improved MM5 meteorology using analysis nudging was able to better simulate ozone~~
90 chemistry as reflected in ~~ozone-model-measurement~~ statistics. ~~Better~~ ~~Their results indicated that~~
91 ~~better~~ “model skill” scores were achieved for daily maximum 1-hr ozone mixing ~~ratios~~ after
92 analysis nudging over a 35-day ~~period~~ ~~simulation episode~~. Byun et al. (2008) performed over a
93 dozen tests on ~~observation-obs-~~nudging (with analysis nudging turned on) and showed
94 ~~observation-obs-~~nudging improved both winds and temperature in MM5 simulations. The study
95 also gave an example in which improved wind fields on a given day ~~led~~ ~~helped the~~ CMAQ
96 ~~to model~~ better capture the ~~high~~ ozone ~~area~~ ~~hotspot~~ southwest of Houston. Ngan et al. (2012)
97 compared results from several ~~MM5-CMAQ~~ simulations ~~and showed~~ ~~coupled to the MM5 model~~
98 ~~which included nudging. Their results indicated~~ that fully nudged (with both analysis nudging
99 and ~~observation-obs-~~nudging implemented) simulations ~~outperformed a forecast run in~~
100 ~~performed better with respect to~~ both meteorology and ~~ozone~~ chemistry. ~~Their study location~~
101 ~~was Houston Texas, the same as in this study. No detailed~~ ~~However, the~~ statistics ~~were presented~~
102 ~~on the quantitative improvements from the nudging~~ ~~their study cannot be used for interpreting the~~
103 ~~sensitivity of obs-nudging since its base WRF case is a forecast run which used a different~~
104 ~~analysis input.~~ Previous ~~work~~ ~~studies~~ by the current authors (e.g., Rappenglueck et al. 2011;
105 Czader et al. 2013) showed that ~~observation-obs-~~nudging ~~helps to~~ ~~helped~~ correct errors in model
106 wind fields, ~~which are~~ critical to the transport ~~process of air~~ pollutants, ~~as well as the~~ ~~and~~
107 production of secondary pollutants. To the best of the authors’ knowledge, there is no
108 comprehensive ~~existing~~ study on the impact of ~~observation-obs-~~nudging on ~~chemistry, especially~~
109 ~~when air quality simulation using the meteorological WRF model is WRF-.~~

110 This study intends to fill up the gap ~~in the studies mentioned above~~ by investigating the
111 sensitivity of WRF- ~~and subsequently,~~ CMAQ simulations to ~~the use of~~ observation nudging.
112 ~~Although not elaborated here, the WRF-CMAQ sensitivity to different observation nudging~~
113 ~~frequencies was also explored.~~ In theory, higher frequency of ~~observation-obs-~~nudging input
114 should have a higher probability to capture small scale events, such as local wind shifts. These
115 events may only slightly impact local weather, yet ~~they can~~ have a ~~large~~ ~~marked~~ effect on
116 chemistry ~~since it. This is well known that~~ ~~because~~ local stagnation and wind

117 convergence/reversals can contribute to the pollutant build-up (~~e.g., as indicated by~~ Banta et al.
118 ~~(1998);~~ Cheung and Wang ~~(2001);~~ and Tucker et al. ~~(2010)~~).

119 There is a significant presence of ~~petro-chemical~~petrochemical facilities, power plants and motor
120 vehicles in the Houston-Galveston-Brazoria (HGB) region located in southeastern Texas
121 (SETX). The major pollutant in the region is ozone due to the abundant emissions of precursors
122 like nitrogen oxide (NO_x) and Volatile Organic Compounds (VOCs). During the long and hot
123 summer, ozone concentrations often ~~rises~~rise above the ~~threshold level as stipulated in the~~
124 National Ambient Air Quality ~~Standards~~Standard (NAAQS). Consequently, HGB has been
125 designated as an ozone ~~non-attainment~~nonattainment region by the US Environmental Protection
126 Agency (USEPA) (~~http://www3.epa.gov/airquality/greenbook/hnacs.html#TEXAS~~). The ~~petro-~~
127 ~~chemical~~petrochemical plants are largely concentrated in the Houston Ship Channel (HSC) area -
128 just north of the Galveston Bay. The VOCs emitted from the HSC area are highly reactive and
129 have been shown to contribute greatly to the high regional ozone episodes ~~in HGB~~ (e.g.
130 Kleinman et al. 2002; Daum et al. 2003). Depending on the local meteorology, the plumes from
131 HSC may be carried to different locations in HGB and trigger high ozone events on its path.
132 Metropolitan Houston has a high level of NO_x emissions partly due to heavy vehicular traffic in
133 the city. As a result of the large amount of precursor emissions and favorable weather, relatively
134 frequent high ozone events occur in the area. ~~Ngan and Byun (2011) gave an analysis on the~~
135 ~~relationships between the high ozone frequency and underlying weather patterns. They derived~~
136 ~~the weather patterns from a classification scheme using large scale 850 hPa synoptic flow as~~
137 ~~input.~~

138 ~~The~~Due to the reasons listed above, the Houston-Galveston-Brazoria region has been the
139 ~~location~~focus of ~~interest of many~~several air quality studies in the recent past (e.g., Banta et al.
140 2005; Parrish et al. 2009; Lefer and Rappengluck 2010; Olaguer et al. 2013; Czader et al. 2013,
141 Choi et al. 2012; Choi 2014; Choi and Sourì, 2015; Pan et al. 2015). It is a good place for
142 studying ozone production and transport due to the existence of a dense surface monitoring
143 network, as well as several intensive measurement field campaigns which provide ample
144 observational data. For example, in September 2013, the National Aeronautics and Space
145 Administration (NASA), joined by a number of agencies and universities, conducted a field
146 measurement campaign in SETX as part of its the Deriving Information on Surface conditions

147 from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ)
148 program. ~~The NASA (<http://www-air.larc.nasa.gov/missions/discover-aq/discover-aq.html>).~~
149 ~~This~~ program has conducted several air quality and meteorology measurements at ~~several~~
150 different locations in the U.S. The availability of dense surface observations is important ~~in OA's~~
151 ~~capability for obs-nudging~~ to correct erroneous local winds in the model. ~~Without a rich set of~~
152 ~~observations, the~~ The performance of OAobs-nudging will be handicapped without a rich set of
153 observations.

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

164

165 **2. Observational Data and Model Configurations**

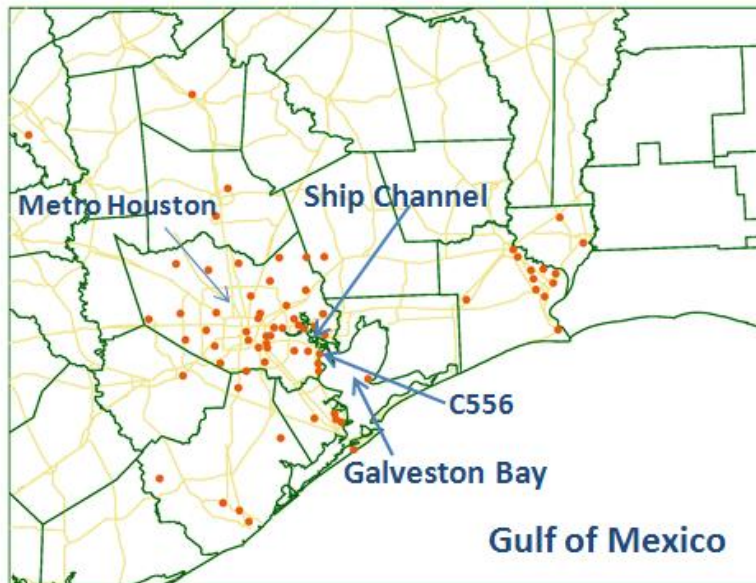
166 ~~For evaluation of the results, this study used regular measurements from the Continuous Ambient~~
167 ~~Monitoring Station (CAMS), operated by the Texas Commission on Environmental Quality~~
168 ~~(TCEQ), as well as PBL and aloft ozone measurements from DISCOVER AQ campaign. For~~
169 ~~observation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

171 **2.1 Observational Data**

172 This study used regular measurements from the Continuous Ambient Monitoring Stations
173 (CAMS) operated by the Texas Commission on Environmental Quality (TCEQ). Additionally,
174 PBL and aloft ozone measurement data were obtained from the DISCOVER-AQ campaign. For

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175 observation nudging, CAMS data and several data streams from the Meteorological Assimilation
176 Data Ingest System (MADIS) were used. The CAMS measurement network collected real-time
177 meteorology and chemistry pollutant data. The measured parameters differ from station to station.
178 The station density at South East Texas (SETX) is relatively high. There ~~are~~were 63 sites
179 having with meteorological measurements and 52 sites having with ozone measurements in the 4-
180 km domain ~~(. The network is represented in Figure 1) during DISCOVER AQ time period.~~ The
181 stations sites are represented by dots, with the La Porte (C556) site labeled. All CAMS
182 observations are accessible at TCEQ website: [http://www.tceq.state.tx.us/cgi-](http://www.tceq.state.tx.us/cgi-bin/compliance/monops/daily_summary.pl)
183 [bin/compliance/monops/daily_summary.pl](http://www.tceq.state.tx.us/cgi-bin/compliance/monops/daily_summary.pl)
184 [http://www.tceq.state.tx.us/cgi-](http://www.tceq.state.tx.us/cgi-bin/compliance/monops/daily_summary.pl)



185
186
187 **Figure 1.** Locations of CAMS sites (dots) in CMAQ 4-km modeling domain during September
188 2013. Metro Houston, Houston Ship Channel, Galveston Bay and Gulf of Mexico are labeled.

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

193 ~~only at this site.~~ For analysis of ~~ozone aloft on September 25~~ ozone, we also used measurements
194 from aircraft P-3B, part of the rich datasets collected during DISCOVER-AQ campaign
195 (~~http://www.air.larc.nasa.gov/missions/discover-aq/discover-aq.html~~). The P-3B data had over
196 100 parameters ~~and which~~ are accessible ~~from the website~~ online.

197 **2.2 Model Configurations**

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

206 **2.2.1. WRF Configurations Setup**

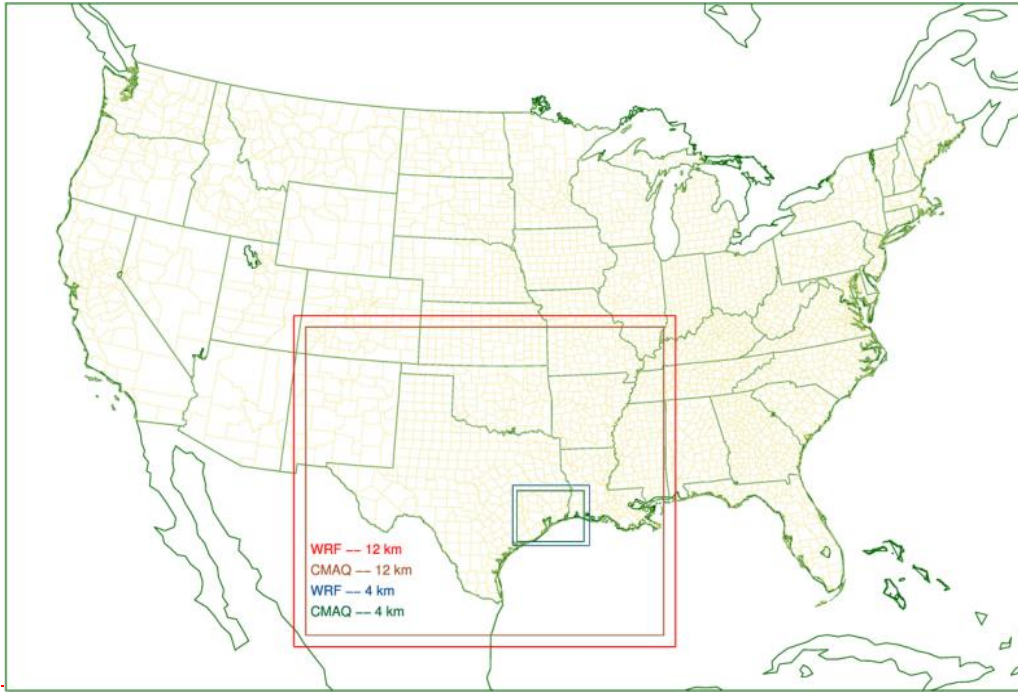
207 Both WRF simulations used the same nested domain and NARR (North American Regional
208 Reanalysis) as input, with grid nudging turned on.

209 **2.2.1.1. Domain Setup**

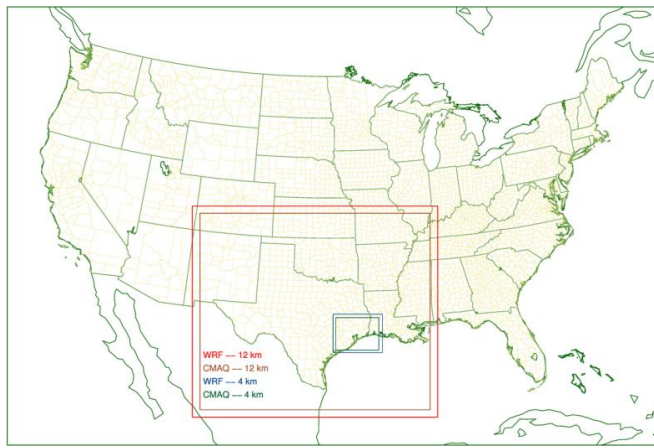
210 Figure 2 depicts the horizontal domain setup. ~~There were two~~ Two nested domains ~~were used,~~
211 with 12-km and 4-km resolution respectively. The 4-km domain covered SETX and a small
212 portion of Louisiana. The 12-km domain (red box) encompassed Texas and ~~parts of~~ a few
213 neighboring states ~~(or parts)~~. The ~~number of grid sizes~~ cells for the 12-km and 4-km domains
214 were 161×145 (E-W by N-S), and 95×77 respectively. The projection type ~~is was~~ Lambert conic
215 conformal (LCC). Three projection parameters, ~~were considered: namely~~ first latitude, the
216 (33°N), second latitude (45°N) and the standard longitude, are 33°N, 45°N and (97°W degrees
217 respectively). The USEPA used the same projection parameters to develop emission inventories
218 for air quality modeling. ~~Vertically both (Mason et al. 2010). Both~~ domains had a vertical
219 resolution of 27 eta layers based on dry hydrostatic pressures. The model top is ~~set to be~~ 100 hPa,
220 corresponding to top layer pressure of the input NARR data.

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222



223 **Figure 2.** Horizontal domains of WRF and CMAQ simulation at 4km4 km and 12km12 km grid
224 resolution (the bigger domains are for 12km12 km WRF and CMAQ and the smaller domains for
225 4km4 km WRF and CMAQ).

226

2.2.1.21. Input Data

227 ~~Both~~The NARR data used for WRF simulations ~~were retrospective runs using NARR analysis as~~
228 ~~input, is~~ downloadable from: ~~http://rda.ucar.edu/datasets/ds608.0/~~. The NARR
229 ~~http://rda.ucar.edu/datasets/ds608.0/~~. The data were based on an Eta 221 grid at 29 pressure
230 levels. Its horizontal resolution was 32-km and the frequency was 3- hourly. The initial and
231 boundary conditions were generated from the NARR analysis by WRF. An alternative to NARR
232 was the Eta-NAM analysis data. However, the data temporal frequency was lowered from 3-
233 hourly to 6-hourly starting 2013. Our ~~testtests~~ showed that it was not as good as NARR ~~for WRF~~
234 ~~input, dataset~~ - likely because of lower temporal resolution.

235 **2.2.1.32. Physics and FDDA Options**

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

251 **2.2.1.43. Observation Nudging with MADIS and CAMS data in WRF**

252 ~~As mentioned in the introduction, observation nudging is regarded as a low-cost and effective~~
253 ~~method for improving meteorological model performance, but it requires additional~~Additional
254 observational data. ~~In this study, we acquired~~ are required to implement obs-nudging and OA. To
255 ~~generate~~ the input ~~files for the OBSGRID program, we processed the~~ observation data ~~and~~

256 | ~~generating files in “little_r” format using similar procedures found in the approach of~~ Ngan et al.
257 | (2012) and Czader et al. (2013). Observational data came from the MADIS and TCEQ CAMS.
258 | MADIS (<https://madis.ncep.noaa.gov/>); is a National Oceanic and Atmospheric Administration
259 | (NOAA) program, which collects, integrates, quality-controls, and distributes observations from
260 | NOAA and other organizations. Additional information is available online.
261 | <https://madis.ncep.noaa.gov/>. The four MADIS datasets used for ~~observation_obs-~~nudging were
262 | NOAA Profiler Network (NPN), Cooperative Agency Profilers (CAP), Meteorological Terminal
263 | Aviation Routine (METAR) weather report and NOAA Radiosonde (RAOB). The METAR
264 | dataset was collected by mostly first-order, METAR reporting, surface monitoring stations.
265 | NPN, RAOB and CAP were the most commonly used upper air datasets.

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

273 | Theoretically, ~~observation_obs-~~nudging updating at a higher frequency should enhance the
274 | model’s performance. A typical frequency of input analysis data is 3-hourly while the frequency
275 | for observational data is hourly. The 3-hourly frequency of input analyses may be the reason for
276 | the default 3-hour time_ interval in WRF’s OBSGRID settings for generating the ~~observation~~
277 | ~~obs-~~nudging files. Since there were few existing ~~OA_obs-nudging~~ studies related to air quality
278 | and we are not aware of any reference to the adoption of 1-hour input frequency, we assume that
279 | all the existing studies used the default 3-hour interval. As the WRF model allows the interval to
280 | be set to 1-hour or smaller when corresponding observational data were available, we tested both
281 | 1-hour and 3-hour scenarios. The results indicated that 1-hour ~~OA_obs-nudging~~ had slightly better
282 | performance than the 3-hour one. As a result, this study adopted 1-hour temporal frequency for
283 | observation nudging. The quantities that were nudged were temperature, moisture, and the two
284 | wind components (U-WIND and V-WIND). Obs-nudging for moisture was not performed in

285 this study. This was based on our past experiences since performing moisture nudging sometimes
286 trigger excessive artificial thunderstorms which disrupted model flow fields.

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

294 ~~In WRF, there were a few namelist variables controlling the frequency of grid nudging and~~
295 ~~observation nudging. The first one was “interval_seconds”, which should match the interval of~~
296 ~~input grid nudging files (“met_em”). The second one was “sgfdda_interval_m”, matching the~~
297 ~~interval of surface grid nudging files (“sgfdda”). In our simulation, both intervals were equal to~~
298 ~~3 hours. The third one was “auxinput11_interval”, controlling the updating interval for~~
299 ~~observation nudging files (“OBS_DOMAIN”). The last one, “obs_ionf”, determined the nudging~~
300 ~~frequency relative to internal integration time step. For example, if the integration time step for~~
301 ~~the coarse domain is 30 seconds, setting “obs_ionf” to 1 means performing OA every 30~~
302 ~~seconds, while setting “obs_ionf” to 3 means performing OA every 90 seconds. In our~~
303 ~~simulation, “obs_ionf” is set to 1.~~

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

307 2.2.2. EmissionEmissions Processing

308 For anthropogenic sources we utilized the National EmissionEmissions Inventory of 2008
309 (NEI2008) generated by the USEPA. ~~The mobile~~ (USEPA, 2011). Motor vehicle emissions for
310 this inventory were processed ~~with EPA's using the EPA's~~ Motor Vehicle EmissionEmissions
311 Simulator (MOVES). ~~Using~~ (USEPA, 2015). The inventory was processed using the Sparse
312 Matrix Operator Kernel Emissions (SMOKE) Modeling System_model v3.1 ~~the inventory was~~
313 converted to obtain gridded emission rates ~~as well as to emission species as listed in and~~

314 ~~speciated for~~ the Carbon Bond 05 (CB05) chemical mechanism ~~that is used for use~~ in ~~the~~ CMAQ
315 ~~modeling model~~. The biogenic emissions were ~~estimated modeled~~ using the Biogenic Emissions
316 Inventory System (BEIS) ~~v-3v3~~.14. Although NEI2008 might have overestimated NO_x emissions
317 in Houston (e.g., Choi 2012; Czader et al. ~~2015~~ ~~which could have impacted on ozone formation~~
318 ~~in the region, 2015~~), we used base NEI2008 without adjustment because the adjustment of the
319 NO_x emission also has large uncertainty. Pan et al. (2015) showed that the CMAQ ozone
320 performance using NEI2008 appears reasonable.

321 2.2.3. CMAQ Configurations

322 The USEPA's CMAQ (Byun and Schere 2006) version 5.0.1 was adopted for this study;
323 ~~following the choice of several other Houston~~. ~~Several~~ air quality ~~modeling~~ studies ~~focusing on~~
324 ~~the Houston area have used this model~~ (e.g., Foley et al. 2010; Czader et al. 2013, 2015; Choi
325 2014; Pan et al. 2015). CMAQ horizontal domains were slightly smaller than the WRF
326 counterpart in order to avoid the discontinuity near the domain boundary. The domains were
327 shown in Figure 2 as green and brown boxes. The chemical boundary conditions for all the
328 species in the 4-km domain were derived from 12-km domain air quality forecasting results
329 ~~(http://spock.geosc.uh.edu)~~. ~~Vertically, CMAQ inherited~~ ~~(http://spock.geosc.uh.edu)~~. ~~The model~~
330 ~~used~~ the same ~~layers from vertical structure as~~ WRF ~~without layer collapsing~~. Major CMAQ
331 configurations ~~were described are listed~~ in Table 2. ~~The texts in the parentheses were the values~~
332 ~~in the CMAQ build script~~.

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

338

339 3. Evaluation Metrics

340 To assess model performance against observations, we computed a set of five statistics including
341 Pearson correlation, index of agreement (IOA, Willmott 1981), mean bias (MB), root mean

342 square error (RMSE), and Mean Absolute Error (MAE),). This list is similar to one used by Li et
343 al (2008) for model performance evaluation. The goal is to have a comprehensive comparison
344 between model and observation time series. ~~These~~The set of five statistics ~~have been frequently~~
345 ~~used for performance evaluation in modeling community.~~was divided into three groups:

346 ~~The set~~1) Evaluation of ~~five statistics was divided into three groups:~~

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

- 349 • Mean Bias (MB)
- 350 • Mean Absolute Error (MAE)
- 351 • Root Mean Square Error (RMSE)

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

- 353 • Correlation

354 3) A composite performance index, index of agreement (IOA or d)~~suggested by Willmott~~
355 ~~(1981)~~, unitless

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

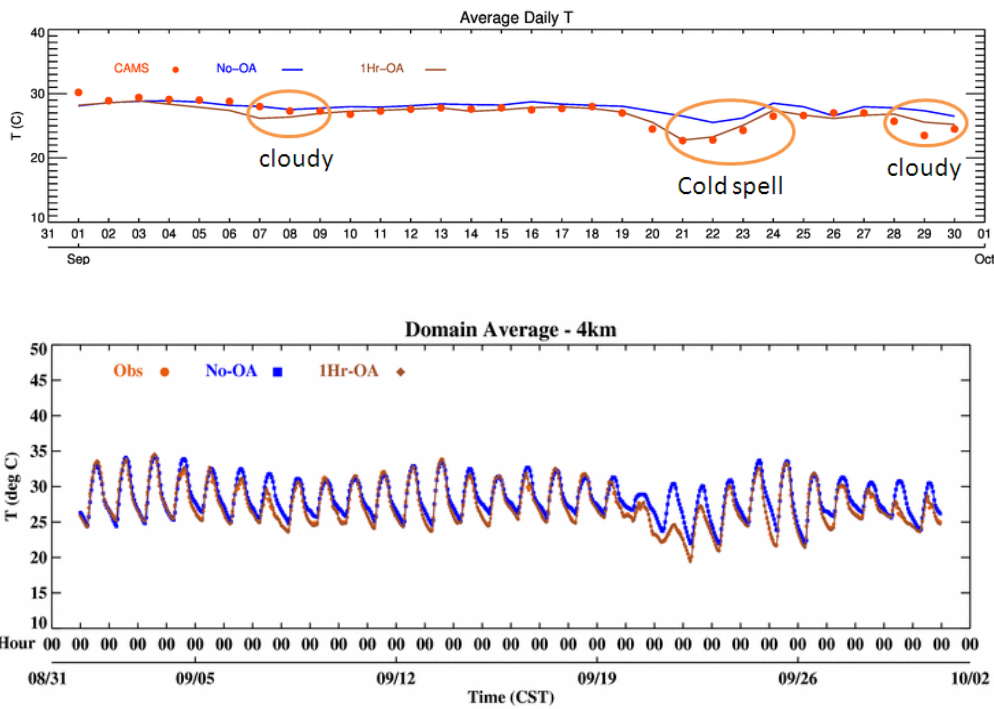
360 ~~Additionally, the mean and the standard deviation (Std. Dev.) of model values and observations~~
361 ~~were included as a reference.~~

362

363 **4. General Meteorological and Ozone Conditions in September 2013**

364 The weather during ~~the~~ September 2013 ~~simulation period~~ was relatively dry with mostly
365 southerly, easterly or southeasterly winds. From 09/05 to 09/19 ~~(all dates are in MM/DD~~
366 ~~format)~~, September, there was a lack of influence of strong synoptic weather systems. Shifting

367 wind patterns were observed during the period: light northeasterly in the early morning gradually
 368 turned clockwise to southeasterly in the afternoon and evening hours. In this period, winds
 369 shifted from southeast to near east and there were more clouds after 09/10 September. The only
 370 cold front arrived on the early morning of 09/21 September. Figure 3 shows the daily-regional
 371 average temperatures and periods marked with for the period and it can be seen that 21
 372 September has the lowest daily high temperature drop. Although not very significant to
 373 photochemistry, temperature drop is usually a good proxy for the critical factors affecting ozone
 374 production or transport such as cloudiness, wind. The influences of the cold air intrusion lasted
 375 till early 25 September. Winds turned into southerly in the afternoon of the 25th and
 376 precipitation warming continued in the next few days until the 28th.



377

378

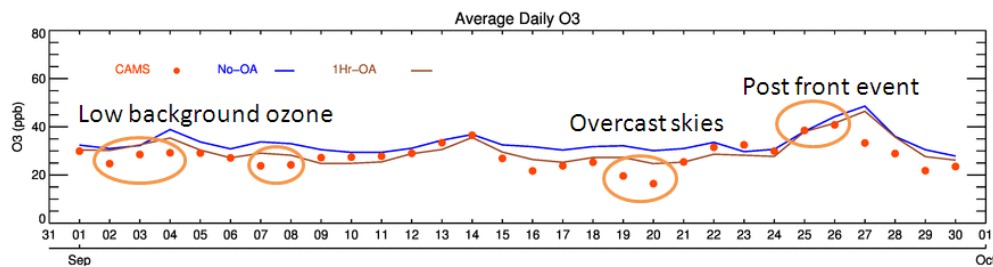
379 **Figure 3.** Regional dailyhourly temperature averaged over all available (typically around 1200)
 380 hourly CAMS observations, two model cases also included for September of 2013.

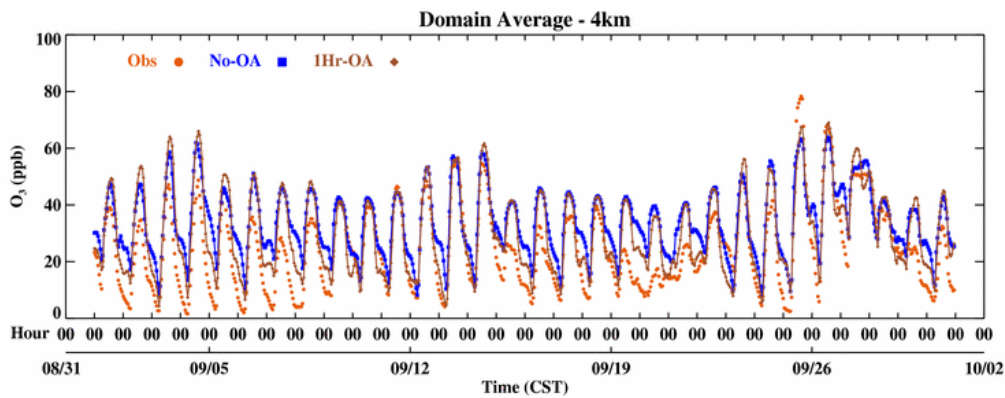
381 ~~Rain~~Light rain events occurred on 09/02, 09/10, 09/16, 09/19 to 09/21 and 09/28 to 09/30. ~~None~~
382 ~~of them was heavy.~~ The 09/20 and 09/21 events consisted of widespread light to medium
383 showers. Besides the above-mentioned dates, there were a few other days with sporadic drizzles.

384 A majority of the days between 09/01 and 09/20 were ~~mostly~~either sunny ~~to mostly~~or cloudy.
385 The periods from 09/08 to 09/10 and 09/18 to 09/20 had more clouds than other days. The period
386 from 09/21 to 09/30 was influenced by a cold front passage. The days between 09/22 and 09/24
387 were sunny and ~~cool.~~ ~~Then the cold.~~ ~~The~~ surface wind reversed direction during ~~mid~~midday of
388 09/25 and brought clouds back from 09/26 to 09/30.

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

393 Figure 4 ~~shows~~plots the ~~daily~~hourly regional averaged ozone. On most days, the ~~observed in-situ~~
394 averaged ozone ~~fell~~concentrations were below ~~30~~70 ppb. Since the winds after dawn consistently
395 pushed the precursors from the industrial area to the southwest of the city, the wind pattern did
396 not favor the local ozone production. The daytime winds also contained a persistent easterly
397 component which moved the pollutants away from the Houston metropolitan area. In the first 10-
398 day period, ~~less~~low background ozone originating from the Gulf of Mexico contributed to the
399 low-ozone days. With overcast skies on the 19th and the 20th, ~~hourly high~~ ozone values dipped
400 below ~~20~~30 ppb. The two highest ozone days; characterized by post-frontal ozone events; were
401 the 25th and the 26th.





403
 404 **Figure 4.** The dailyhourly regional averaged ozone for the two cases (No-OA and 1hr-OA) at the
 405 stations which include observation surface O₃ over the 4km domain for September of 2013.

406
 407 **5. 5. Evaluation of Simulation Results**

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

413 **5.1. Meteorology**

414 **5.1.1. Temperature**

415 The comparison of regional ~~averaged daily temperatures~~ average hourly temperature for the
 416 analyzed timesimulation period is shown in Figure 3. The regional observed averaged
 417 daily surface temperature was calculated by averaging the hourly temperature from ~60 CAMS
 418 sites in the 4-km model domain. ~~Despite the differences in~~ The base case temperature was too
 419 high compared to the in-situ measurements. For example, the days with more
 420 clouds/precipitation, No-OA maximum temperature for the simulated averaged temperatures
 421 tracked 21st was 30°C compared to 25°C for the in-situ data very well. It was also evident that,

422 ~~The high biases in the base case are sharply reduced in~~ the “1Hr-OA” case ~~and temperature~~
423 ~~matched better with the observations~~ for several time periods, especially for September 20-23.

424 ~~The statistics of hourly surface temperature are presented~~listed in Table 3. With higher IOA and
425 lower mean biases (MB), the “1Hr-OA” case was clearly better than the base case “No-OA”. The
426 IOA of “1Hr-OA” was about 9% higher than the base case.

427 5.1.2. Winds

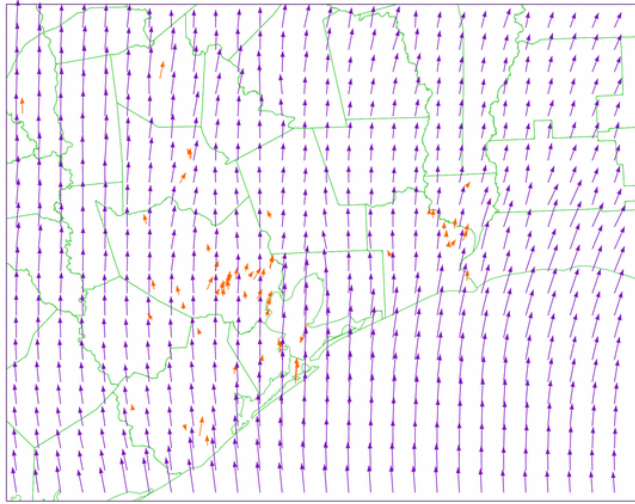
428 ~~Wind fields are known to significantly affect chemistry (e.g., Banta et al. 2005, 2011; Darby~~
429 ~~2005).~~In ozone chemistry, winds affect the accumulation of precursors and hence the resulting
430 ozone production.~~Winds (e.g., Banta et al. 2005, 2011; Darby 2005). They~~ are also responsible
431 for dispersing high ozone and bringing in background ozone. ~~In HGB, prevailing~~ Prevailing
432 summer time southerly to southeasterly winds in the summer time~~HGB region~~ significantly
433 ~~lowered~~lower the ozone ~~level~~concentrations in the ~~metr~~metropolitan area. Therefore, high
434 ozone events usually occur when such wind ~~pattern changes~~patterns change. Cold front
435 ~~intrusion, intrusions~~ coming as early as late August, ~~blows~~ blow pollutants to the south. As a
436 result, an area of high ozone develops in the Gulf. ~~A few days later,~~ Following cold fronts
437 ~~weaken~~weakening and the weather warming up, reversing winds can bring high ozone back to
438 land. High ozone may also ~~occur~~occur during intra-day ~~pollutant~~ recirculation events when
439 pollutants previously blown away from industrial zone are brought back by reversing winds. ~~The~~
440 high Correctly simulating these recirculation events is particularly important in predicting the
441 high ozone event caused by post-front conditions. The ozone event in the HSC area on 09/25 was
442 likely due to a combination of local recirculation caused by onset of the bay breeze and increased
443 background ozone brought in by ~~the much larger scale southerly flow from the Gulf~~ transport.

444 Due to the land-water thermal contrast and the different size of the Galveston Bay and the Gulf
445 of Mexico, the western shore of the Galveston Bay often experiences a successive onset of bay
446 breeze and sea breeze in the summer. The bay breeze is typically a weaker easterly while sea
447 breeze is a stronger southeasterly. Sea breeze usually comes one to a few hours later after the bay
448 breeze. The bay breeze and the subsequent sea breeze phenomena in Houston were described by
449 Banta et al. (2005).

450 The statistics of zonal (U-WIND) and meridional (V-WIND) wind components are listed in
451 Table 3. The purpose of choosing U and V over wind speed and direction is to avoid the
452 anomalies in the wind direction statistics. For example, although wind direction of 5 and 355
453 degrees are close, the statistics suggest that they are distinctively different.

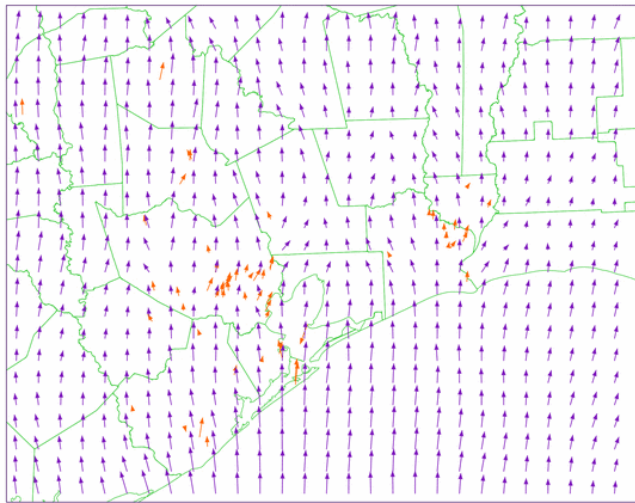
454 For both U and V components of wind, “1Hr-OA” had higher correlation and IOA than “No-
455 OA”. The model performance on U and V are similar, with the correlation in a range of 0.76 to
456 0.81 for all the cases. ~~As a reference~~For comparison, the performance of the OA case (“M1”) in
457 Ngan et al. (2012) is very close to that in this study, with a correlation of 0.75 for U and 0.82 for
458 V. In terms of IOA, the OA case had a larger lead over the base case, ahead by 5-6% in U and
459 10-11% in V over the base case. This can be explained by the much reduced wind biases in the
460 OA case.

461 The base case had consistently stronger winds, especially the southerly component, than the
462 observation. This was reflected in the mean bias “MB”, as well as the model mean “M_M”.
463 Winds were reduced significantly after OA was performed. Interestingly, the high southerly bias
464 in “No-OA” turned slightly negative after OA. Winds originating from the Gulf were also
465 stronger in base case, which played a role in raising the ozone level ~~in comparing to the~~
466 area-sensitivity case. Figure 5 illustrated the slowing down of southerly winds after observation
467 nudging. As a result, ~~winds of nudging, the wind vectors~~ matched better to the observations.



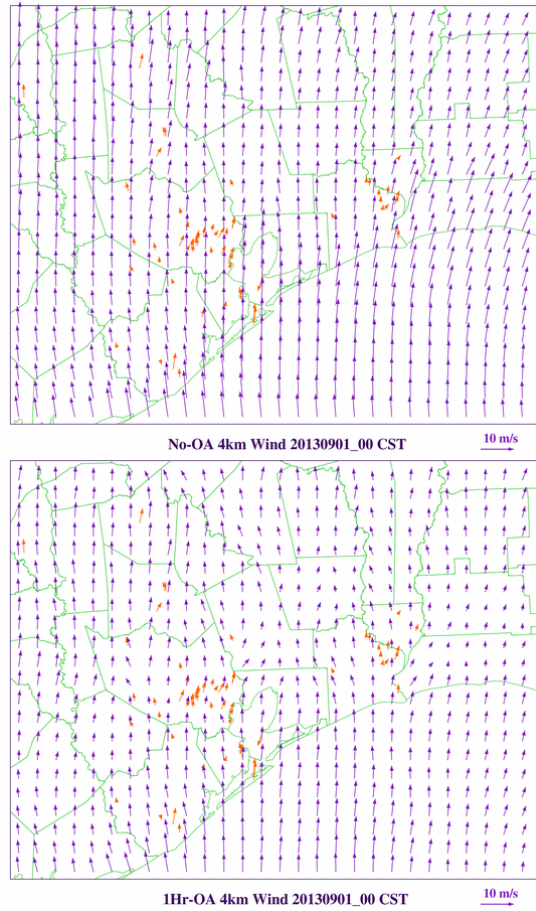
No-OA 4km Wind 20130901_00 CST

10 m/s



1Hr-OA 4km Wind 20130901_00 CST

10 m/s



469

470 **Figure 5.** Model and observed winds at 09/01_00 CST: No-OA (top) and 1Hr-OA (bottom).
 471 Model winds are blue arrows and the observations are orange arrows. Stronger southerly winds,
 472 especially along coastal region, were reduced in the OA case.

473 5.1.3. PBL height

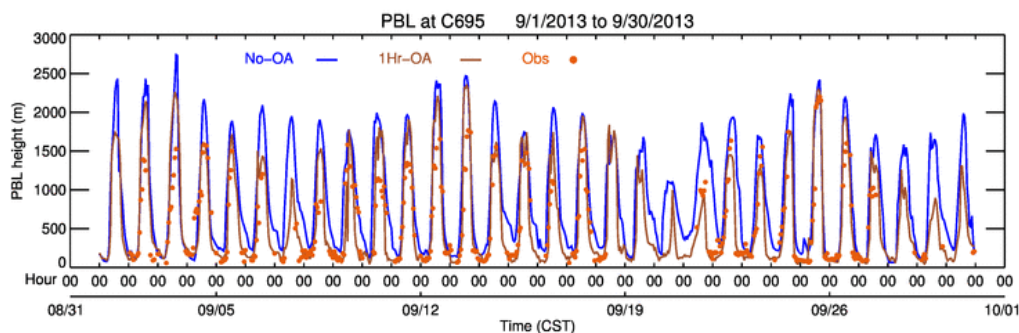
474 Atmospheric pollutants are largely confined in the PBL as most of the emissions sources are
 475 close to the ground level. Hence the PBL height plays a critical role in mixing and spreading the
 476 pollutants. Haman et al. (2014) studied the relationship between ozone level and PBL height at a
 477 Houston CAMS site and found that nighttime and early morning PBL heights were consistently
 478 lower on high ozone days than on low ozone days. Czader et al. (2013) pointed out that the

479 model underprediction of PBL during nighttime may have caused the CO overprediction at the
480 same site. CO is a good proxy for understanding model's transport since it has low reactivity and
481 a relatively long life time in the troposphere.

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

487 ~~The PBL height data were taken at an urban site very close to CAMS site C695, located on~~
488 ~~University of Houston campus. A study by~~ Haman et al. (2012) showed that ~~Houston's the~~ daily
489 maximum PBL height ~~at the University of Houston site indicated previously~~ reached its highest
490 values of slightly over 2000 m in August. In September, typical daily maximum PBL height was
491 1500 m at 15 CST while daily minimum was just below 200 m between 00 CST and 06 CST.

492 The comparison of observed and model PBL height is shown at Figure 6. ~~The Our results~~
493 ~~indicated that the~~ model tended to overpredict the daily maximum ~~and OAPBL height; obs-~~
494 ~~nudging~~ helped to reduce the ~~overprediction overprediction~~. For the daily minimum PBL height,
495 "No-OA" ~~case~~ had slightly high biases while the OA case matched quite well with
496 ~~observations in-situ height data~~. The observed minimum PBL height was lower than that reported
497 by Haman et al. (2012), likely due to the cloudy ~~condition conditions prevailing~~ in September
498 2013. There was no apparent explanation on the reduced daytime PBL biases in the OA case
499 than the base case, but it is likely the results of improved winds and temperatures in PBL.

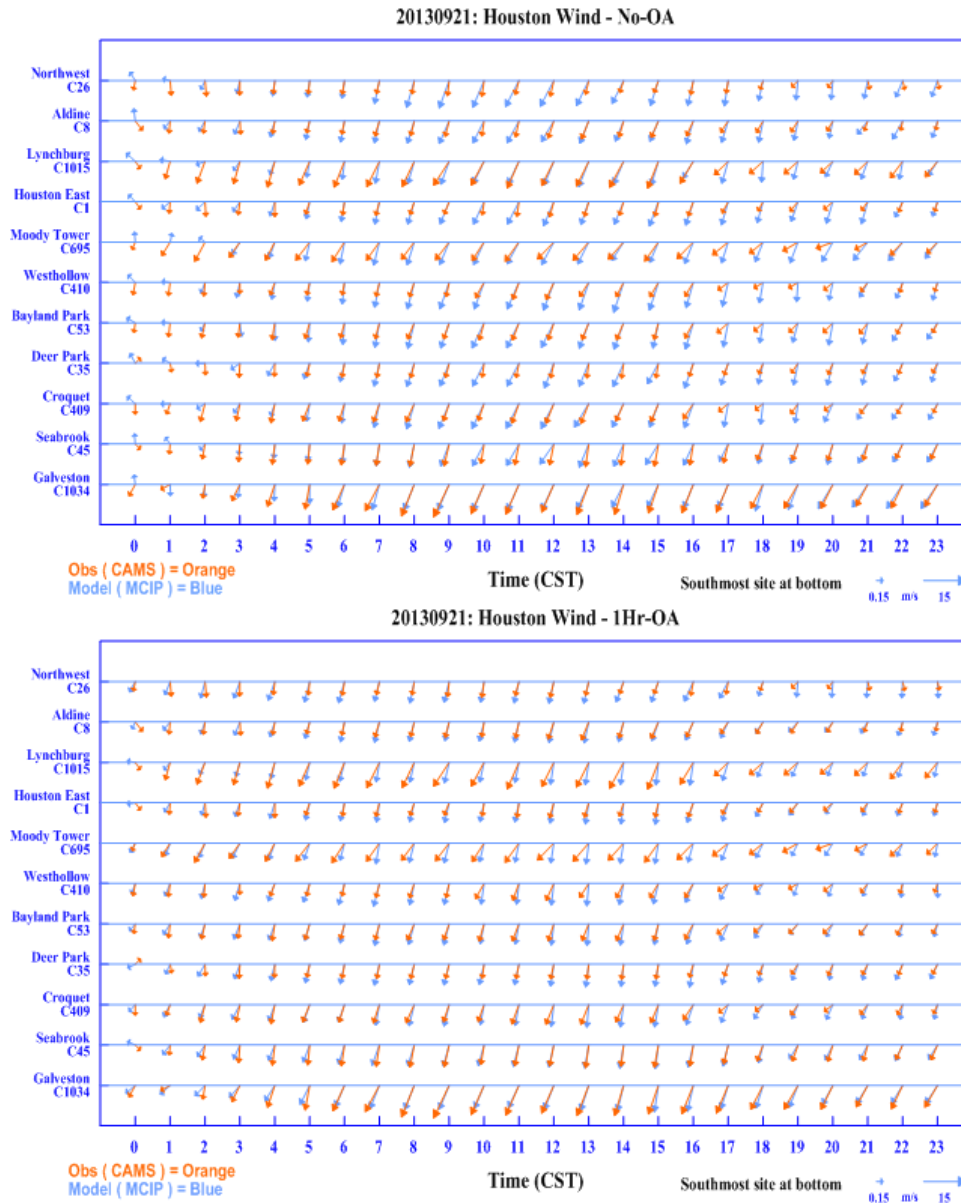


501 **Figure 6.** Planetary Boundary Layer (PBL) height time series at CAMS C695 for September
502 2013.

503 **5.1.4. Cold Front Passage**

504 The surface winds on 09/20 were overwhelmingly southerly in the region and reversed on ~~09/21~~
505 September due to the arrival of a cold front. The hour-by-hour wind shifts for 11 sites in HGB on
506 ~~09/21~~ September are plotted in Figure 7. The sites are sorted by latitude with the southernmost
507 site, Galveston C1034, located at the bottom row. There was only one site, Deer Park C35,
508 showing weak southerly at 00 CST while all the others had mostly weak northerly. Starting from
509 01 CST, winds in the entire HGB area turned northerly to northeasterly and continued gaining
510 strength in the next few hours, indicating cold air had taken over the region.

511 Both cases performed reasonably well on 09/21 and the timing of wind shift was captured quite
512 accurately; although “No-OA” lagged ~~about an hour behind by ~ 1 hr~~. The winds turned weak
513 northerly at 00 CST for most sites ~~and but the~~ “No-OA” ~~case~~ still showed ~~the wind direction to be~~
514 all southerly. Besides the timing, ~~OA also helped moderate the winds as~~ the northeasterly winds
515 in “No-OA” case sometimes were too strong; ~~obs-nudging helped moderate the winds~~. The
516 ~~reduced~~ V-wind bias ~~in “1Hr-OA” was also evident in the wind model-measurement statistics on~~
517 ~~09/21 is reduced from -2.5 m/s to -0.6 m/s after OA was performed. The performance of the OA~~
518 ~~case during cold front passage was consistent with our past simulations. September.~~



519

520 | **Figure 7.** Hourly model (blue) and CAMS (orange) winds at 11 sites on ~~09/21~~ September: No-
 521 OA (top) and 1hr-OA (bottom). The 1hr-OA case is better in 00 CST to 02 CST and 17 CST to
 522 20 CST.

523 5.2. Ozone

524 5.2.1. Regional ~~Daily~~ Average Hourly Ozone

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

534 ~~Although model had high biases for majority of the days, biases were consistently lower for the~~
535 ~~OA case during two periods: 09/07 a reasonably good job on capturing the timing of intra-day~~
536 ~~variations. However, both cases tended to 09/09 overpredict the daily highs and 09/17 to 09/21.~~
537 ~~The reduced biases were likely due to daily lows, especially in the first 8 days and between 15~~
538 ~~and 21 September. An obvious departure is the 25th – both cases missed the daily high. During~~
539 ~~the model high bias period, the OA case usually did better in reaching the daily low although it~~
540 ~~overpredicted the high a bit more than the base case. The night time biases were reduced likely~~
541 ~~because the lower southerly winds in the OA case since model had higher background transported~~
542 ~~less ozone originated from the Gulf to the land.~~

543 ~~In Figure 4, the first three orange circles showed the days with high model biases. The first two~~
544 ~~circles consisted of days with lower Our results suggested that the modeled ozone concentrations~~
545 ~~were likely higher in the Gulf than “normal” background ozone actual. However during the 2nd –~~
546 ~~4th and 7th-8th of September, the incoming ozone from the Gulf was markedly lower. Since the~~
547 ~~model ozone had fixed boundary values, the model was unable to capture the daily ozone~~
548 ~~variation at the boundary. The third circle consisted of days with model showed the highest~~
549 ~~biases during period of the 19th -20th likely due to overcast skies. The high model biases were~~
550 ~~likely the result of problems and uncertainties in model's cloud fields and high background~~
551 ~~ozone values. Despite the overprediction, the biases in OA case are notably lower during the~~

552 | ~~nights of 19th and 20th.~~ A future study to upgrade the accuracy of cloud fraction using remote
553 | sensing data (e.g., MODIS) should be helpful in explaining the biases.

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

560 | **5.2.2. Performance Statistics**

561 | The ozone statistics ~~were displayed~~are listed in Table 4. Both cases had very close correlation of
562 | 0.72 and 0.73. However, the mean biases in the OA case were lower by 3.2 ppb, which helped
563 | raise the IOA from 0.78 to 0.83. The model standard deviation increased in the OA case and
564 | matched better with ~~observation~~that of the in-situ data. The improvement in IOA was slightly
565 | less ~~was compared to that for~~ temperature and winds.

566 | **5.2.3. High ozone episode after the passage of a front**

567 | In SETX, high ozone events during the fall season usually occurred after the passage of a cold
568 | front (e.g., Rappenglück et al. 2008; Ngan and Byun, 2011; Ngan et al. 2012; Haman et al.
569 | 2014). Two factors may have contributed to the post-front ozone events: 1) ~~following~~Following a
570 | cold spell ~~winds reverse direction and subsequent,~~ light winds and sunny skies create an ideal
571 | condition for ozone production and accumulation. 2) ~~wind~~Wind reversal ~~transports~~may transport
572 | back the pollutants that were previously blown into the Gulf ~~previously, a phenomenon~~
573 | commonly known as recirculation.

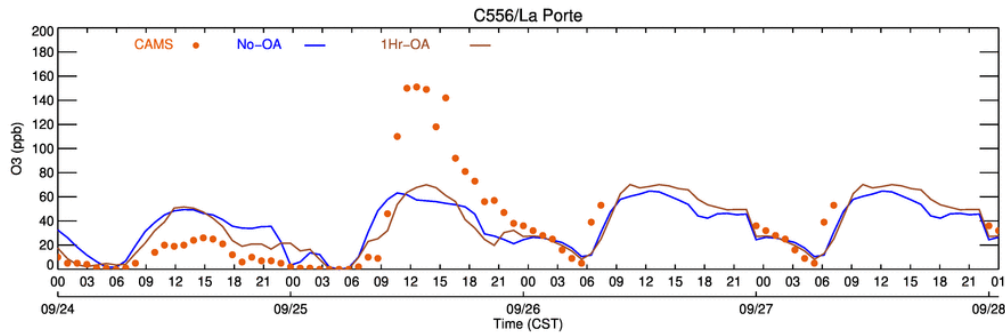
574 | During the DISCOVER-AQ period, the two days with highest ozone concentrations were
575 | ~~09/25~~the 25th and ~~the day 09/26 (26th of September as indicated in~~ Figure 4), ~~but the two days~~
576 | ~~exhibited different patterns~~. The 1-hour maximum ozone on ~~09/25~~the 25th was localized and
577 | higher by about 40 ppb ~~than the 26th~~. In addition to heightened background ozone on the 25th,
578 | the major contributor was the production resulting from favorable weather conditions: sunny,
579 | overall light winds and shifting winds over the industrial area. The light morning land breeze

580 | carried pollutants from ship channel area to the Galveston Bay. As the day warmed up, the bay
581 | breeze started to develop and carry pollutants back to the land. This localized circulation was
582 | described by Banta et al. (2005). Ngan et al. (2012) reported the same phenomenon in their
583 | Texas Air Quality Study-II 2006 study. ~~09/26 is characterized by elevated background ozone~~
584 | ~~from early morning to late night.~~

585 | Figure 8 shows the ozone time series ~~of for the~~ La Porte (C556), in Figure 1) site located in the
586 | HSC area ~~(Figure 1). In September, the~~. The highest hourly ozone ~~of for September,~~ 151 ppb
587 | occurred ~~at C556 here~~ at 13 CST ~~of 09/25. From 9 CST to 12 CST, ozone on the 25th.~~ Ozone
588 | rose from 10 ppb to 150 ppb. ~~The large between 09-12 CST. Such a dramatic~~ increase in ozone
589 | was likely the result of ~~chemical production~~ increased photochemical activity under favorable
590 | meteorological ~~condition~~ conditions in an area with accumulated precursors. Figures 9 and 10
591 | depict the wind and ozone concentrations at 08 CST and 13 CST.

592 | ~~From the~~ The wind plots of Figure 9, ~~we can see~~ indicate that the winds in the HGB region at 8
593 | CST were light northerly for sites located on the north side while ~~winds they~~ were ~~mostly~~
594 | westerly for the sites in the middle and south. The base case winds were all northerly while the
595 | OA case had northwest winds for north side and west winds for the middle and south. ~~The~~ Hence,
596 | the model winds in OA case ~~were much~~ are more realistic than the winds in base case. The 909
597 | CST winds were similar to those of 808 CST. As a result, the ozone statistics in Table 5 showed
598 | that the OA case had much better correlation and IOA than the base case during 8-908-09 CST.
599 | This example demonstrated ~~OA's~~ the ability of obs-nudging to correct erroneous winds.
600 | However, later events showed ~~OA~~ it may not always be able to perform consistently.

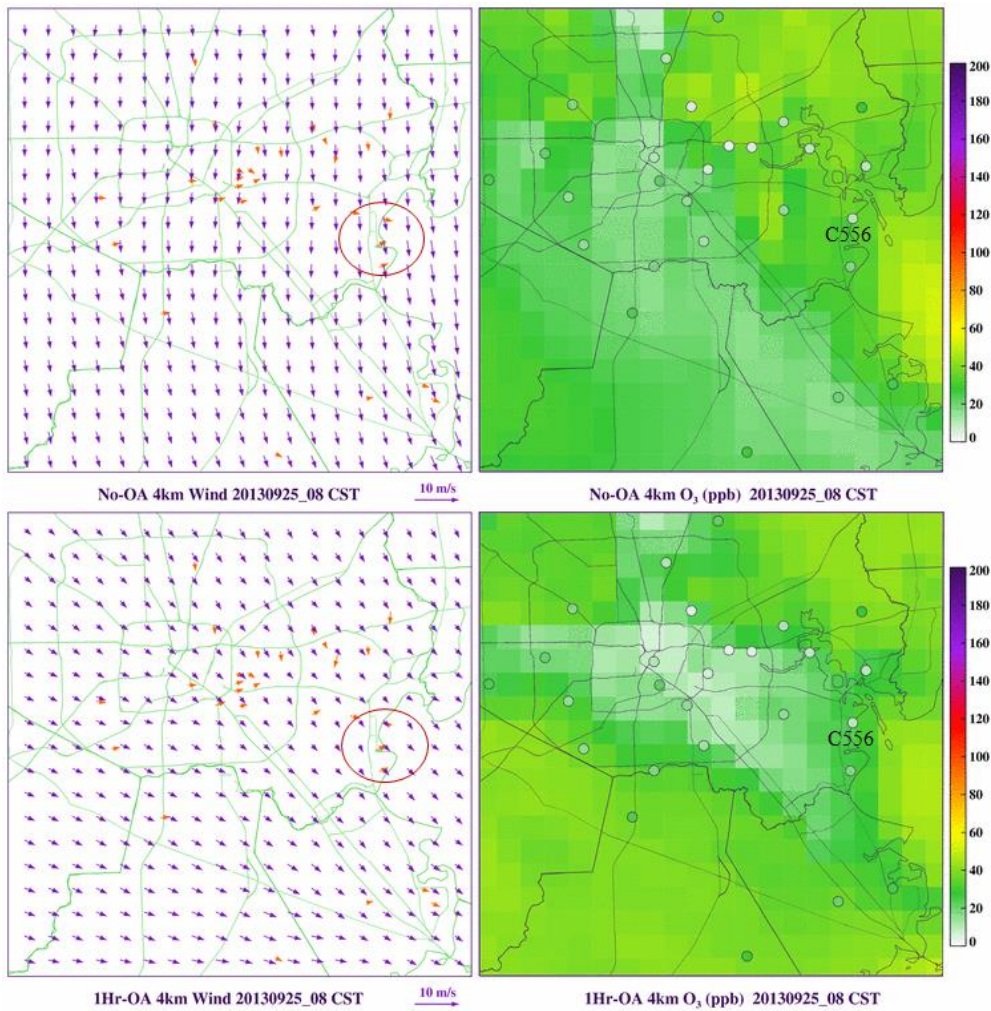
601 | The bay breeze started to develop at 10 CST near the C556 site. The early onset was likely to be
602 | related to ~~the~~ warming up on the previous afternoon on 09/24 ~~(as indicated in Figure 3).~~ At 10
603 | CST most other sites to the west of HSC experienced light northwest winds while ~~winds those~~ at
604 | HSC ~~were~~ originated from the northeast. Combined with the easterly bay breeze, a convergence
605 | zone was formed just below C556, where emissions from the HSC area stalled and accumulated.
606 | At 13 CST, the whole region had light winds and the bay breeze was well developed. The
607 | highest ozone indeed appeared in C556 and its vicinity. The rapid increase of ozone
608 | concentration for C556 between 909-13 CST is shown in Figure 8.



609

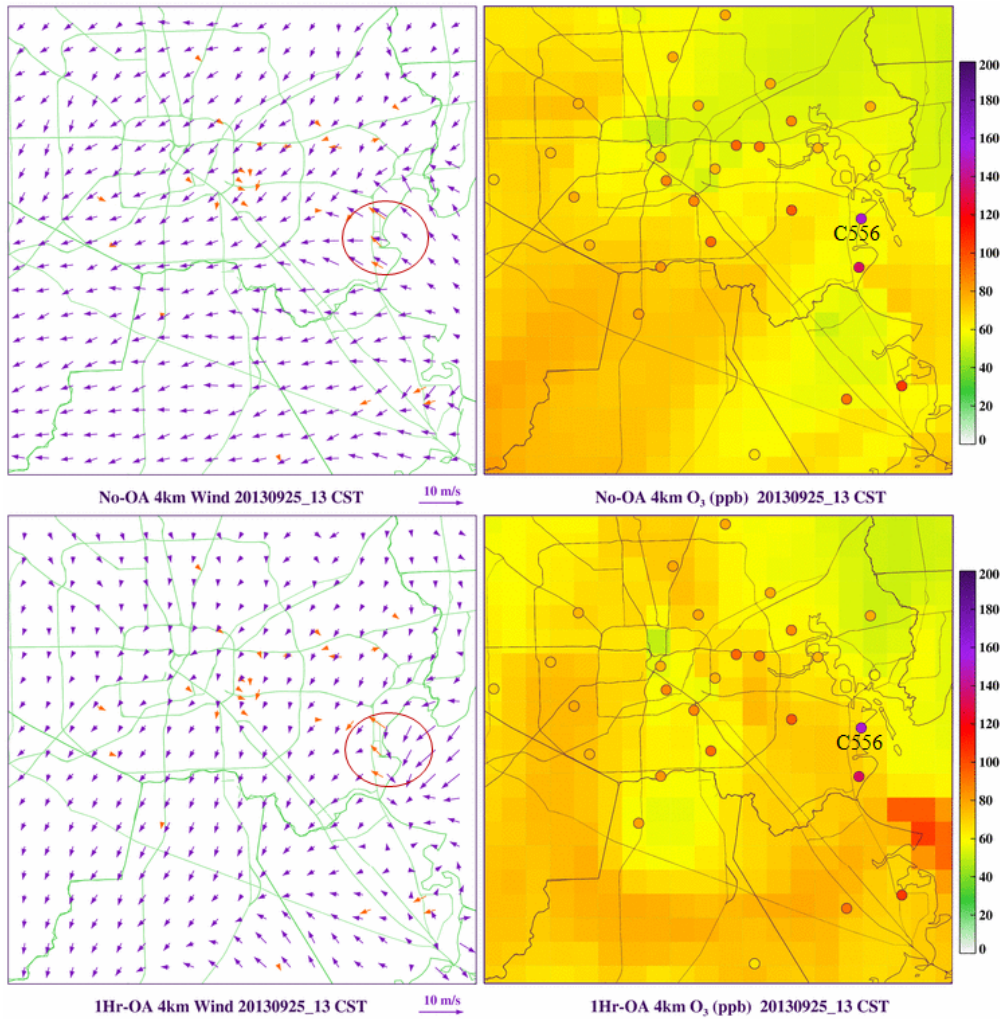
610 **Figure 8.** Ozone time series of La Porte (C556) between 09/24_00 to 09/28_00 CST of 2013.

611 It is important to note that both modeled cases missed the wind shifts in the HSC area, and the
 612 ~~resulted~~resulting convergence zone near C556. This could explain the model's inability to
 613 recreate the sharp ozone increase at C556. Figure 9 shows that the ozone level~~concentrations~~
 614 around HSC area ~~is~~are quite low (~10 ppb) at 08 CST. A further examination showed that while
 615 both model cases missed the wind shift and convergence, ~~though~~ the patterns were different. The
 616 base case had flawed winds for most of the morning: instead of a weak ~~northwesterly~~westerly, it
 617 had stronger ~~northeasterly~~northwesterly to northerly. By 08 CST, winds were almost uniformly
 618 northerly in the base case while they were weak west-northwesterly in the OA case (Figure 9).
 619 The oval in Figure 9's top-left panel shows the mismatch of winds around C556 in the base case.
 620 As a result, the NO_x produced in the city was carried further to the southeast in the model in the
 621 base case. Until 13 CST, base case winds did not shift directions by much. The OA case got the
 622 early hour weak northwesterly right, but missed the bay breeze onset between 10 and 13 CST
 623 (oval in Figure 10). The OA case could not reproduce the small-scale wind reversal near C556,
 624 suggesting there is a limitation in the current WRF OA's capability. On the other hand, the OA
 625 case did improve the spatial ozone pattern, as the high ozone area was closer to HSC after OA
 626 (Figure 10).



627

628 **Figure 9.** Zoom-in ozone concentrations (right) and wind plots (left) at ~~09/25_0813~~ 09/25_0813 CST of
 629 201325 September for “No-OA” (top) and “1Hr-OA” (bottom). Ozone observation is in small
 630 circle; wind observation is indicated by an orange arrow. La Porte site C556 is labeled. The
 631 ~~value~~numerical range of right-side colour scale is 0 to 200 ppb. Higher value than 200 ppb has
 632 the same colour as 200 ppb.

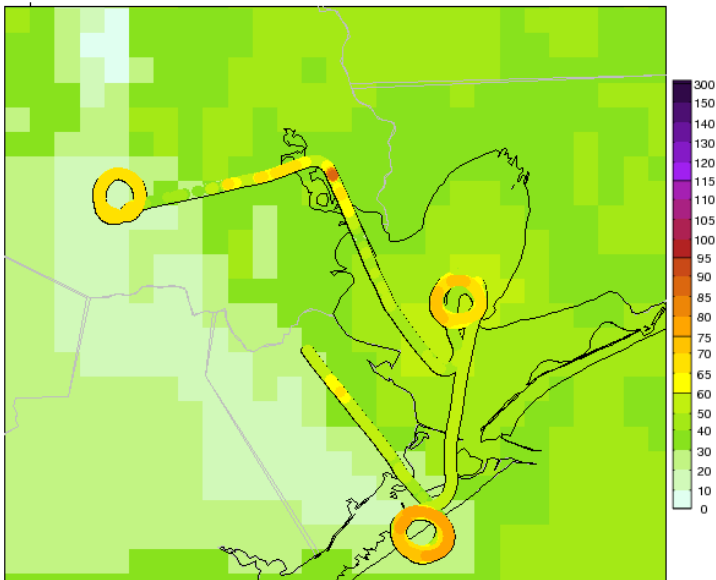


633
 634
 635 **Figure 10.** Zoom-in ozone concentrations (right) and wind plots (left) at 09/25_13 CST of
 636 201325 September for “No-OA” (top) and “1Hr-OA” (bottom). Ozone observation is in small
 637 circle; wind observation is indicated by an orange arrow. ~~La Porte site C556 is labeled.~~ Bay
 638 breeze is shown in the orange oval.

639 The ozone measurements from aircraft P3-B provided a more complete picture for 09/25's the
 640 ozone evolution on 09/25. During the day, ~~P-3B~~ the aircraft flew around the industrial area,
 641 Galveston Bay, and Galveston Island for about 9 hours. Figures 11 and 12 ~~showed~~ plot the ozone
 642 concentrations along aircraft tracks at 08 and 13 CST, ~~with surface.~~ Surface layer ozone from the

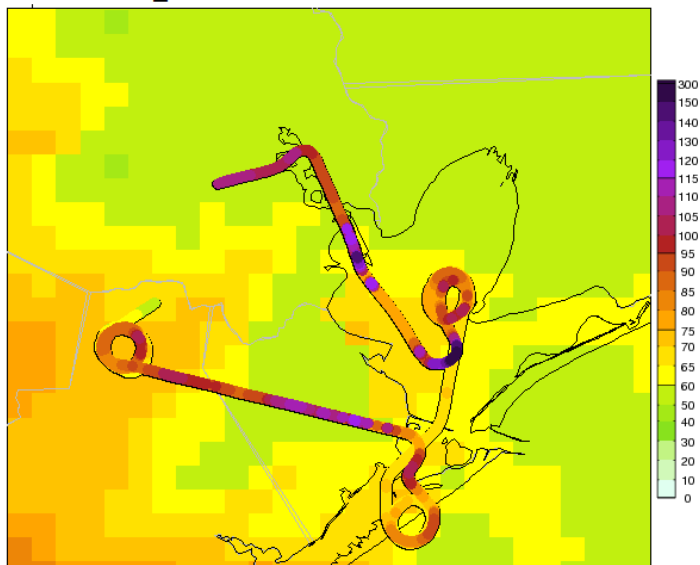
643 | “No-OA” case is provided as background. ~~The background was only intended as a for~~ reference.
644 | At 08 CST, ozone level of 60-80 ppb aloft was already observed at three locations (three loops in
645 | Fig.11): Galveston Island, Smith Point and inner city. Another high of ~90 ppb could be seen
646 | above the HSC area. Ozone sonde observations over HGB showed the aloft ozone aloft
647 | concentrations were ~~normally typically~~ ~40-50 ppb (e. g., Li and Rappengluck 2014) at the
648 | height level. The higher-than normal ozone aloft suggested a post-front ozone recirculation
649 | condition. Such high ozone aloft might raise surface ozone level as a growing PBL downwardly
650 | mixed the air aloft with near surface air. At 13 CST, high ozone over 100 ppb was observed at
651 | multiple locations. The highest aloft ozone aloft, of ~ 160 ppb, occurred southwest of Smith Point
652 | in the Galveston Bay. Such level of ozone high increase in ozone concentrations was likely the
653 | result of active production photochemistry in the industrial zone and around Galveston Bay;
654 | indicating a high level of precursor accumulation in the area.

2013-09-25_08 CST P3B Ozone with No-OA Surface



655 |
656 | **Figure 11.** Ozone along aircraft tracks at 08 CST of September 25th, overlaid upon model No-
657 | OA surface ozone.

2013-09-25_13 CST P3B Ozone with No-OA Surface



658

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

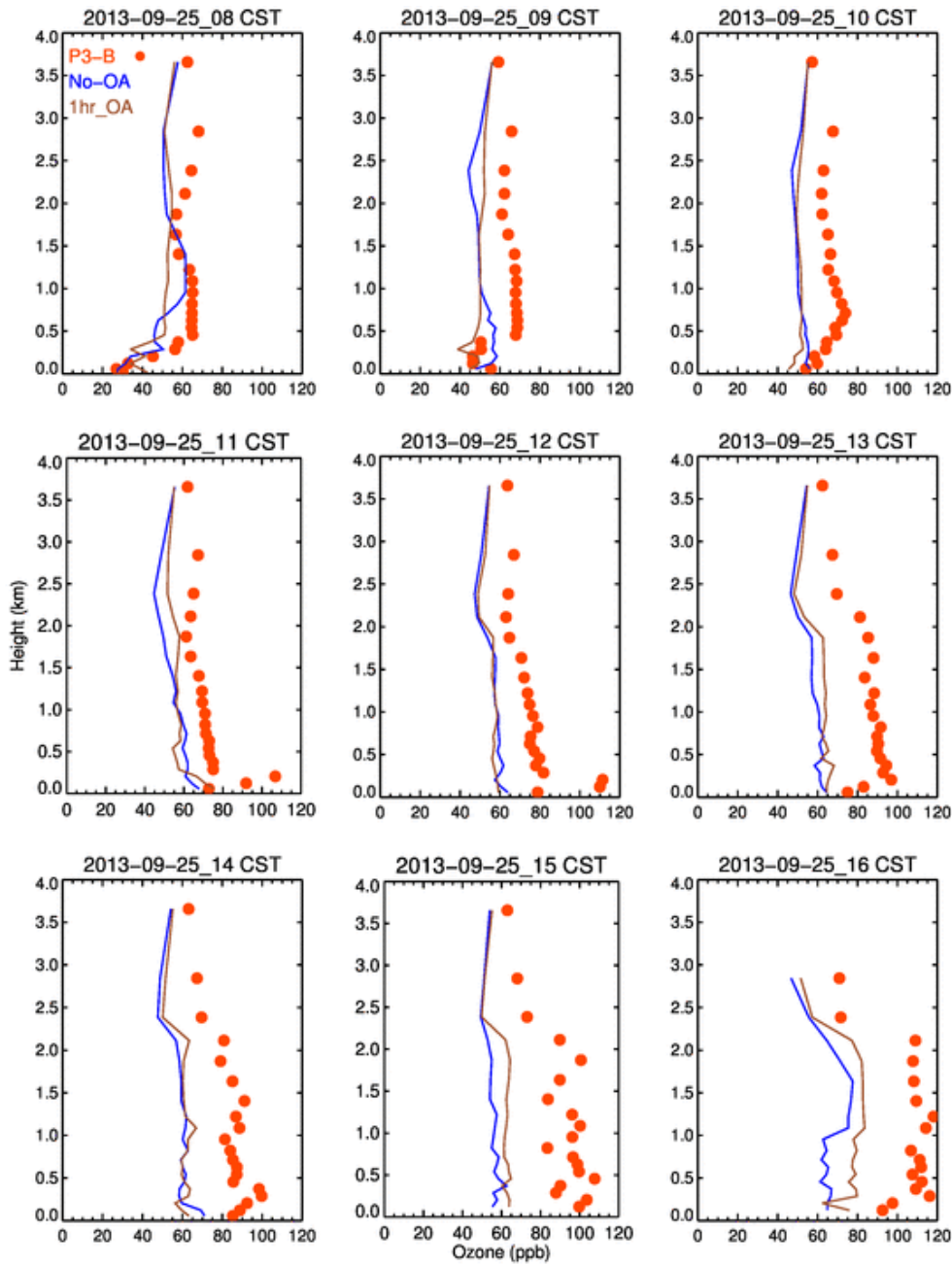
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661 Figure 13 shows hourly ozone vertical profiles from 08 CST to 16 CST ~~of on~~ September 25th,
662 with ozone being displayed on the x-axis and height on the y-axis. ~~One observation dot was~~
663 ~~averaged over all the grid cells in the same model layer. For example, during 08-09 CST, aircraft~~
664 ~~flew passing 30 cells at model's 5th layer. The 5th layer had a mid-layer height of 287.5 m. The~~
665 ~~averaged ozone of the 30 cells was 56 ppb. It should be noted that the~~ ~~The~~ observed ozone was
666 averaged over multiple measurements in the same model cell, ~~such so~~ that they could be properly
667 compared to model ~~output. Next, both model and observed ozone values, were averaged over all~~
668 ~~the grid cells in the same model layer, such that one dot represents the average ozone of all the~~
669 ~~cells in the same layer.~~ The 08 and 09 CST profiles showed there was a high ozone layer with
670 average ozone of ~65 ppb, stretching from 450 m to 1200 m height. In comparison, all model
671 runs had lower ozone in this layer. The model biases, as shown in Figure 14, were about -10 ppb
672 at 08 CST and grew to -20 ppb at 09 CST. The ~~discrepancies~~ ~~large discrepancy~~ between low
673 surface ozone and ozone aloft ~~was unusual and~~ may be explained by the ~~earlier reversal arrival~~ of
674 ~~wind~~ ~~high ozone air mass~~ aloft: ~~winds at surface layer still showed a light northwesterly in the~~

675 | ~~early morning while winds aloft already changed to southerly~~. The observed ozone rose
676 | continuously in following hours yet model simulated ozone stagnated around 60 ppb from
677 | surface up to 2000 m until 15 CST. At 16 CST, the ozone of OA case in the lowermost (0-1 km)
678 | layer rose 20 ppb over the previous hours yet the base case ozone increased only a few ppb.
679 | Although different in magnitude, ~~ozone~~the aloft ozone had a few similar features to the surface
680 | ozone. Firstly, the model missed the observed high ozone in the afternoon by a large margin. For
681 | example, the base case underpredicted the 0-1 km level ozone by up to 50 ppb. The primary
682 | cause for the lower ozone production was likely model's wind fields as both model and
683 | ~~observation~~observations had a clear sky in industrial area and Galveston Bay. Secondly, nudging
684 | clearly helped reducing the ozone biases aloft. In most plots of Figure 14, the OA case had lower
685 | biases than the base case. The largest difference was at 16 CST; when nudging reduced biases
686 | from ~45 ppb to ~30 ppb in the 300 – 1000 m layer.

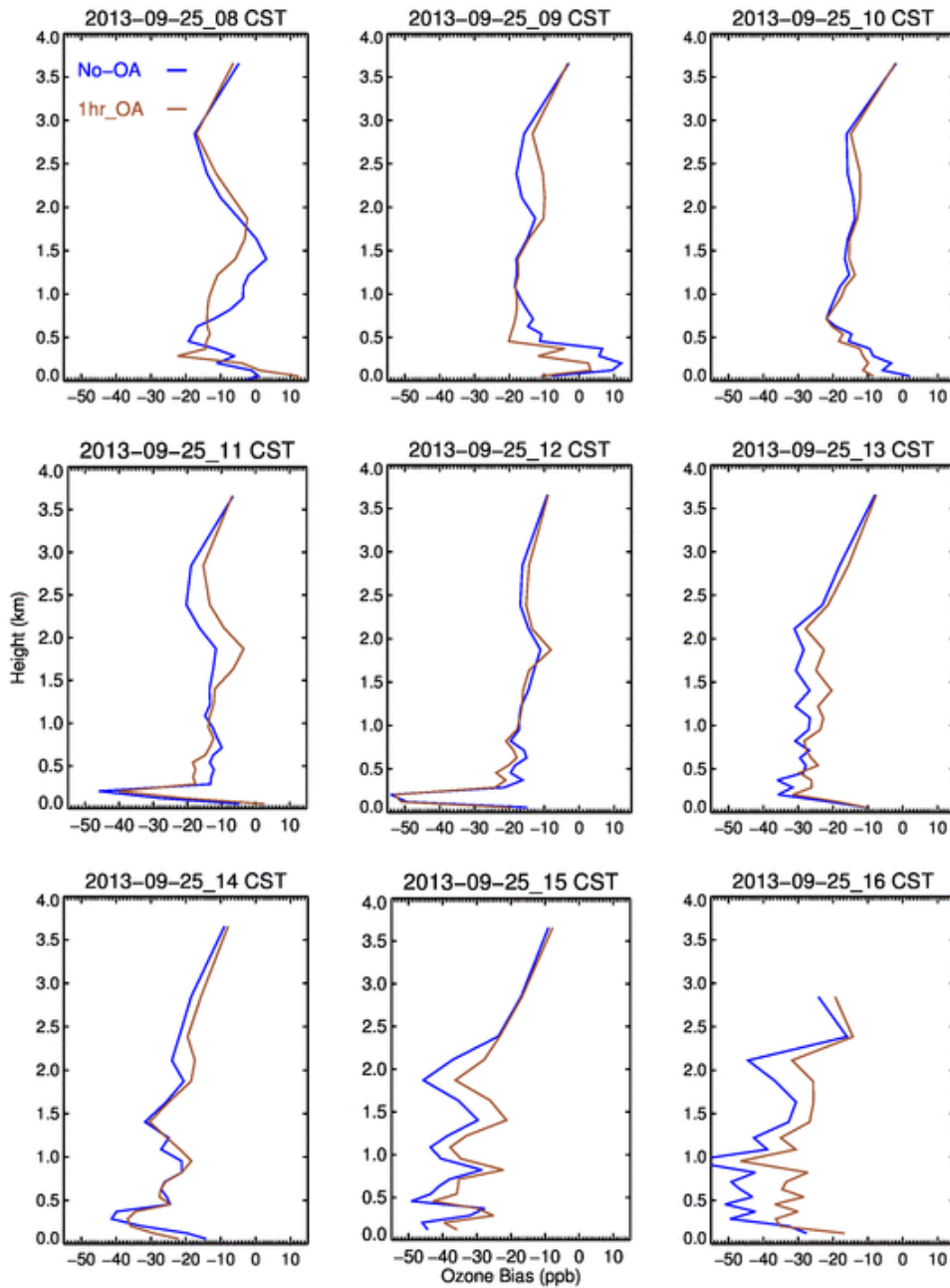
687 | While it is easy to understand the improvements in temperature and winds after obs-nudging was
688 | applied, it is more difficult to explain how other variables such as precipitation and clouds
689 | reacted to obs-nudging. The indirect impact of these meteorological variables on ozone was
690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

697



698

699 **Figure 13.** Vertical ozone profiles from 09/25_08 CST to 09/25_16 CST of 2013 for two cases
 700 of No-OA and 1Hr-OA compared with corresponding observations.



701

702 **Figure 14.** Model vertical ozone biases from 09/25_08 CST to 09/25_16 CST of 2013 for two
 703 cases of No-OA and 1Hr-OA.

704 6. Conclusions and Discussions

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

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

729 The only high ozone episode in the simulation period was related to the cold front passage. The
730 small-scale winds and high aloft ozone aloft concentrations on 09/25, likely contributed to the
731 ozone exceedance in the area. It is also possible that an unreported emission event played a role.
732 Since the maximum surface ozone at La Porte was much higher than the morning-time aloft
733 ozone ~~aloft~~, the active local ozone production was likely the dominant factor. Analyses of aloft

734 | ozone ~~aloft~~ on 09/25 showed while there was high aloft ozone ~~aloft~~ and large negative model
735 | biases, the OA case tended to have smaller biases, especially in late hours.

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

750 | **Acknowledgement**

751 | **Acknowledgements**

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754 | AQ team for the aircraft data, Vanessa Caicedo for LIDAR data, and the TCEQ CAMS site team
755 | for the in-situ ozone and meteorological data.

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926 Table 1. Major WRF physics and FDDA Options, the numbers in the parentheses are the related
927 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 (5)
Surface Layer Option	Monin-Obukhov with CB viscous sublayer scheme (+)
Land-Surface Option	Unified Noah LSM (2)
Urban Physics	None
Boundary Layer Scheme	YSU (+)
Cumulus Cloud Option	Kain-Fritsch (+)
FDDA	Grid nudging on for all; Observation-nudging on for the OA case

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

CMAQ version	V5.0.1
Chemical Mechanism	eb05tuel_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 (aem2)
Chemistry solver	EBI (Euler Backward Iterative) (ebi_eb05tuel)
Aerosol	AERO5 for sea salt and thermodynamics (aero5)
Cloud Option	ACM cloud processor for AERO5 (eloud_aem_ae5)
Boundary conditions	Default static profiles

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 939 Table 3 Statistics of surface T, U-wind and V-wind for three WRF simulations: N – data points;
 940 Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean
 941 Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M –
 942 Model Mean; SD – Standard Deviation; Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD:
 943 degree C
 944
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Surface temperature T										
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

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948 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

949

950 Table 5 Statistics of ozone on 09/25/2013, all day and hour 0 to 13. Both correlation and index of
 951 agreement are unitless. The red numbers indicate the three hours (07 CST to 09 CST) when the
 952 ozone in 1Hr-OA case is significantly better than the No-OA case due to much improved winds.

		No-OA		1Hr-OA	
	N	Corr	IOA	Corr	IOA
Hr All	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

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