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

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4 Xiangshang Li<sup>1</sup>, Yunsoo Choi<sup>1</sup>, Beata Czader<sup>1</sup>, Anirban Roy<sup>1</sup>, Hyuncheol Kim<sup>2,3</sup>, Barry Lefer
5 <sup>1</sup>, Shuai Pan<sup>1</sup>

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<sup>1</sup>Department of Earth and Atmospheric Sciences, University of Houston, Houston, TX, 77204,
USA

9 <sup>2</sup>NOAA Air Resources Laboratory, College Park, MD 20740, USA

<sup>3</sup>University of Maryland, Cooperative Institute for Climate and Satellite, College Park, MD,
USA

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

## 13 Abstract

14 Accurate meteorological fields are imperative for correct chemical transport modeling. 15 Observation nudging, along with objective analysis, is generally considered as a low-cost and 16 effective technique to improve meteorological simulations. However, the meteorological impact 17 of observation nudging on chemistry has not been well characterized. This study involved two 18 simulations to analyze the impact of observation nudging on the simulated meteorology and 19 ozone concentrations during the 2013 Deriving Information on Surface conditions from Column 20 and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) Texas 21 campaign period, using Weather Research and Forecasting (WRF) and Community Multiscale 22 Air Quality (CMAQ) models. The results showed improved correlations between observed and 23 simulated parameters from the sensitivity case. The index of agreement (IOA) improved by 24 about 9% for surface temperature and 6-11% for surface zonal (U-WIND) and meridional (V-25 WIND) winds when observation nudging was employed. Analysis of a cold front event indicated 26 that it improved the timing of wind transition during the front passage. Employing observation

27 nudging also reduced the model biases for the planetary boundary height predictions. For CMAQ simulations, the IOA improved by 6% in the sensitivity case for surface ozone during the entire 28 simulation period. The high ozone episode on September 25<sup>th</sup> was a post-front ozone event in 29 30 Houston. The small-scale morning wind shifts near the Houston Ship Channel combined with 31 higher aloft ozone early morning likely caused the day's ozone exceedance. While observation 32 nudging did not recreate the wind shifts on that day and failed to reproduce the observed high ozone, analyses of surface and aircraft data found that observation nudging helperpodel to yield 33 improved ozone prediction a two-hour period during the event, substantially better winds in 34 the sensitivity case noticeably improved the ozon Further work on improving the capability of 35 nudging to reproduce local meteorological events could enhance a chemical transport model's 36 37 capability to predict high ozone events.

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

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# 40 **1. Introduction**

41 Meteorological variables such as cloud fraction, winds, planetary boundary layer (PBL) heights 42 and precipitation significantly impact air quality. They influence the production, transport, and deposition of various chemical species (e.g., Pour-Biazar et al. 2007 Danta et al. 2005; Cuchiara 43 44 et al. 2014). Hence accurate meteorological inputs are imperative for air quality modeling. 45 Common approaches of improving meteorological simulations include the selection of updated 46 and high resolution terrain data (e.g., Cheng and Byun 2008), optimization of physics and 47 dynamics options (e.g., Zhong et al. 2007) and the implementation of four dimensional data assimilation (FDDA 48

FDI continuously merges new observational data into model simulation such that the model's predictions do not drift away from observations. There are several FDDA methods including nudging (e.g., Stauffer and Seaman 2004) and Variational Methods (3D-VAR or 4D-VAR; e.g., Le Dimet and Talagrand 1986; Huang et al. 2009). 4D-VAR obtains optimal states of the atmosphere using multi-time-level observations by globally adjusting a model solution to all available observations over an interval of time. Nudging is a simple yet flexible FDDA method originally developed by Stauffer and Seaman (1990, 1994), and implemented in the Fifth-

56 Generation PSU/NCAR Mesoscale Model (MM5). Not intended for optimal adjustment, nudging 57 is less computationally intensive but needs special care for the nudging coefficients. Nudging 58 involves adding an artificial tendency term to one or more model prognostic equations that 59 reflect the difference between the best estimate of the observed state and the model state at a given location and time. In short, the goal is to "nudge" del state towards observed state. 60 There are several types of nudging such as 3D analysis nudging, surface analysis nudging, and 61 62 observation nudging (obs-nudging). In the case of analysis nudging, the model state is nudged 63 toward gridded analysis. The difference between 3D and surface analysis nudging is that 3D 64 analysis (at all model levels except for a face) data are used to improve 3D fields while surface analysis data are used to improve surface fields. In observation nudging, the model predictions 65 are nudged to match better with observations at individual locations both surface and aloft. The 66 67 MM5 nudging codes were later improved and incorporated into the Weather Research and 68 Forecasting (WRF) model by Liu et al. (2005, 2006). The enhancements enable obs-nudging to 69 assimilate a large variety of direct or derived observations. In WRF, the inputs for obs-nudging are generated by MF OBSGRID program. This program also performs Objective Analysis 70 71 (OA) to improve the quality of analysis nudging files. Objective Analysis updates first guess 72 meteorology analysis by incorporating observational data. Since obs-nudging is usually 73 performed along with OA (as in this study) to maximize the benefits of assimilating 74 observations, we also use OA to denote the combined Objective Analysis and obs-nudging 75 processes in case names.

76 The benefit of applying nudging to improve meteorological simulations has been demonstrated 77 in many studies (e.g., Deng 2009; Gilliam and Pleim 2010). However, the impact of the 78 improved fields on air quality simulations has been investigated by relatively fewer studies. Otte 79 (2008) showed that the Community Multiscale Air Quality (CMAQ) model with improved MM5 80 meteorology using analysis nudging was able to better simulate ozone chemistry as reflected in 81 model-measurement statistics. Their results indicated that better "model skill" scores were 82 achieved for daily maximum 1-hr ozone mixing ratios after analysis nudging over a 35-day 83 simulation episode. Byun et al. (2008) performed over a dozen tests on obs-nudging (with 84 analysis nudging turned on) and showed obs-nudging improved both winds and temperature in 85 MM5 simulations. The study also gave an example in which improved wind fields on a given 86 day helped the CMAQ model better capture the ozone hotspot southwest of Houston. Ngan et al.

87 (2012) compared results from several CMAQ simulations coupled to the MM5 model which 88 included nudging. Their results indicated that fully nudged (with both analysis nudging and obs-89 nudging implemented) simulations performed better ith respect to both meteorology and ozone 90 chemistry. However, the statistics from their study cannot be used for interpreting the sensitivity 91 of obs-nudging since its base WRF case is a forecast run which used a different analysis input. 92 Previous studies by the current authors (e.g., Rappenglueck et al. 2011; Czader et al. 2013) 93 showed that obs-nudging helped correct errors in model wind fields, critical to the transport of 94 pollutants and production of secondary pollutants. To the best of the authors' knowledge, there is 95 no comprehensive study on the impact of obs-nudging on air quality simulation using the WRF 96 model.

97 This study intends to fill up the gap in the studies mentioned above by investigating the

98 sensitivity of WRF and subsequently, CMAQ simulations to observation nudging. In theory,

higher frequency of obs-nudging input should have a higher probability capture small scale

100 events, such as local wind shifts. These events may only slightly impact local weather, yet have a

101 marked effect on chemistry. This is because local stagnation and wind convergence/reversals can

102 contribute to the pollutant build-up, as indicated by Banta et al. (1998), Cheung and Wang

103 (2001) and Tucker et al. (2010).

104 There is a significant presence of petrochemical facilities, power plants and motor vehicles in the

105 Houston-Galveston-Brazoria (HGB) region located in southeastern Texas (SETX). The major

106 pollutant in the region is ozone due to the abundant emissions of precursors like nitrogen oxid

107 (NO<sub>x</sub>) and Volatile Organic Compounds (VOCs). During the long and hot summer, ozone

108 concentrations often rise above the National Ambient Air Quality Standard (NAAQS).

109 Consequently, HGB has been designated as an ozone nonattainment region by the US

110 Environmental Protection Agency (USEPA)

111 (<u>http://www3.epa.gov/airquality/greenbook/hncs.html#TEXAS</u>). The petrochemical plants are

112 largely concentrated in the Houston Ship Channel (HSC) area - just north of the Galveston Bay.

- 113 The VOCs emitted from the HSC area are highly reactive and have been shown to contribute
- greatly to the high regional ozone episodes (e. Kleinman et al. 2002; Daum et al. 2003).

115 Depending on the local meteorology, the plumes from HSC may be carried to different locations

116 in HGB and trigger high ozone events  $rac{1}{5}$  s path. Metropolitan Houston has a high level of NO<sub>x</sub>

emissions partly due to heavy vehicular traffic in the city. As a result of the large amount of precursor emissions and favorable weath relatively frequent high ozone events occur in the area.

120 Due to the reasons listed above, the Houston-Galveston-Brazoria region has been the focus of 121 several air quality studies in the recent past (e.g., Banta et al. 2005; Parrish et al. 2009; Lefer and 122 Rappengluck 2010; Olaguer et al. 2013; Czader et al. 2013, Choi et al. 2012; Choi 2014; Choi 123 and Souri, 2015; Pan et al. 2015). It is a good place for studying ozone production and transport 124 due to the existence of a dense surface monitoring network, as well as several intensive 125 measurement field campaigns which provide ample observational data. For example in 126 September 2013, the National Aeronautics and Space Administration (NASA), joined by a 127 number of agencies and universities, conducted a field measurement campaign in SETX as part 128 of its the Deriving Information on Surface conditions from Column and Vertically Resolved 129 Observations Relevant to Air Quality (DISCOVER-AQ) program (http://www-130 air.larc.nasa.gov/missions/discover-aq/discover-aq.html). This program has conducted several 131 air quality and meteorology measurements at different locations in the U.S. The availability of 132 dense surface observations is important for obs-nudging to correct erroneous local winds in the 133 model. The performance of obs-nudging will be handicapped without a rich set of observations. 134 This study involved performing two sets of WRF and CMAQ model simulations for the 2013 135 DISCOVER-AQ Texas time period in order to understand the impact of obs-nudging. The data 136 for nudging included multiple sets of observation data from both surface and aloft measurements.

137 We evaluated model-measurement performance statistics for both WRF and CMAQ output

# 138 2. Observational Data and Model Configurations

#### 139 2.1 Observational Data

140 This study used regular measurements from the Continuous Ambient Monitoring Stations

141 (CAMS) operated by the Texas Commission on Environmental Quality (TCEQ). Additionally,

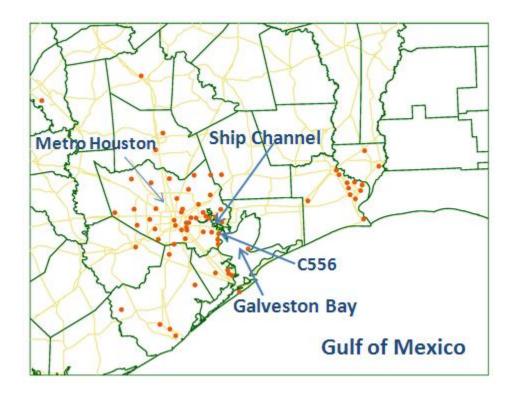
142 PBL and aloft ozone measurement data were obtained from the DISCOVER-AQ campaign. For

143 observation nudging, CAMS data and several data streams from the Meteorological Assimilation

144 Data Ingest System (MADIS) were used. The CAMS measurement network collected real-time

145 meteorology and pollutant data. The measured parameters differ from station to station. The

- 146 station density at South East Texas (SETX) is relatively high. There were 63 sites with
- 147 meteorological and 52 sites with ozone measurements in the 4-km domain. The network is
- 148 represented in Figure 1. The sites are represented by dots, with the La Porte (C556) site labeled.
- 149 All CAMS observations are accessible at TCEQ website: <u>http://www.tceq.state.tx.us/cgi-</u>
- 150 <u>bin/compliance/monops/daily\_summary.pl</u>.



**Figure 1**. Locations of CAMS sites (dots) in CMAQ 4-km modeling domain during September

154 2013. Metro Houston, Houston Ship Channel, Galveston Bay and Gulf of Mexico are labeled

155 Additionally, PBL height measurements for September were recorded at a site at the University

156 of Houston. The PBL height was measured using the Light Detection and Ranging (LIDAR)

157 system. The PBL data is currently available only at this site. For analysis of aloft ozone, we also

158 used measurements from aircraft P-3B, part of the rich datasets collected during DISCOVER-

159 AQ campaign. The P-3B data had over 100 parameters which are accessible online.

# 160 2.2 Model Configurations

161 The modeling system consists of the WRF meteorological model (Skamarock et al., 2008), the

162 Sparse Matrix Operator Kernel Emissions (SMOKE) model for emissions modeling (Houyoux et

al., 2000) and the CMAQ model (Byun and Schere, 2006) for chemical transport modeling. The
details about model configurations are presented in the following sections. Two sets of
simulations were conducted, one set with obs-nudging and OA and the other without. The base
case, referred as "No-OA", did not employ obs-nudging or OA. The second case, "1Hr-OA",
performed obs-nudging and OA using hourly nudging input.

168 **2.2.1. WRF Setup** 

169Both WRF simulations used the same nested domain and NARR (North American Regional

170 Reanalysis) as input, with grid nudging turned on. Figure 2 depicts the horizontal domain setup.

171 Two nested domains were used, with 12-km and 4-km resolution respectively. The 4-km domain

172 covered SETX and a small portion of Louisiana. The 12-km domain (red box) encompassed

173 Texas and parts of a few neighboring states. The number of grid cells for the 12-km and 4-km

domains were 161×145 (E-W by N-S), and 95×77 respectively. The projection type was Lambert

175 conic conformal (LCC). Three projection parameters were considered: namely first latitude

- 176 (33 N), second latitude (45 N) and standard longitude (97 W). The USEPA used the same
- 177 projection parameters to develop emission inventories for air quality modeling (Mason et al.
- 178 2010). Both domains had a vertical resolution of 27 eta layers based on dry hydrostatic pressures.
- 179 The model top is 100 hPa, corresponding to top layer pressure of the input NARR data.

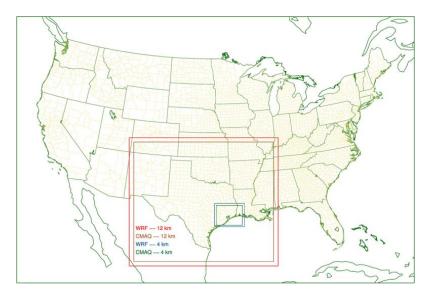


Figure 2. Horizontal domains of WRF and CMAQ simulation at 4 km and 12 km grid resolution
(the bigger domains are for 12 km WRF and CMAQ and the smaller domains for 4 km WRF and
CMAQ).

#### 184 **2.2.1.1. Input Data**

185 The NARR data used for WRF simulations lownloadable from

186 <u>http://rda.ucar.edu/datasets/ds608.0/</u>. The data were based on an Eta 221 grid at 29 pressure

- 187 levels. Its horizontal resolution was 32-km and the frequency was 3 hourly. The initial and
- 188 boundary conditions were generated from the NARR analysis by WRF. An alternative to NARR

189 was the Eta-NAM analysis data. However, the data temporal frequency was lowered from 3-

190 hourly to 6-hourly starting 13. Our tests showed that it was not as good as ARR dataset -

191 likely because of lower temporal resolution.

# 192 **2.2.1.2.** Physics and FDDA Options

193 Major physics options used in the model are listed in Table 1. Our past modeling experiences 194 indicated that employing the Yonsei University (YSU) for BL scheme and the Kain-Fritsch (K-F) for mulous scheme gave the best results for the Houston area 195 196 the two PBL schemes recommended by Cuchiara et al. (2014). The K-F scheme is "drier" than 197 others and produces less number of "false" convectional thunderstorms. For grid nudging options, we generally followed the recommendations in the WRI Jser Guide. For example, the 198 199 mass fields (temperature and moisture) were nudged only at layers above the PBL while wind 200 fields were adjusted at all layers including the surface layer.

#### 201 **2.2.1.3.** Observation Nudging with MADIS and CAMS data in WRF

Additional observational data are required to implement obs-nudging and OA. To generate the input files for the OBSGRID program, we processed the observation data using the approach of Ngan et al. (2012) and Czader et al. (2013). Observational data came from the MADIS and TCEQ CAMS. MADIS is a National Oceanic and Atmospheric Administration (NOAA) program which collects, integrates, quality-controls and distributes observations from NOAA and other organizations. Additional information is available online, <u>https://madis.ncep.noaa.gov/</u>.

208 The four MADIS datasets used for obs-nudging were NOAA Profiler Network (NPN),

209 Cooperative Agency Profilers (CAP), Meteorological Terminal Aviation Routine (METAR)

210 weather report and NOAA Radiosonde (RAOB). The METAR dataset was collected by mostly

211 first-order, METAR reporting, surface monitoring stations. NPN, RAOB and CAP were the most

212 commonly used upper air datasets.

213 The processed input observation data were fed into OBSGRID to update the domain analyses

and generate additional surface analyses and text nudging files. Actuarys-nudging was

215 performed by the main WRF program after obs-nudging namelist variables are properly set. The

216 namelist for OBSGRID and relevant WRF section settings came largely from recommended

217 values or RF User's Guide and a previous study by Ngan et al. (2012).

218 Theoretically, obs-nudging updating at a higher frequency should enhance the model's 219 performance. A typical frequency of input analysis data is 3-hourly while the frequency for 220 observational data is hourly. The 3-hourly frequency of input analyses may be the reason for the 221 default 3-hour time interval in WRF's OBSGRID settings for generating the obs-nudging files. 222 Since there were few existing obs-nudging studies related to air quality and we report aware of any reference to the adoption of 1-hour input frequency, we assung that all the existing studies 223 224 used the default 3-hour interval. As the WRF model allows the interval to be set to 1-hour or 225 smaller when corresponding observational data were available, we tested both 1-hour and 3-hour 226 scenarios. The results indicated that 1-hour obs-nudging had slightly better performance than the 227 3-hour one. As a result, this study adopted 1-hour temporal frequency for observation nudging. 228 The quantities that were nudged were temperature, moisture, and the two wind components (U-WIND and V-WIN Obs-nudging for moisture was not performed in this study. This was 229 230 based on our past experiences since performing moisture nudging sometimes triggenergy 231 artificial thunderstorms which disruption del flow fields.

#### 232 2.2.2. Emissions Processing

For anthropogenic sources we utilized the National Emissions Inventory of 2008 (NEI2008)

234 generated by the USEPA (USEPA, 2011). Motor vehicle emissions for this inventory were

processed using the EPA's Motor Vehicle Emissions Simulator (MOVES) (USEPA, 2015). The

236 inventory was processed using the Sparse Matrix Operator Kernel Emissions (SMOKE) model

v3.1 to obtain gridded emission rates and speciated for the Carbon Bond 05 (CB05) chemical

238 mechanism for use in the CMAQ model. The biogenic emissions were modeled using the

239 Biogenic Emissions Inventory System (BEIS) v3.14. Although NEI2008 might have

240 overestimated NO<sub>x</sub> emissions in Houston (e.g., Choi 2012; Czader et al. 2015), we used base

241 NEI2008 without adjustment because the adjustment of the NO<sub>x</sub> emission also has large

uncertain Pan et al. (2015) showed that the CMAQ ozone performance using NEI2008 appears
 reasonable.

#### 244 2.2.3. CMAQ Configurations

245 The USEPA's CMAQ (Byun and Schere 2006) version 5.0.1 was adopted for this study. Several 246 air quality studies focusing on the Houston area have used this model (e.g., Foley et al. 2010; 247 Czader et al. 2013, 2015; Choi 2014; Pan et al. 2015). CMAQ horizontal domains were slightly 248 smaller than the WRF counterpart in order to avoid the discontinuity near the domain boundary. 249 The domains were shown in Figure 2 as green and brown box 250 conditions for all the species in the 4-km domain were derived from 12-km domain air quality 251 forecasting results (http://spock.geosc.uh.edu). The model used the same vertical structure as 252 WRF. Major CMAQ configurations are listed in Table 2. Chemical processes were simulated 253 with the available in CMAQ CB05 chemical mechanism with cloud/aqueous chemistry, active chlorine chemistry and dated toluene mechanism. For aerosol modeling, the fifth-generation 254 255 CMAQ aerosol mechanism (AE5) which includes sea salt modeling was selected. The total 256 number of included species is 132, with 70 reactive gas-phase, 49 aerosol and 13 non-reactive 257 species.

#### **3. Evaluation Metrics**

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

1) Evaluation of the magnitude of model results vis-a-vis in-situ da

266	٠	Mean Bias (MB)
267	•	Mean Absolute Error (MAE)
268	•	Root Mean Square Error (RMSE)

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

• Correlation

3) A composite performance index, index of agreement (IOA or d), unitless

272 IOA is considered a better performance index than correlation as it takes into account the

273 difference in the means and standard deviation. For example, when correlations are similar,

274 lower model biases would yield higher IOA values. Additionally, the mean and the standard

275 deviation of model values and observations were included as a reference

# 4. General Meteorological and Ozone Conditions in September 2013

277 The weather during September 2013 was relatively dry with mostly southerly, easterly or 278 southeasterly winds. From 5 to 19 September, there was a lack of influence of strong synoptic 279 weather systems. Shifting wind patterns were observed during the period: light northeasterly in 280 the early morning gradually turned clockwise to southeasterly in the afternoon and evening 281 hours. In this period, winds shifted from southeast to near east and there were more clouds after 282 10 September. The only cold front arrived on the early morning of 21 September. Figure 3 283 shows the regional average temperatures for the period and it can be seen that 21 September has 284 the lowest daily high temperature. The influences of the cold air intrusion lasted till early 25 September. Winds turned into southerly in the afternoon of the 25<sup>th</sup> and warming continued in 285 the next few days until the  $28^{\text{th}}$ . 286

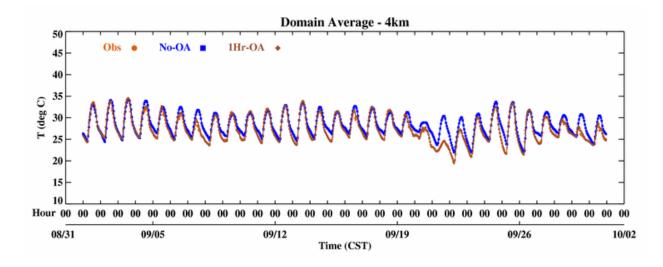
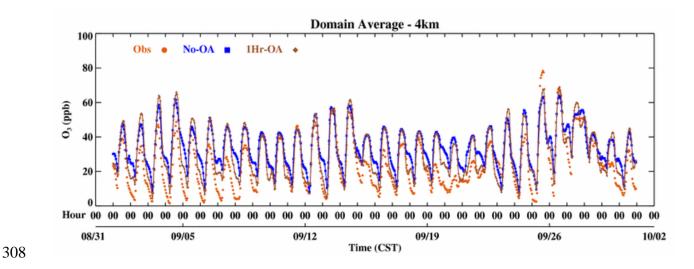


Figure 3. Regional hourly temperature averaged over all available hourly CAMS observations,
two model cases also included for September of 201

Light rain events occurred on 09/02, 09/10, 09/16, 09/19 to 09/21 and 09/28 to 09/3 the 09/20 290 291 and 09/21 events consisted of widespread light to medium showers. Besides the above-292 mentioned dates, there were a few other days with sporadic drizzles. Amajority of the days 293 between 09/01 and 09/20 were either sunny or cloudy. The periods from 09/08 to 09/10 and 294 09/18 to 09/20 had more clouds than other days. The period from 09/21 to 09/30 was influenced 295 by a cold front passage. The days between 09/22 and 09/24 were sunny and cold. The surface 296 wind reversed direction during midday of 09/25 and brought clouds back from 09/26 to 09/30. 297 High ozone events in SETX during fall are typically associated with a passage of cold front (e.g., Rappenglueck et al. 2008). The only ozone event with hourly surface ozone exceeding 120 ppb 298 (parts per billion) in September which occurred on the 25<sup>th</sup> fell in this category. 299 300 Figure 4 plots the hourly regional averaged ozone. On most days, the in-situ averaged ozone

301 concentrations were below 70 ppb. Since the winds after dawn consistently pushed the 302 precursors from the industrial area to the southwest of the city, the wind pattern did not favor the 303 local ozone production. The daytime winds also contained a persistent easterly component which 304 moved the pollutants away from the Houston metropolitan area. In the first 10-day period, low 305 background ozone originating from the Gulf of Mexico contributed to the low-ozone days. With 306 overcast skies on the 19<sup>th</sup> and the 20<sup>th</sup>, hourly high ozone values dipped below 30 ppb. The two 307 highest ozone days characterized by post-frontal ozone events were the 25<sup>th</sup> and the 26<sup>th</sup>.



**Figure 4**. The hourly regional averaged ozone for the two cases (No-OA and 1hr-OA) at the stations which include observation surface  $O_3$  over the 4km domain for September of 2013.

# **5. Results**

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

#### 317 **5.1.** Meteorology

# 318 **5.1.1. Temperature**

319 The comparison of regional average hourly temperature for the simulation period is shown in 320 Figure 3. The regional observed averaged surface temperature was calculated by averaging the 321 hourly temperature from ~60 CAMS sites in the 4-km model domain. The base case temperature 322 was too high compared to the in-situ measurements. For example, the No-OA maximum temperature for the 21<sup>st</sup> was 30°C compared to 25°C for the in-situ data. The high biases in the 323 base case are sharply reduced in the "1Hr-OA ase and temperature matched better with the 324 325 observations for several time periods, especially for September 20-23. The statistics of hourly 326 surface temperature are listed in Table 3. With higher IOA and lower mean biases (MB), the

327 "1Hr-OA" case was clearly better than the base case "No-OA". The IOA of "1Hr-OA" was about
328 9% higher than the base case.

#### 329 **5.1.2.** Winds

330 In ozone chemistry, winds affect the accumulation of precursors and hence the resulting ozone 331 production (e.g., Banta et al. 2005, 2011; Darby 2005). They are also responsible for dispersing 332 high ozone and bringing in background ozone. Prevailing summer time southerly to 333 southeasterly winds in the HGB region significantly lower the ozone concentrations in the 334 metropolitan area. Therefore, high ozone events usually occur when such wind patterns change. 335 Cold front intrusions coming as early as late August blow pollutants to the south. As a result, an 336 area of high ozone develops in the Gulf. Following cold fronts weakening and the weather 337 warming up, reversing winds can bring high ozone back to land. High ozone may also occur 338 during intra-day recirculation events when pollutants previously blown away from industrial 339 zone are brought back by reversing winds. Correctly simulating these recirculation events is 340 particularly important in predicting the high ozone event caused by post-front conditions. The 341 ozone event in the HSC area on 09/25 was likely due to a combination of local recirculation 342 caused by onset of the bay breeze and increased background ozone brought in by transport.

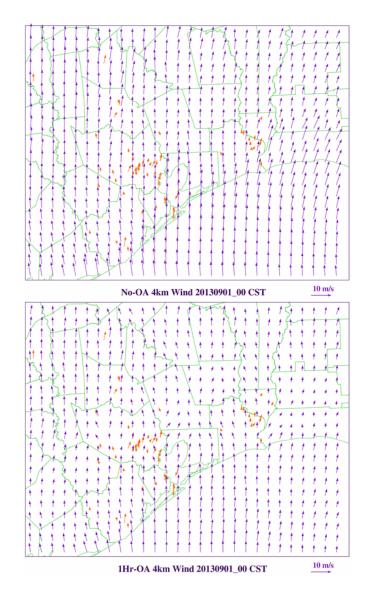
Due to the land-water thermal contrast and the different size of the Galveston Bay and the Gulf of Mexico, the western shore of the Galveston Bay often experiences a successive onset of bay breeze and sea breeze in the summer. The bay breeze is typically a weaker easterly while a breeze is a stronger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

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

For both U and V components of wind, "1Hr-OA" had higher correlation and IOA than "No-OA". The model performance on U and V are similar, with the correlation in a range of 0.76 to

355 0.81 for all the cases. For comparison, the performance of the OA case ("M1") in Ngan et al.

- 356 (2012) is very close to that in this study, with a correlation of 0.75 for U and 0.82 for V. In terms
- of IOA, the OA case had a larger le ver the base case, ahead by 5-6% in U and 10-11% in V
- 358 over the base case. This can be explained by the much reduced wind biases in the OA case.
- 359 The base case had consistently stronger winds, especially the southerly component, than the
- observation This was reflected in the mean bias "MB", as well as the model mean "M\_M".
- 361 Winds were reduced significantly after OA was performed. Interestinging the high southerly bias
- 362 in "No-OA" turned slightly negative after OA. Winds originating from the Gulf were also
- 363 stronger in secase, which played a role in raising the ozone level comparing to the sensitivity
- 364 case. Figure 5 illustrated the slowing down of southerly winds after observation nudging. As a
- 365 result of nudging, the wind vectors matched better to the observations.



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

# 370 **5.1.3. PBL height**

371 Atmospheric pollutants are largely confined in the PBL as most of the emissions sources are 372 close to the ground level. Hence the PBL height plays a critical role in mixing and spreading the 373 pollutants. Haman et al. (2014) studied the relationship between ozone level and PBL height at a 374 Houston CAMS site and found that nighttime and early morning PBL heights were consistently 375 lower on high ozone days than on low ozone days. Czader et al. (2013) pointed out that the 376 model underprediction of PBL during nighttime may have caused the CO overprediction at the 377 same site. CO is a good proxy for understanding mod transport since it has low reactivity and 378 a relatively long life time in the troposphe Cuchiara el al. (2014) conducted four WRF/Chem 379 sensitivity tests using different PBL schemes over southeast Texas. While no preferred PBL 380 scheme was identified for WRF simulations, the YSU scheme performed better than others in 381 terms of ozone prediction.

382 Haman et al. (2012) showed that the daily maximum PBL height at the University of Houston 383 site indicated previous eached its highest values of slightly over 2000 m in August. In 384 September, typical daily maximum PBL height was 1500 m at 15 CST while daily minimum was 385 just below 200 m between 00 CST and 06 CST. The comparison of observed and model PBL 386 height is shown at Figure 6. Our results indicated that the model tended to overpredict the daily 387 maximum PBL height; obs-nudging helped to reduce the overprediction. For the daily minimum 388 PBL height, "No-OA" case had slightly high biases while the OA case matched quite well with 389 in-situ height data. The observed minimum PBL height was lower than that reported by Haman 390 et al. (2012), likely due to the cloudy conditions prevailing in September 2013. There was no 391 apparent explanation on the reduced daytime PBL biases in the OA case than the base case, but it 392 is likely the results of improved winds and temperatures in PBL.

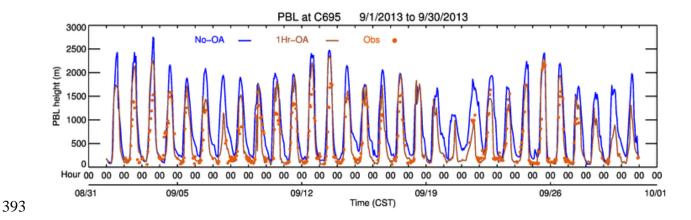
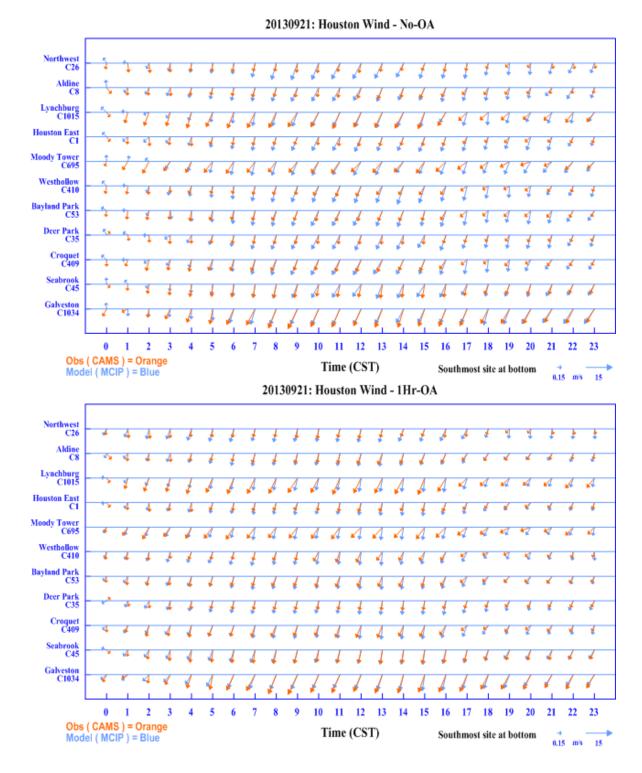


Figure 6. Planetary Boundary Layer (PBL) height time series at CAMS C695 for September2013.

# 396 5.1.4. Cold Front Passage

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

- 404 Both cases performed reasonably well on 09/21 and the timing of wind shift was captured qui
- 405 accurately; although "No-OA" lagged behind by ~ 1 hr. The winds turned weak northerly at 00
- 406 CST for most sites but the "No-OA" case still showed the wind direction to be all southerly.
- 407 Besides the timing, the northeasterly winds i No-OA" case sometimes were too strong; obs-
- 408 nudging helped moderate the winds. The reduced V-wind bias in "1Hr-OA" was also evident in
- 409 the wind model-measurement statistics on 21 September.



411 Figure 7. Hourly model (blue) and CAMS (orange) winds at 11 sites on 21 September: No-OA
412 (top) and 1hr-OA (bottom). The 1hr-OA case is better 0 CST to 02 CST and 17 CST to 20

413 CST.

#### 414 **5.2. Ozone**

#### 415 5.2.1. Regional Average Hourly Ozone

416 Figure 4 plots the regional average hourly ozone, which was defined similarly to the average 417 temperature. Overall, observed ozone concentrations were low and the model did a reasonably 418 good job on capturing the timing of intra-day variations. However, both cases tended to 419 overpredict the daily highs and daily lows, especially in the first 8 days and between 15 and 21 September. An obvious departure is the  $25^{th}$  – both cases missed the daily high. During the 420 421 model high bias period, the OA case usually did better in reaching the daily low although it 422 overpredicted the high a bit more than the base case. The night time biases were reduced likely because the lower southerly winds in the OA case transported less ozone from the Gulf to the 423 land  $\bigcirc$ 424

425 Our results suggested that the modeled ozone concentrations were likely higher in the Gulf than actual However during the  $2^{nd} - 4^{th}$  and  $7^{th} - 8^{th}$  of September, the incoming ozone from the Gulf 426 was markedly low Since the model ozone had fixed boundary values, the model was unable to 427 capture the daily ozone variation at the boundary. The model showed the highest biases during 428 priod of the 19<sup>th</sup> -20<sup>th</sup> likely due to overcast skies and uncertainties in model your fields and 429 430 high background ozone values. Despite the overprediction, the biases in OA case are notably lower puring the nights of 19<sup>th</sup> and 20<sup>th</sup>. A future study to upgrade the accuracy of cloud fraction 431 using remote sensing data (e.g., MOD should be helpful in explaining the biases. 432

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

## 439 **5.2.2.** Performance Statistics

440 The ozone statistics are listed in Table 4. Both cases had very closed porrelation of 0.72 and 0.73.

441 However, the mean biases in the OA case were low (1) y 3.2 ppb, which helped raise the IOA

442 from 0.78 to 0.83. The model standard deviation increased in the OA case and matched better

443 with that of the in-situ data. The improvement in IOA was slightly less as compared to that for

444 temperature and wind

#### 445 **5.2.3.** High ozone episode after the passage of a front

In SETX, high ozone events during the fall season usually occurrent for the passage of a cold front (e.g., Rappenglück et al. 2008; Ngan and Byun 2011; Ngan et al. 2012; Haman et al. 2014). Two factors may have contributed to the post-front ozone events: 1) Following a cold spell, light winds and sunny skies create an ideal condition for ozone production and accumulation. 2) Wind reversal may transport back the pollutants that were previously blown into the Gulf.

451 During the DISCOVER-AQ period, the two days with highest ozone concentrations were the 25<sup>th</sup> and 26<sup>th</sup> of September as indicated in Figure 4. The 1-hour maximum ozone on the 25<sup>th</sup> was 452 localized and higher by about 40 ppb than the 26<sup>th</sup>. In addition to heightened background ozone 453 454 on the 25<sup>th</sup>, the major contributor was the production resulting from favorable weather 455 conditions: sunny, overall light winds and shifting winds over the industrial area. The light 456 morning land breeze carried pollutants from ip channel area to the Galveston Bay. As the day 457 warmed up, the bay breeze started to develop and carry pollutants back to the land. This 458 localized circulation was described by Banta et al. (2005). Ngan et al. (2012) reported the same 459 phenomenon in their Texas Air Quality Study-II 2006 study.

Figure 8 shows the ozone time series for the La Porte (C556 in Figure 1) site located in the HSC

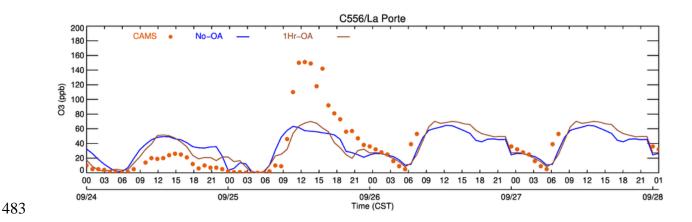
461 area. The highest hourly ozone for September, 151 ppb occurred here at 13 CST on the 25<sup>th</sup>.

462 Ozone rose from 10 ppb to 150 ppb between 09-12 CST. Such a drama
463 likely the result of increased photochemical activity under favorable meteorological conditions in

likely the result of increased photochemical activity under favorable meteorological conditions in
an area with accumulated precursors. Figures 9 and 10 depict the wind and ozone concentrations
at 08 CST and 13 CST.

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

475 The bay breeze started to develop at 10 CST near the C556 site. The early onset was likely to be 476 related to warming up on the previous afternoon on 09/24 as indicated in Figure 3. At 10 CST 477 most other sites to the west of HSC experienced light northwest winds while those at HSC 478 originated from the northeast. Combined with the easterly bay breeze, a convergence zone was 479 formed just below C556, where emissions from the HSC area stalled and accumulated. At 13 480 CST, the whole region had light winds and the bay breeze was well developed. The highest 481 ozone indeed appeared in C556 and its vicinity. The rapid increase of ozone concentration for 482 C556 between 09-13 CST is shown in Figure 8.



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

485 It is important to note that both modeled cases missed the wind shifts in the HSC area, and the 486 resulting convergence zone near C556. This could explain the model's inability to recreate the 487 sharp ozone increase at C556. Figure 9 shows that the ozone concentrations around HSC area are 488 quite low (~10 ppb) at 08 CST. A further examination showed that while both model cases missed the wind shift and convergence, the patterns were different. The base case had flaw 489 490 winds for most of the morning: instead of a weak westerly, it had stronger northwesterly to 491 northerly. By 08 CST, winds were almost uniformly northerly in the base case while they were 492 weak west-northwesterly in the OA case (Figure 9). The oval in Figure 9's top-left panel shows

the mismatch of winds around C556 in the base case. As a result, the NO<sub>x</sub> produced in the city was carried further to the southeast in the model in the base case. Until 13 CST, base case winds did not shift directions by much. The OA case got the early hour weak northwesterly right, but missed the bay breeze onset between 10 and 13 CST (oval in Figure 10). The OA case could not reproduce the small-scale wind reversal near C556, suggesting there is a limitation in the current WRF OA apability. On the other hand, the OA case did improve the spatial ozone pattern, as the high ozone area was closer to HSC after OA (Figure 10).

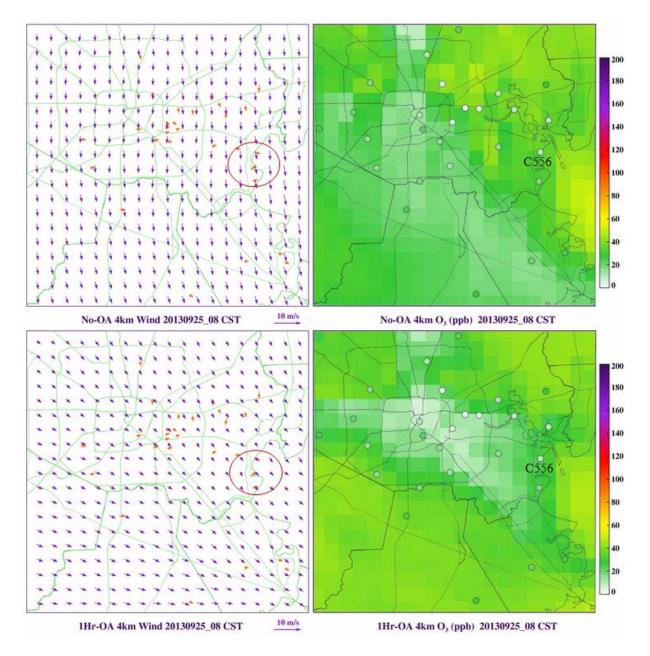
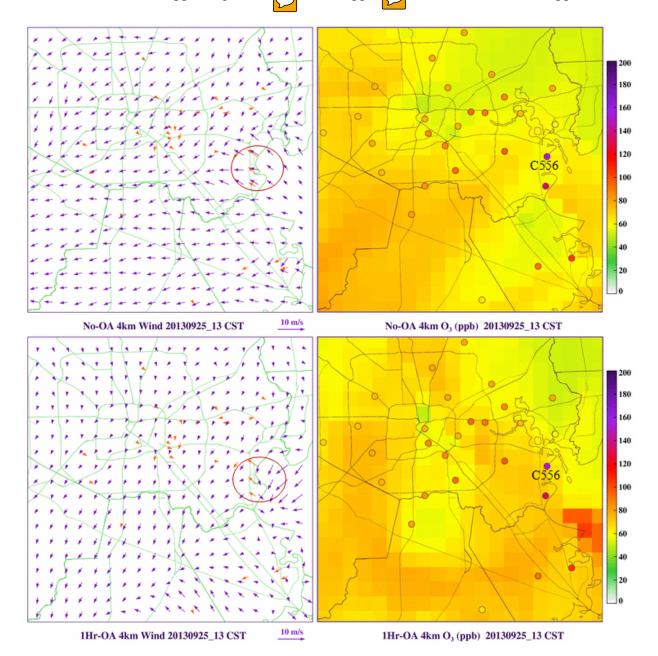


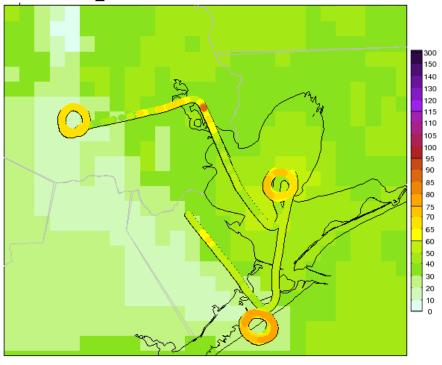
Figure 9. Zoom-in ozone concentrations (right) and wind plots (left) at 13 CST 25 September for "No-OA" (top) and "1Hr-OA" (bottom). Ozone observation is inspall circle; wind observation is indicated by an orange arrow. La Porte site C556 is labeled. The numerical range of point-side colour scale is 0 to 200 ppb. Higher valor han 200 ppb (on the same colour as 200 ppb.)

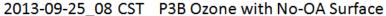


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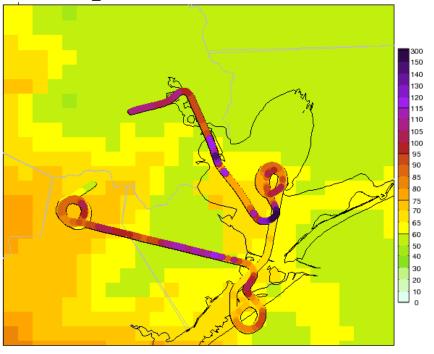
507 **Figure 10**. Zoom-in ozone concentrations (right) and wind plots (left) at 13 CST 25 September 508 for "No-OA" (top) and "1Hr-OA" (bottom). Ozone observation is included by an orange arrow. Bay breeze is shown in the orange ova

510 The ozone measurements from aircraft P3-B provided a more complete picture for the ozone 511 evolution on 09/25. During the day, the aircraft flew around the industrial area, Galveston Bay 512 and Galveston Island for about 9 hours. Figures 11 and 12 plot the ozone concentrations along 513 aircraft tracks at 08 and 13 CST. Surface layer ozone from the "No-OA" case is provided as 514 background for reference. At 08 CST one level of 60-80 ppb aloft was already observed at 515 three locations (three loops in Fig.11): Galveston Island, Smith Point an mer city. Another 516 high of ~90 ppb could be seen above the HSC area. Ozonesonde observations over HGB showed 517 the aloft ozone concentrations were typically ~40-50 ppb (e.g., Li and Rappengluck 2014) at the 518 height leven The higher-than normal ozone aloft suggested a post-front ozone recirculation 519 condition. Such high ozone aloft might raise surface ozone as a growing PBL downwardly mixed 520 the air aloft with near surface air. At 13 CST, high ozone over 100 ppb was observed at multiple 521 locations. The highest aloft ozone of ~ 160 ppb occurred southwest of Smith Point in the 522 Galveston Bay. Such high increase in ozone concentrations was likely the result of active 523 photochemistry in the industrial zone and around Galveston Bay; indicating a high level of 524 precursor accumulation in the area.





- 526 Figure 11. Ozone along aircraft tracks at 08 CST of September 25th, overlaid upon model No-
- 527 OA surface ozon



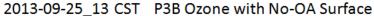


Figure 12. Ozone along aircraft tracks at 09/25\_13 CST of September 25<sup>th</sup>, overlaid upon model
"No-OA" surface ozone. Plumes can be seen as dark purple circles in Galveston Bay.

Figure 13 shows hourly ozone vertical profiles from 08 CST to 16 CST on September 25<sup>th</sup>, with 531 532 ozone being displayed on the x-axis and height on the y-axis. The observed ozone was averaged 533 over multiple measurements in the same model cell, so that they could be compared to model 534 output. Next, both model and observed ozone values were averaged over all the grid cells in the 535 same model layer, such that one dot represents the average ozone of all the cells in the same 536 layer. The 08 and 09 CST profiles showed there was a high ozone layer with average ozone of 537 ~65 ppb stretching from 450 m to 1200 register. In comparison, all model runs had lower ozone in this layer. The model biases as shown in Figure 14 were about -10 ppb at 08 CST and grew to 538 539 -20 ppb at 09 CST. The large discrepancy between low surface ozone and ozone aloft was 540 unusual and may be explained by the arrival or hozone air mass aloft. The observed ozone 541 rose continuously in llowing hours yet model simulated ozone stagnated around 60 ppb from Trace up to 2000 m until 15 CST. At 16 CST, the ozone of A case in the lowermost (0-1 km) 542

543 layer rose 20 ppb over the previous hours yet the base case ozone increased only a few ppb.

544 Although different in magnitude, the aloft ozone had a few similar features to the surface ozone.

545 Firstly, the model missed the observed high ozone in the afternoon by a large margin. For

546 example, the base case underpredicted the 0-1 km level ozone by up to 50 ppb. The primary

547 cause for the lower ozone production was likely total s wind fields as both model and

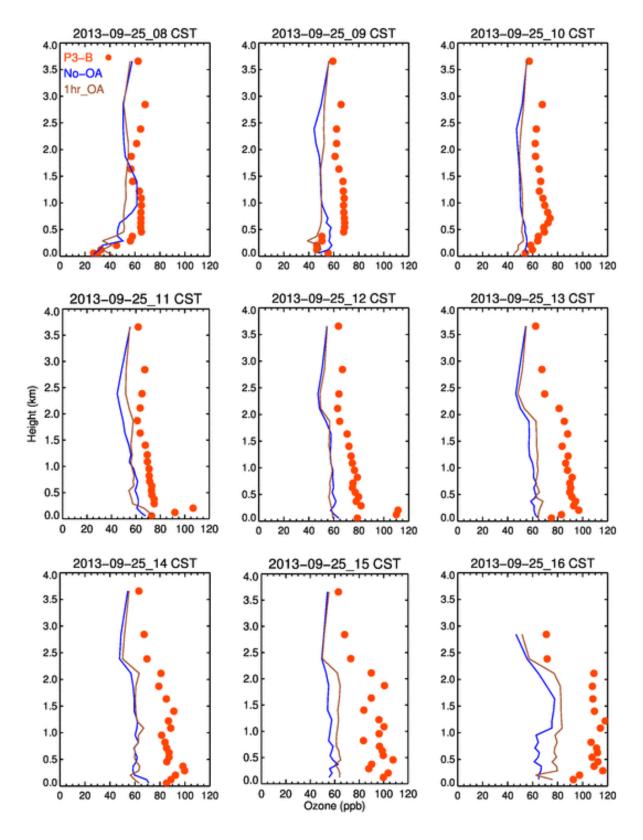
548 observations had a clear sky industrial area and Galveston Bay. Secondly, nudging clearly

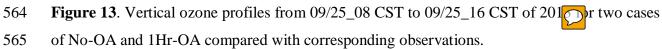
549 helped reducing the ozone biases aloft. In most plots of Figure 14, the OA case had lower biases

than the base case. The largest difference was at 16 CST when nudging reduced biases from ~45

551 ppb to  $\sim$ 30 ppb in the 300 – 1000 m layer.

552 While it is easy to understand the improvements in temperature and winds after obs-nudging was 553 applied, it is more difficult to explain how other variables such as precipitation and clouds 554 reacted to obs-nudging. The indirect impact of these meteorological variables on ozone was 555 harder to assess. In our study, we did not evaluate clouds quantitatively as there were no 556 digitized cloud fraction data available for our modeling domains. A preliminary analysis on convection showed that there were occasions in which model missed the convection or 557 precipitation and there were other occasions in which del created artificial convection. The 558 559 convection cells were usually visible as 3 ar-burst" from surface wind vector plots – arrows 560 going out to different directions from a center. However, the mismatch in convection appeared to 561 be not a serious issue since only a few occurrences were observed in the month of September.





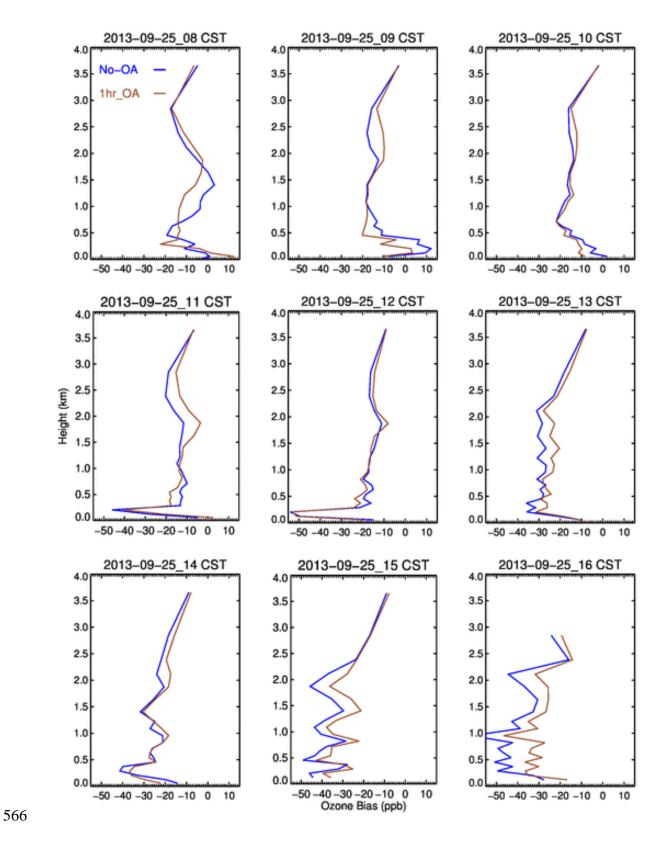


Figure 14. Model vertical ozone biases from 09/25\_08 CST to 09/25\_16 CST of 2013 for two
cases of No-OA and 1Hr-OA.

#### 569 **6.** Conclusions and Discussions

570 In this study, we performed two Weather Research and Forecasting (WRF) and Community 571 Multiscale Air Quality (CMAQ) model simulations to explore model sensitivity to observation 572 nudging. In evaluating meteorological and ozone conditions, we found that obs-nudging 573 improved the meteorology and ozone performance as shown in the index of agreement (IOA) of 574 temperature, winds, and ozone. While the base case winds were overall well simulated, obs-575 nudging significantly reduced the high wind biases (especially the meridional wind) shown in the 576 base case. For planetary boundary layer height, obs-nudging reduced high biases in both daily 577 maximum and daily minimum values. In the end, the combined changes in meteorology lowered 578 the ozone biases by about 3 ppb, a 35% reduction. There were short time periods (such as between 07 and 09 CST on 09/ when the simulated base case model winds differed 579 580 significantly from observational data and obs-nudging significantly corrected the meteorological 581 simulation problems, leading to much better ozone simulation. However, model ozone biases are 582 also impacted by emissions and lateral boundary conditions.

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

590 Small-scale meteorological events are frequently cited for their contributions to high ozone 591 events. Mode capability in reproducing these events is critical in simulating such high ozone 592 episodes. The base case did not recreate the 25 September small-scale events likely due to the 593 complex winds and a lack of local information which can be used to steer model state closer to 594 reality. On the other hand, the inability of the sensitivity case to replicate the local winds is likely 595 a result of the imperfection of the nudging process pending further investigation. An ongoing 596 study by the current authors suggests that errors in the metrological fields from the default grid 597 nudging files are important sources. Methods are being tested to improve the quality of grid 598 nudging files. Early results showed that the bay breeze which caused the wind reversal around La

- 599 Porte was well captured through improved grid nudging files. In addition, more observational
- 600 data (e.g., more sites and higher data frequency) and more testing on the combination of nudging
- 601 settig hould help improve the obs-nudging performance. Also, the impact of obs-nudging on
- 602 precipitation and clouds should be further investigated to understand their characteristics of the state of the state
- 603 chemistry.

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- 748 Res.-Atmos., 112, doi:10.1029/2006jd008274, 2007.

- 751 Table 1. Major WRF physics and FDDA Options, the numbers in the parentheses are the related
- 752 settings in RF namelist file.

WRF Version	V3.5.1
Microphysics	Lin et a heme
Long-wave Radiation	RRTMG
Short-wave Radiation	New Goddard scheme
Surface Layer Option	Monin-Obukhov with CB viscous sublayer scheme
Land-Surface Option	Unified Noah LSM
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

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

CMAQ version	V5.0.1					
Chemical Mechanism	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 inline					
Horizontal advection	YAMO (Yamartino)					
Vertical advection	WRF omega formula					
Horizontal	Multiscale					
mixing/diffusion						
Vertical mixing/diffusion	Asymmetric Convective Model (ACM) version 2					
Chemistry solver	EBI (Euler Backward Iterative)					
Aerosol	AERO5 for sea salt and thermodynamics					
Cloud Option	ACM cloud processor for AERO5					
Boundary conditions	Default static profiles					

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Table 3 Statistics of surface T, U-wind and V-wind for three WRF simulations: N – data points;
Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean
Absolute Error; MB – Mean Bias; O – Observation; M - Model; O\_M – Observed Mean; M\_M –
Model Mean; SD – Standard Deviation; Units for RMSE/MAE/MB/O\_M/M\_M/O\_SD/M\_SD:
degree C

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

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

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
No-OA	33308	0.72	0.78	14.9	12.3	9.3	24.4	33.7	16.5	14.1
1Hr-OA	33308	0.73	0.83	13.8	11.0	6.1	24.4	30.6	16.5	17.4

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

		No-	-OA	1Hr	-0A
	Ν	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