OZONE SIMULATIONS FOR HGB AREA USING DIFFERENT CHEMICAL MECHANISMS WITHCAMX

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ABSTRACT

Areas with air pollution problems often tend to use sophisticated Air Quality Models (AQM) and these models simulate the emissions, dispersion, chemical reactions, and removal of pollutants in the troposphere by solving different equations for each chemical species. Chemical mechanisms play a critical role in predicting the pollutant concentrations. In this study Comprehensive Air quality Model with Extensions (CAMx), photochemical dispersion model is used to predict the air quality of Houston-Galveston-Brazoria (HGB) area. This area has been a non-attainment area for ozone (O_3), which is a secondary pollutant. Accurate prediction of air quality can be very effective in reducing harmful air pollutants and help policy makers to make better emission control strategies. In this study, two different versions of CAMx;CAMx 4.53 and CAMx 5.40 simulation results are evaluated for predication of ozone (O_3). These models use different chemical mechanisms namely, CAMx 4.53 uses Carbon bond 5 (CB5) and CAMx 5.40 uses Carbon bond 6 (CB6). CAMx 4.53 and CAMx 5.40 results are then compared with the observations from TCEQ monitoring sites in the HGB area. CAMx 5.40 (CB6) is found to give an optimal prediction of ozone (O_3). On 9th June, 2006, CAMx 4.53 predictions of ozone were 15% lower than the maximum ozone (O_3) concentration from CAMx 5.40 simulations for HGB area.

Keywords: Air quality, CAMx 4.53, CAMx 5.40, CB5, CB6, Ozone

I. INTRODUCTION

Urbanization and industrial development is causing serious air pollution problems in many areas of the world. Air quality control has become very important to protect public health and environment. Sophisticated Air Quality Models (AQM)are widely used nowadays to study and understand air pollution problems and various control strategies. Dispersion modeling, photochemical modeling, receptor modeling are some of the popular AQMs. Among these models, photochemical models are more appropriate for areas like Houston-Galveston-Brazoria (HGB) whereozone (O_3) pollution is and has been a major concern.This secondary pollutant is produced from the photochemical reaction of Nitrogen Oxides (NO_x) and Highly Reactive Volatile Organic Compounds (HRVOC) [1]. Ozone concentration in HGB is found to be higher than 0.075 parts per million (ppm), the 8-hour average ozone standard from National Ambient Air Quality Standards (NAAQS) [2]. To improve air quality and determine proper air quality control strategies and planning,modeling air quality and being able to model various scenarios is of great value. Air quality models simulate the emissions, dispersion, chemical reactions, and removal of pollutants in the troposphere by solving simultaneously different equations for each chemical species. In this study Comprehensive Air Quality Model with Extensions (CAMx), a popular photochemical dispersion model is used to predict the air quality in the Houston-Galveston-Brazoria (HGB) area.Two versions of CAMx; CAMx 4.53 and CAMx 5.40 are used to simulate the air quality. These models use different chemical mechanisms. CAMx 4.53 uses Carbon bond 5 (CB5) and CAMx 5.40 uses the revised Carbon bond 6 (CB6)mechanism[3]. Several additional chemical species were added to the CB6 mechanism for CAMx 5.40 version, which is supposed to give more accuracy for optimal ozone (O_3) predictions.

Presence of sunlight favors ground level ozone formation[4]. June 9,2006 isselected for this study from Texas Commission on Environmental Quality (TCEQ) summer episodes base case scenarios. CAMx results show that maximum hourly ozone concentration is higher than the NAAQS on June 9, 2006 for most of the daytime. In comparison, CAMx 5.40 (CB6) shows higher hourly ozone concentration than CAMx 4.53. During ozone formation hours, CAMx 4.53 is found to predict about 15% lower maximum ozone (O_3) concentration for HGB area than CAMx 5.40.The model results are also compared with the observed ozone concentrations at TCEQ monitoring sites.

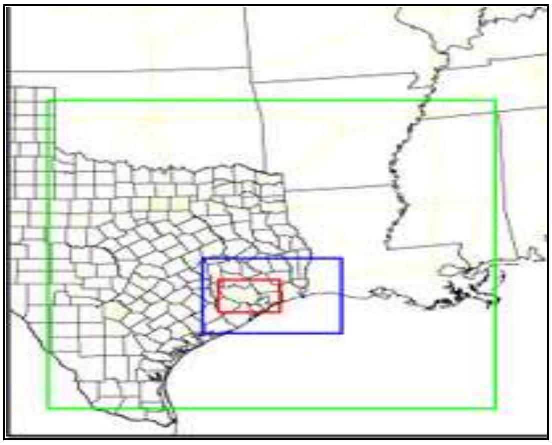
II. MODEL DESCRIPTION

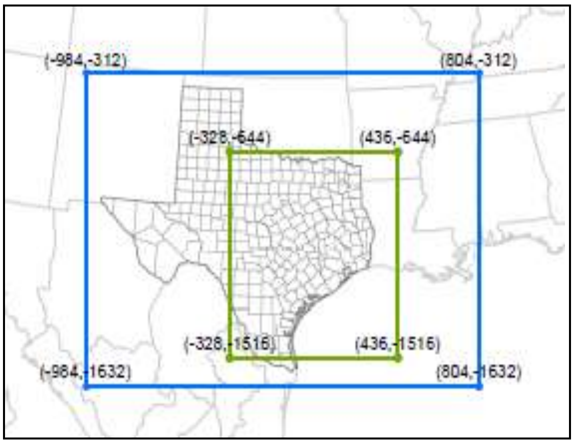
Comprehensive Air quality Model with Extensions (CAMx) is a three-dimensional photochemical dispersion model. CAMx uses a nested grid system and Eulerian continuity equation to simulate the emissions, dispersion, chemical reactions, and removal of pollutants in the troposphere for each chemical species. CAMx model output can have up to 28 layers ranging from 0 to 16,000 meter above the ground. The first layer is 33.9 meter above the ground. In HGB area ground level Ozone is a major concern, so while extracting the data from the CAMx simulation output, the air pollutant concentration of the first layer was used.

The major difference between CAMx 4.53 and CAMx 5.40 is their chemical mechanisms other than general revisions. CAMx 4.53 uses Carbon bond 5 (CB5) mechanism, which comprises of 156 reactions and up to 89 species (54 state gases, up to 22 state particulates, and 13 radicals) whereas CAMx 5.40 uses chemical mechanism 7, known as Carbon bond 6 (CB6). This mechanism uses 218 reactions and up to 114 chemical species (69 state gases, up to 22 state particulates, and 23 radicals) [3].

In CB6, major revisions to the chemistry for aromatics, isoprene, alkenes, alkanes and oxygenates. To improve oxidant formation propane, acetone, benzene and ethyne (acetylene) are included in CB6. This mechanism modified peroxy radical chemistry, which improved formation of hydrogen peroxide (H_2O_2) [5]. In several studies, sensitivity analysis of ozone (O_3) to NO_x and VOC was conducted by using photochemical indicator ratio of [H_2O_2] to [HNO_3] [6]. The inclusion of formation mechanism of hydrogen peroxide (H_2O_2) in CB6 improves ozone (O_3) prediction.

In this work, CAMx Lambert Conformal Conic (LCC) map projection is used. CAMx uses nested grid domain for simulations, i.e. master grid input data moves into finer grid input data. CAMx 4.53 and CAMx 5.40 modeling domain parameters are shown in Table 1and Table 2 respectively. For CAMx 4.53, HGB/BPA Sub-domain 4 km grid is available [7], shown in Fig. 1(a). CAMx 5.40 Tx_4km domain covers Houston-Galveston-Brazoria (HGB) area and portion of surrounding states. Due to lack of input data file for HGB sub-domain, tx_4km data is used for data interpretation [8], as shown in Fig. 1(b).





(a) **(b)**

Figure 1: (a) CAMx 4.53HGB/BPA Sub-domain 4 km grid (blue rectangle) (b) CAMx 5.40 Texas 4km domain (Green rectangle)

Table 1: Modeling domain CAMx 4.53 [7]

Domain (km)	Easting (E)	Northing (N)	Number of cells (E)	(N)
eus_36km	-108,2376	-1584,828	69	67
etx_12km	-12,1056	-1488, -42	89	89
hgbpa_04km	-356,688	-1228,-968	83	65

Table 2: Modeling domain CAMx 4.53 [8]

Domain (km)	Easting (E)	Northing (N)	Number of cells (E)	(N)
rpo_36km	-2735,2592	-2088,1944	148	112
tx_12km	-984,804	-1632, -312	149	110
tx_4km	-328, 436	-1536,-644	191	218

III. METHODOLOGY

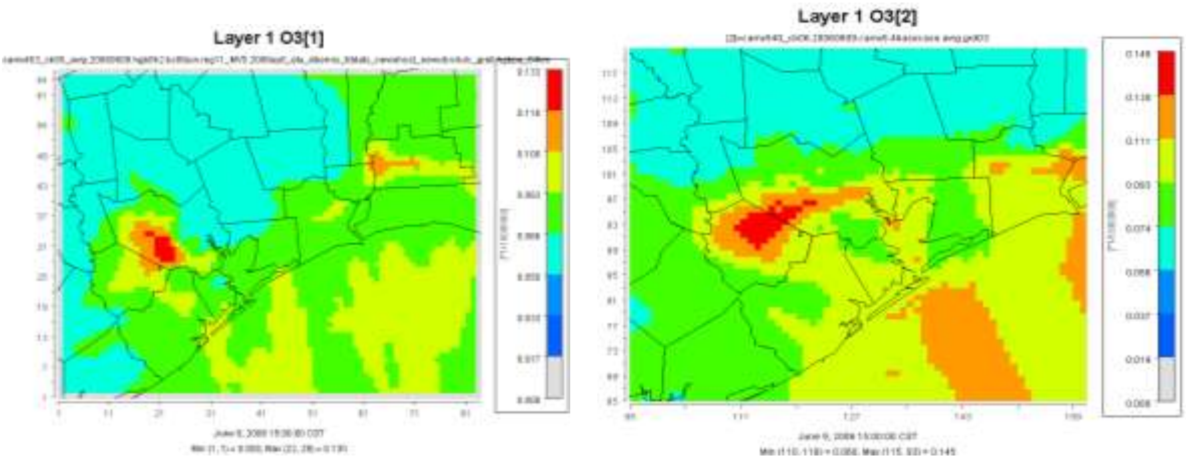
Air quality modeling for the Houston-Galveston-Brazoria (HGB) area was done using two different versions of Comprehensive Air Quality Model with Extensions, namely; CAMx 4.53 and CAMx 5.40. Model inputs were processed by Texas Commission on Environmental Quality (TCEQ) and the Base case from May 31 to July 2, 2006 episode is used for this simulation [7].

CAMx requires input files that configure each simulation, define the chemical mechanism, and describe the photochemical conditions, surface characteristics, initial and boundary conditions, emission rates, and various meteorological fields over the entire modeling domain.In meteorology inputs temperature, wind, pressure, humidity, diffusivity, cloud data are incorporated. WRF and GEOS-Chem models are used to generate meteorological data and boundary condition data files, respectively.Point source, area source, on-road source, non-road source and biogenic source emissions are considered for preparing emission data file which were generated by Emission Processing System (EPS3), MOtor Vehicle Emission Simulator (MOVES), NON-ROAD and Global Biogenic Emissions and Interactions System (GloBEIS) model, respectively [9].

Model simulation results are compared to observations from TCEQ monitoring sites toevaluate the effectiveness of predicting ozone concentrations using CAMx 4.53 and CAMx 5.40. Daily maximum eight-hour ozone averages for June 9th, 2006 for forty one monitoring sites of HGB area [10] are compared to the simulation values obtained from the two versions of CAMx.

IV. CAMXSIMULATIONS, ANALYSIS AND DISCUSSIONS

The output from CAMx is visualized using Visualization Environment Rich Data Interpretation (VERDI) [12]. Tile plots of CAMx 4.53 HGB/BPA Sub-domain 4 km grid and Interpreted HGB area from CAMx 5.40 Texas 4 km grid are shown in Fig. 2 (a) and 2 (b). Tile plots show the spatial maximum ozone concentration for each hour. As shown in Fig. 2(a), CAMx 4.53 (CB5) predicted maximum ozone concentration of 130 ppb at 15:00 CST for June 9, 2006. CAMx 5.40 (CB6) predicted maximum ozone concentration 145 ppb at 15:00 CST for the same day.



(a) (b)

Figure 2: Maximum ozone (O_3) concentration at 15:00 CST for June 9, 2006 (a) CAMx 4.53 (CB5), (b) CAMx 5.40 (CB6)

To analyze the ozone concentration differences for CAMx 4.53 (CB5) andCAMx 5.40 (CB6), maximum ozone concentration values are collected for the June 9, 2006. During mid-day when abundant sunlight is present, ozone production is usually at peak during these conditions. Table 3 shows maximum ozone concentration values for this day using both CB5 and CB6 mechanisms. AS can be seen from the table, CB6 mechanism used in CAMx 5.40 model predicted much higher ozone concentration than CB5, used in CAMx 4.53. From this data, it is found that CB6, CAMx 5.40 predicted about 16% more of ozone concentration than CB5, CAMx 4.53.

Table 3: Maximum Ozone Concentration Values for the June 9, 2006

Time (CST)	Ozone CB5 (ppb)	Ozone CB6 (ppb)
10	84	111

11	96	116
12	103	127
13	112	134
14	122	140
15	130	145
16	122	148
17	120	142

Houston-Galveston-Brazoria (HGB) area consisting eight counties; Brazoria, Chambers, Fort Bend, Galveston, Harris, Liberty, Montgomery, and Waller Counties have about 41 monitoring sites. Daily maximum eight-hour ozone concentrations from all these sites are monitored [10]. For most of the sites, Air Quality Index (AQI) values ranged between 60-100 (minimum 62, maximum 106). AQI range explains that if the value is between 51-100, it indicates a mean 8 hour ozone value in the range of 0.06 - 0.075 ppm [10]. At three of the stations, ozone exceeded 8-hour ozone AQI of 100 (ozone concentration range of 0.076 - 0.095). On average 8 hour ozone concentration is 0.080 ppm.

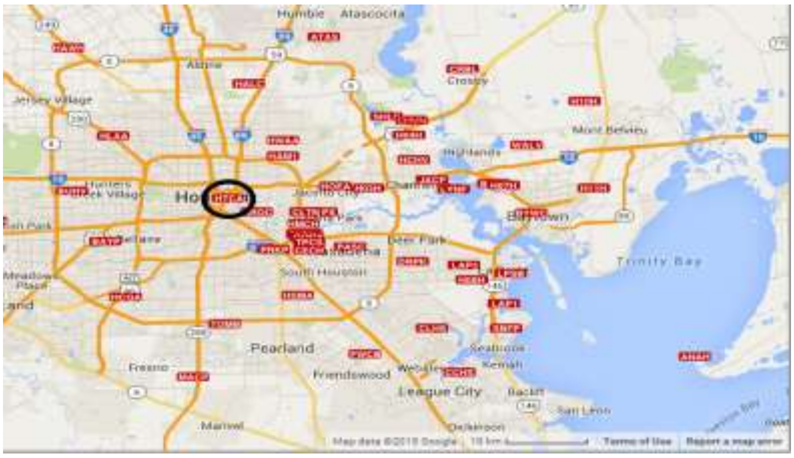


Figure3: TCEQ Air Quality monitoring Stations in HGB area (Black circle: Houston Texas Avenue Station, C411) [11]

The main objective of this study is to assess the role of the revised chemical mechanism (CB6) used with the CAMX 5.40 compared to the older CB5 mechanism used with CAMx 4.53 and its influence on the pollutant concentrations. To compare the model results with TCEQ monitoring station data, Houston Texas Avenue Station C411 (HTCA-C411) is selected. This station is within the Houston-Galveston-Brazoria (HGB) area and provided measured hourly averages for ozone (O_3) pollutant [13]. Table 4 shows the hourly averages for ozone (O_3) concentration in that station on June 9, 2006.

Table 4: Hourlyobserved Ozone Values for selected Monitoring Station on June 9, 2006 [13]

Time (CST)	Ozone (ppb)		Time (CST)	Ozone (ppb)		Time (CST)	Ozone (ppb)
Midnight	28		8	15		16	87
1	28		9	31		17	77
2	28		10	47		18	81

3	26	11	62	19	69
4	19	12(noon)	75	20	48
5	6	13	77	21	34
6	5	14	77	22	39
7	8	15	89	23	42

To compare model results with observed ozone concentrations, CAMx 5.40 and CAMx 4.53 results were plotted in time series. Time series graph in Fig. 3 shows, CB5, CAMx 4.53 ozone concentration values for June 9th, 2006. Maximum average ozone value is 0.070 ppb.Fig. 4 represents time series ozone concentrations predicted by CAMx 5.40 (CB6). The maximum ozone concentration is found 0.075 ppb for June 9th, 2006. From time series graphs, hourly ozone concentrations simulated by CAMx 4.53(CB5) and CAMx 5.40 (CB6) are extracted to compare with the observed values fromHouston Texas Avenue Station C411 monitoring site. It should be noted that the predications are given for broader HGB area where there are 41 monitoring sites and only one such site is selected for this comparison. In Fig. 6, hourly ozone concentration from Houston Texas Avenue Station C411(observed), CAMx 4.53(CB5) and CAMx 5.40 (CB6) are compared for hours CST 12:00 to CST 18:00. Usually peak ozone concentration is found during these hours. From Table 4 and Fig. 6, it is found that maximum ozone concentration observed at Houston Texas Avenue Stationis higher than the CAMx 4.53(CB5) and CAMx 5.40 (CB6) predicted values. Highest ozone concentration is measured at 15:00 CST and value is 89 ppb. Maximum 8-hour ozone value is 79 ppb.

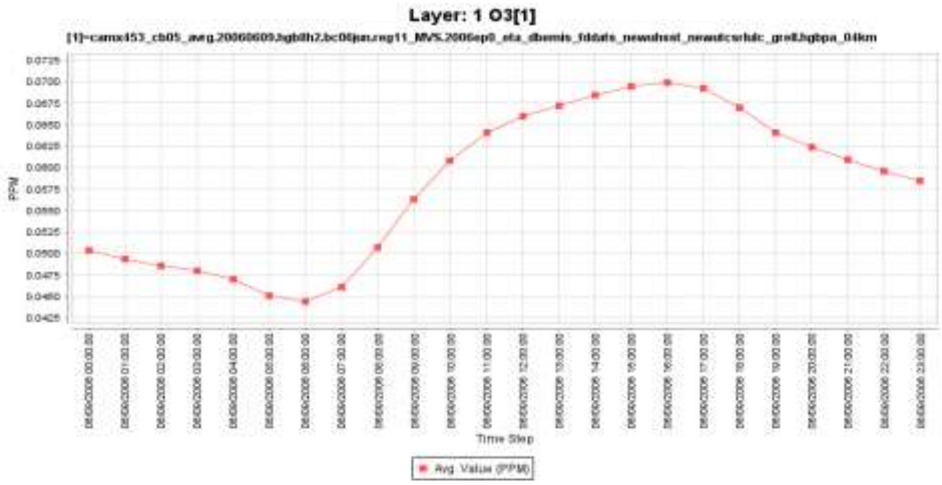


Figure 4: CAMx 4.53 (CB5) Time Series Graph of Ozone Concentration on June 9th, 2006.

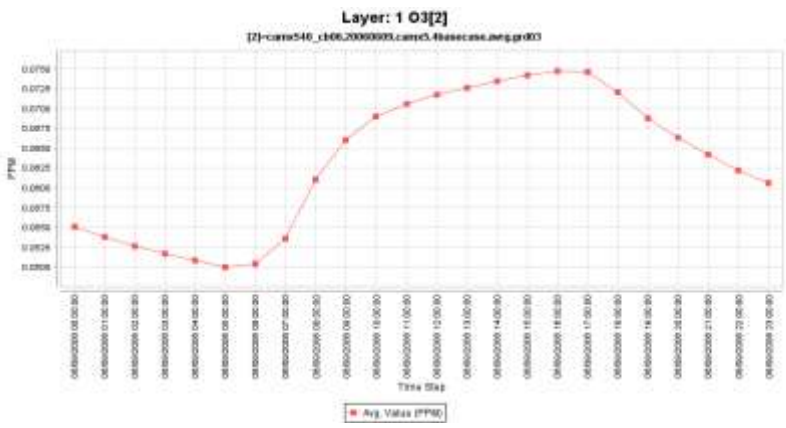


Figure 5: CAMx 5.40 (CB6) Time Series Graph of Ozone Concentration on June 9th, 2006.

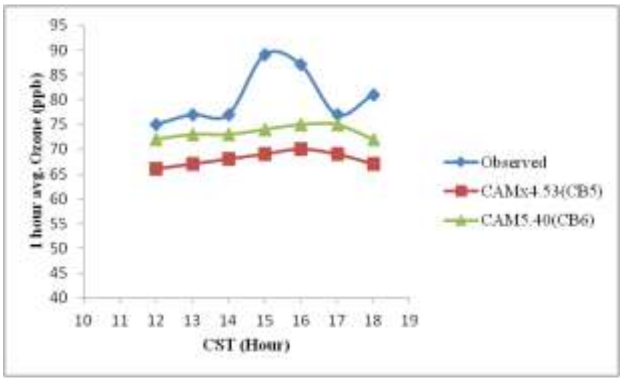


Figure 6: Ozone Concentration Comparison Graph at 12:00 CST to 18:00 CST on June 9th, 2006.

Houston Texas Avenue Stationobserved hourly ozone concentrations are in general higher than the CAMx 4.53(CB5) and CAMx 5.40 (CB6) predicted hourly values. CB6, CAMx 5.40 predicted higher hourly ozone concentrations are in general are higher and more closer to observed values than those predicated fromCB5, CAMx 4.53. It is assumed that even though CB6 has better chemical mechanism to predict air quality than CB5, yet more modifications may be required to improve air quality parameter prediction. As stated earlier, it should be noted here only one monitoring station data is used for comparison here out of the 41 monitoring stations in the HGB area. Plans are currently underway to use the average from the 41 sites for comparison purposes.

V. CONCLUSION

Ozone (O_3) is a secondary pollutant that is produced from complex chemical reactions in the atmosphere. Thus, chemical mechanisms used in the air quality models play a very significant role in predicting the pollutant's concentration.Reliable and precise chemicalmechanisms are necessary to help policy makers to better understand the impact of various emission control strategies. This study is an initial attempt to understand the effect of chemical mechanisms while simulating and analyzing air quality data. CAMx 5.40 (CB6) is found to give better prediction of ozone (O_3) compared to CAMx 4.53 (CB5). From spatial tile plot results, ozone predictions from CAMx 4.53 are found to be about 15% lower than the CAMx 5.40 for HGB area.Chemical mechanism CB6 has improved air quality prediction for CAMx but needs modification to predict accurate pollutant concentration. Due to time constraint only ozone pollutant has been studied. Comprehensive analysis of the other pollutants can give usa better insight to improve CAMx chemical mechanism and also to identifywhich pollutants are responsible for higher ozone production in the HGB area.

VI. ACKNOWLEDGMENTS

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