APPLICATION OF ABACAS-TX FOR OZONE NON-ATTAINMENT IN SOUTHEAST TEXAS

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1. INTRODUCTION

Ground level ozone is one of the six criteria pollutants regulated by the United States Environmental Protection Agency (USEPA) due to its adverse effects on environment and public health(Cao and Thompson 2016). It is formed through the presence of volatile organic compounds (VOCs) and Nitrogen Oxides (NO_x) under sunlight(Lin et al. 2005). Houston-Galveston-Brazoria (HGB) in southeast Texas has been classified as an ozone non-attainment area by the National Ambient Air Quality Standards (NAQQS) since 2004, due to excessive emission of ozone precursors and unfavorable meteorological conditions (i.e., high pressure stagnant air brings dry and sunny weather). Policy makers are seeking for assessment tools for cost-effective emission control strategies to lower ground level ozone concentrations in the HGB non-attainment area, but few policy-oriented software is available for such assessments.

Response modeling methods(Cohan and Napelenok 2011) has been widely applied and demonstrated by many air quality modelers policy analysis, to approximate pollutant concentration as a function of emission change to support policy analysis (e.g., brute-force, decoupled direct method and source apportionment). However, numerous and complicated computation make these methods relative time-consuming for a good performance. Herein, an advanced statistical technique using multidimensional kriging approach called response surface modeling (RSM) is utilized (Foley et al. 2014) to maximize effectiveness while minimizing numbers of cases required for photochemical simulation, making the system an efficient tool in the mean while.

Motivation of this study focuses on the first-time air quality management application of *The Air Benefit and Cost and Attainment Assessment System (ABaCAS)* software package in Southeast Texas ozone non-attainment: A multi-region response surface modeling (RSM) was first developed, with ozone precursors controlled during ozone season of the Year 2015, followed by control strategies assessment for ozone attainment, with public health and economic benefit estimation from ozone reduction.

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2. METHODS

Work flow of this study was mainly the integration of ozone photochemical modeling with ABaCAS streamline for air quality management analysis. And as illustrated in Figure 1, the ultimate result could provide overall benefit-cost ratios for varies of emission control scenarios. To accomplish this, all ozone simulation results must first be well prepared as input of ABaCAS system.

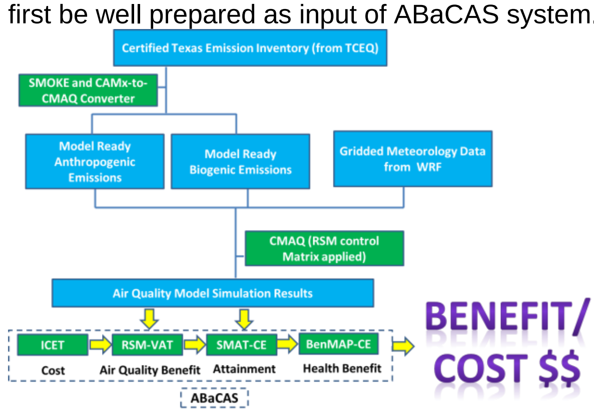

Fig.1. Schematic Diagram Showing Major Model Components Involved in ABaCAS-TX.

2.1 Photochemical Modeling

To build up an RSM model to examine nonlinear response of ground level ozone concentration to emission inventory changes, a photochemical modeling was crucial to accurately simulate ozone concentration at given emission, meteorological, initial and boundary conditions. Community Multiscale Air Quality (CMAQ) model is one of such reliable Eulerian models for gas and particles concentration prediction(Byun and Schere 2006). And in this work, CMAQ v5.2 with emission control built-in module was used. Since we had special interest in ground level ozone activities within Southeast Texas, 191x218 grids domain of 4-km resolution was defined for photochemical modeling, with 20 vertical lays. The model was configured with a CB05 gas phase chemistry and AE6 aerosol chemistry and cloud-ACM-AE6 mechanism. Other important parameters included multiscale advection diffusion, ACM2 horizontal diffusion and M3day deposition scheme. Top 10 maximum daily average eight-hour (MDA8) ozone concentration during model episodes was post-processed within 4-km domain as input of RSM model. High-performance computer cluster (HPCC) with Intel Xeon CPU E5-2620 v4 processors was utilized for emission, meteorological and photochemical modeling under Linux CentOS 7 platform.

2.1.1 Emission Inventory

Emission inventory (EI) data consisted of certified hourly gridded 4km anthropogenic (point, area and mobile) and biogenic emissions provided by TCEQ in CAMx-ready format for ozone season 2012 (downloaded from ftp://amdaftp.tceq.texas.gov/TX/camx). The programs of CAMX2CMAQ (Liu et al. 2015) and Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System were used for conversion of CAMx-formatted emissions into CMAQ-ready I/O API netCDF input files that were compatible for CB05-AE6 CMAQ mechanism. C-shell scripts were written to allocate CMAx-ready elevated point source emissions into netCDF gridded files. Data was visualized with VERDI v1.5 and carefully checked to ensure consistence after EI format conversion.

2.1.2 Meteorological Modeling

Meteorological conditions were simulated with Weather Research and Forecasting (WRF) Model v3.8 (Hegarty et al. 2015). Domains were defined as three nested grids at resolution of 36, 12 and 4 km covering North America, South US (entire Texas with partial surrounding states) and east Texas, respectively. A 20-layer structure was configured with a domain top at 50mb pressure level.

Input NCEP FNL Operational Model Global Tropospheric Analyses data was downloaded from https://rda.ucar.edu/datasets/ds083.2 with the resolution of 1-degree x 1-degree grids and a 6-hour time interval. WRF was initialed with Real-time, global, sea surface temperature (RTG-SST) analysis (data downloaded from ftp://polar.ncep.noaa.gov/pub/history/sst/ophi) Spin-up time was set as 10 days. Configuration of WRF model was for the June through August 2015 episode with parameters determined upon Texas SIP plan and TCEQ contract project for metrological modeling (Hegarty et al. 2015; TCEQ 2016a). Details are shown in Table 1. These settings are aiming at reducing and minimizing bias of temperature, ground level wind direction and especially wind speed, for good photochemical modeling of ground level ozone within 4 km domain of Texas. MCIP v4.1 is used to convert WRF output into meteorological input data ready for CMAQ.

Domain	36 km and 12 km	4 km
Nudging Type	Analysis Nudging	Analysis + Obs Nudging
PBL	YSU	YSU
Cumulus	Kain-Fritsch	Kain-Fritsch
Radiation	RRTM/Dudhia	RRTM/Dudhia
Land-Surface	Pleim-Xiu	Pleim-Xiu
Microphysics	WSM5	WSM6

Table 1. WRF Model Configuration Parameters

2.2 The ABaCAS Streamline

The next step was utilization of ABaCAS for Southeast Texas ozone attainment case study with previous generated modeled MDA8 ozone concentration. This decision making orientated integrated system (Wang et al. 2015) would provide a direct visualization of cost per emission reduction, real-time response of pollutant concentration to emission change (in this case ozone), attainment test after emission adjustment and benefit gained when certain control strategies are applied, ending with assessment of benefit per cost on anthropogenic emission control. All information could be achieved with tools of ICET (International Cost Estimate Tool), RSM, SMAT (Speciated Modeled Attainment Test) and BenMAP (Environmental Benefits Mapping and Analysis Program) in ABaCAS developed by USEPA.

The core software made this system both efficient and effective was RSM-VAT v1.0.7. For RSM development, a 15-dimensional hypercube random sampling was generated on emission factor ranging from 0% to 200% of base case emission level, for point source NOx and VOCs, mobile source NOx and VOCs and area source VOCs in HBG, DFW and other regions of Texas. A total of 83 CMAQ simulations (including one base case and 82 control cases) were run for good RSM performance.

ICET can provide data of cost per % of ozone precursor reduction from all sources. Input data could be prepared with the control strategy model tool CoST v2.13.

A relative reduction factor (RRF) would be calculated from base case and control case ozone concentration simulation in SMAT v0.64. By multiplying this factor by base case ozone design value, future year design value could be estimated, for ozone attainment among all monitoring sites within 4km domain of Texas.

BenMAP v1.3 was for economic and health benefit estimation based on control case ozone peak concentration reduction when compared with base case. Epidemiological study endpoints include school loss days, hospital admissions and emergency room visits and mortality. Valuation of life was calculated by willing to pay approach.

The entire package of ABaCAS version 2.1 is running under windows operating system. Final results will show overall benefit-cost ratio estimation for control scenario cases.

3. RESULTS AND DISCUSSION

3.1 Base Case Model Performance Validation

For WRF simulation results, hourly modeled temperature, wind speed and wind direction were evaluated since their accuracy of great importance to ozone photochemical modeling. Small mean bias and mean error for all parameters suggest a good performance of WRF simulation (see Table 2). In scatter plots, slopes of 1.00 and high correlation coefficients (R^2) of 0.8869, 0.8489 and 0.5939 respectively also suggested perfect matches in between modeled and monitored meteorological data.

	MB (Mean Bias)	ME (Mean Error)
Temperature	0.01 K	0.95 K
Wind Speed	-0.03 m/s	0.35 m/s
Wind Direction	-1.13 deg	16.12 deg

Table 2. Comparison between Modeled and Measured meteorological conditions

For ozone photochemical simulation results, a list of statistical measures was calculated for comparison of modeled ozone concentration with values in the same cell where a monitor is located, among all three regions of HGB, BPT and DFW. As shown in Table 4, modeled 8-hr average ozone concentration matched with measured data well, with a small mean bias less than 2 ppb and MFB less than 10%.

MB (Mean Bias)	1.58 ppb
ME (Mean Error)	7.71 ppb
MFB (Mean Fractional Bias)	9.48%
MFE (Mean Fractional Error	24.56%
MNB (Mean Normalized Bias)	16.82%
MNE (Mean Normalized Error)	29.96%

Table 3. Comparison between Modeled and Measured Ozone Concentration

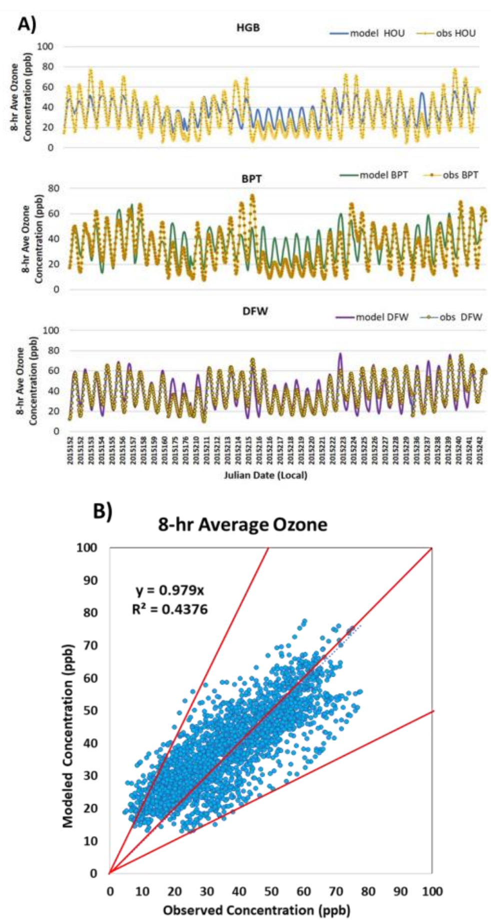

Fig.2. Photochemical Modeling Results Comparison with Observed Ozone Concentration: 2A). Time series plots of for observed and modeled 8-hr average ozone concentrations in HGB BPT and DFW regions; 2B). Scatter plot of modeled vs. observed 8-hr average ozone concentration among all three regions.

Time series and scatter plot (slope=0.98) also showed good agreements in between two sets of data (Fig. 2) during high ozone days. For days when MDA8 ozone concentration was less than 40 ppb, modeled ozone concentrations appeared much higher than observed values. But they would not affect model accuracy since we were only seeking for top 10 of MDA8 ozone during entire episode for RSM input and SMAT attainment test (Foley et al. 2014). Therefore, this base case performance was considered suitable for RSM development and ABaCAS assessment.

3.2 RSM Results Verification

Cross validation was done for RSM for model verification. Mean error was as low as 0.32 ppb with mean normalized error of 0.52%, indicating a good performance of Kriging interpolation.

Performance Metric	Mean	Min	Max
Mean Bias (ppbv)	0.00098	-0.41	0.27
Mean Error (ppbv)	0.32	0.13	1.43
Mean Normalized Bias (%)	0.01%	-0.60%	0.53%
Mean Normalized Error (%)	0.52%	0.20%	2.96%
Mean Fractional Bias (%)	0.01%	-0.68%	0.49%
Mean Fractional Error (%)	0.52%	0.20%	2.95%
Normalized Mean Bias (%)	0.00%	-0.83%	0.45%
Normalized Mean Error (%)	0.54%	0.21%	2.91%

Table 4. RSM Cross Validation Results (83 Cases)

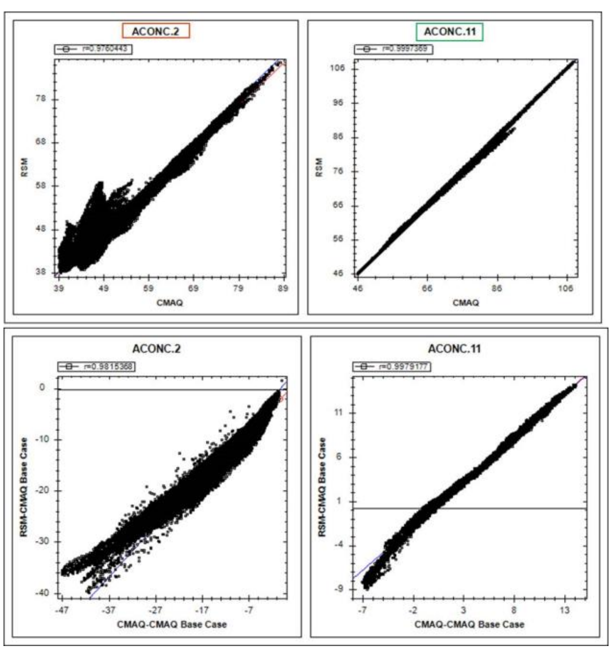

Fig. 3. RSM vs. CMAQ comparisons for Selected Cases

Two cases were selected to compare RSM vs. CMAQ results with each other as illustrated in Figure 3: Case #2 had the highest MNE of 2.96% while Case 11 had the lowest MNE of 0.20%. This was because control matrices of Case #2 were all zeros, which was at the low limit of RSM model. Nevertheless, high correlation coefficient (R>0.97) still indicated a good correlation in between RSM and CMAQ modeled ozone concentration. Selection of control factors to a level not too close to its limit would be helpful to avoid big errors of RSM. In summary, such comparison results supported the fact that this RSM model was suitable for efficient and effective examination of ozone concentration responses to emissions changes from all sources of three Texas regions.

3.3 Control Scenario Case Demonstration

Control case was designed according to TCEQ DFW and HGB SIP plans for 2008 O_3 NAQQS attainment (design value 75 ppb), as well as referring to RSM sensitivity analysis and source apportionment examination (TCEQ 2016a, 2016b).

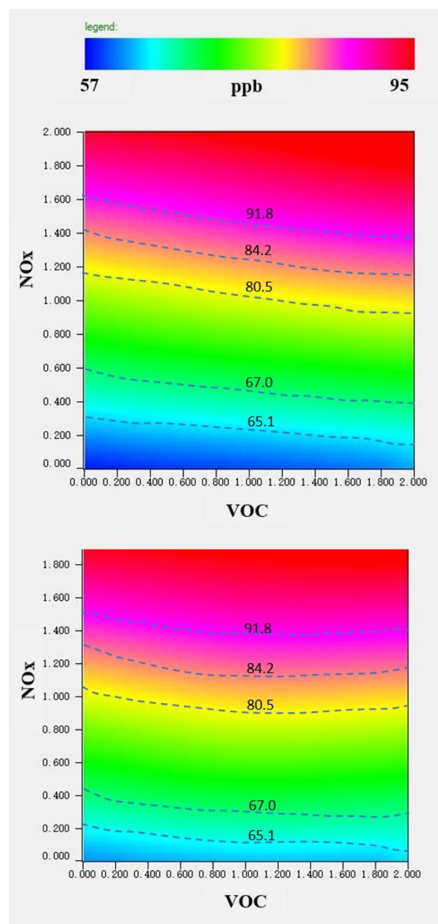

Fig. 4 NOx/VOC ozone isopleth in HGB and DFW

As shown in Figure 4, both DFW and HGB were at the regions where NOx limited production of ozone during high ozone days, which was consistent with the statement from TCEQ SIP plan that most ozone exceedance days were at NOx limited regime while VOC limited production of ozone during low ozone days(TCEQ 2016a). This result suggested that focusing on NOx emission would be the most effective method for ozone pollution management. In Figure 5, source apportionment of ozone reduction was studied with 30% emission reduction of NOx and VOC in the entire Texas. Breakdown contribution information was provided in both areas: HGB mobile source NOx emission was the dominate contributor to ozone formation (54%), followed by HGB point source NOx (22%), mobile (7%) and point (5%) source NOx from regions other than DFW or HGB; In DFW, regional mobile source NOx also made the most contribution to ozone production (54%), however, point source NOx was not at the second place since economy of DFW is not primary relying on oil and chemical industry as HGB.

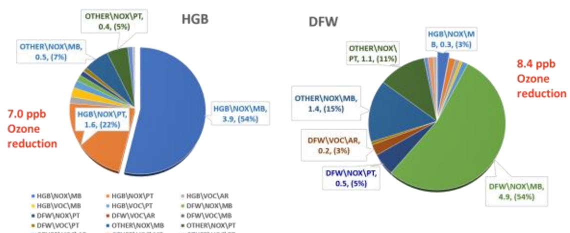

Fig. 5. Ozone Reduction Source Apportionment in HGB

Details of control strategies are shown in Table 5. Strategies are pointing to mobile source NOx reduction in all Texas regions. Such emission controls would be accomplished by existing emission reduction programs in compliance with air regulations in the state of Texas and EPA (*Mass Emissions Cap and Trade Program*, *Highly Reactive Volatile Organic Compound Emissions Cap and Trade Program, Cross-State Air Pollution Rule, etc)*.

Source	Emission Reduction (%)	HGB	DFW	OTHER
Point	NOX	-10	-6	12
Point	VOC	-16	-7	3
Area	VOC	-3	9	2
Mobile	NOX	24	32	10
Mobile	VOC	15	1	1

Table 5. Emission Control Case Designation

As a result, MDA8 ozone reduced by 3.0, 6.0 and 1.8 ppb, respectively in HGB, DFW and other regions of Texas (Figure 6), which lower future year design value from 80 and 83 down to 75 ppb in both DFW and HGB regions in SMAT attainment test (Figure 7). This indicated ozone attainment for 2008 NAQQS. Moreover, benefit gained from ozone reduction spread all over the state, with a high benefit/cost ratio 4.52 and average ratio of 1.33, mainly from its impaction on mortality and acute respiratory symptoms (Figure 8). This control case has successfully demonstrated ozone attainment in HGB and DFW with health benefit gained from ground level ozone reduction in the meantime.

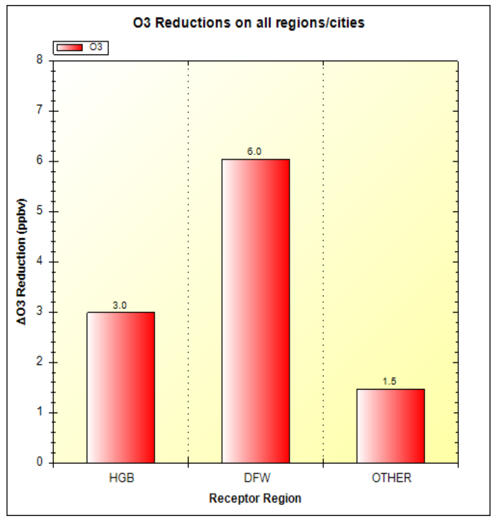

Fig. 6. Real-time Visualization of Regional Ozone Reductions in Emission Control Case

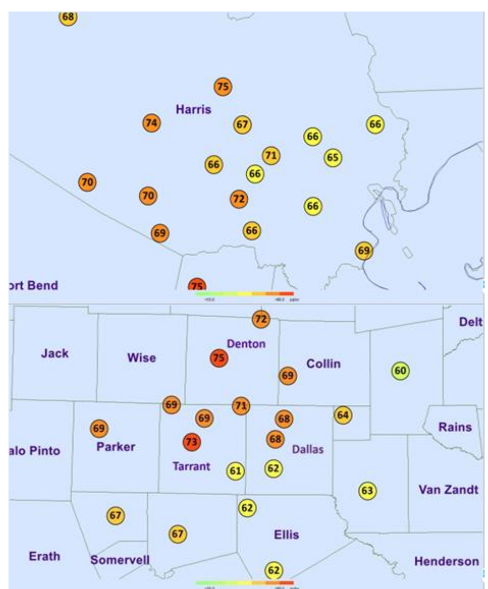

Fig. 7. Attainment Test in HGB and DFW areas

A)

Endpoint	HGB VOC Control Cost	HGB NOx Control Cost	HGB Low Benefit	HGB High Benefit	DFW VOC Control Cost	DFW NOx Control Cost	DFW Low Benefit	DFW High Benefit
Acute Respiratory Symptoms			0.7	4.6			0.8	4.9
School Loss Days			0.2	0.8			0.2	0.9
Hospital Admissions, Respiratory	36.1	0.9	0.5	2.3	34.6	0.6	0.5	2.3
Emergency Room Visits, Respiratory			0.002	0.02			0.002	0.02
Mortality			2.3	237.9			2.5	254.3

(Unit: million dollars)

B)

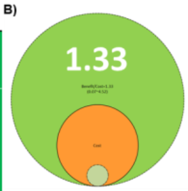

Fig 8. A) Benefit Valuation from Ozone Concentration Reduction in HGB and DFW. B) Benefit/cost for Ozone Reduction in Texas

4. CONCLUSION

This was the first demonstration of ABaCAS for Ozone non-attainment in the State of Texas, with multi-region RSM developed and one emission control scenario case successfully studied. Results suggest that both DFW and HGB high ozone days fall under NO_x-limited regime, where mobile source NO_x emission reduction leads to largest 8-hour peak Ozone reduction. Point source NO_x is also important but not as significant as mobile source NOx emission in both regions. Control of anthropogenic VOC emissions has little impaction on peak ozone reduction. DFW and HGB are relative independent and barely contribute to each other on emission source for ozone production during high ozone days.

Control case demonstration indicated ozone attainment in Texas is anticipated in near future, when emission controls are pointing to mobile source NOx intensive areas. This control scenario can also gain some health and benefit from ozone attainment. Economic development and environmental protection are not exclusive of each other.

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