Quality Assurance Project Plan

Project 14-010

Impact of large-scale circulation patterns on surface ozone concentrations in Houston-Galveston-Brazoria (HGB)

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Summary of Project

QAPP Category Number: III
Type of Project: Research or Development (Modeling)

QAPP Requirements: This QAPP requires descriptions of project description and objectives; organization and responsibilities; scientific approach; quality metrics; data analysis, interpretation, and management; reporting; and references.

QAPP Requirements:

Audits of Data Quality: 10% Required
Report of QA Findings: Required in final report

January 21, 2015

DISTRIBUTION LIST

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1. PROJECT DESCRIPTION AND OBJECTIVES

1.1 Problem Statement

The Houston-Galveston-Brazoria (HGB) area was classified in 2012 as a “marginal” nonattainment zone for ozone (O_3) by the U.S. Environmental Protection Agency (EPA) under the 2008 National Ambient Air Quality Standards (NAAQS) standard (TCEQ, 2012). Previous studies (Nielsen-Gammon et al., 2005a; 2005b; Rappenglück et al., 2008; Tucker et al., 2010; Berlin et al., 2013) have demonstrated the impact of large-scale circulation and associated meteorological factors on surface ozone concentrations and ozone exceedances in HGB. Given that NAAQS for ground-level ozone have become increasingly stringent, it is important to understand and quantify the extent to which the variability in surface ozone concentrations and nonattainment statistics over HGB is associated with the variability in large-scale circulations.

The Bermuda High (BH) is a key driver of large-scale circulation patterns in Southeastern Texas in summer (Figure 1) (Davis et al., 1997). There are two mechanistic linkages between the BH and surface ozone in HGB: first, the west extension of the BH defines the strength of low-level jet (LLJ) of southerly flows that bring marine air with lower ozone background from the Gulf of Mexico (Higgins et al. 1997); second, the high pressure system allows for clear sky and warm temperature conditions that are favorable for local production of ozone. It has been suggested that the late summer maximum of surface ozone in HGB can be explained by a decrease in the strength of LLJ resulting from the reduced intensity of the BH in later summer (Nielsen-Gammon et al., 2005a).

Given the underlying mechanism of BH influencing maritime background O_3 in HGB, it is tempting to explore the observational records for any relationships between BH and O_3. Indeed, Zhu and Liang (2013) has revealed a moderate-to-strong negative correlation between summer interannual anomalies of the BH intensity and maximum daily 8-h average (MDA8) over HGB during the period of 1993-2010 and applied that correlation to evaluate regional climate models. However, there has been no attempt to derive a quantitative relationship of predictability power between the variability of BH and surface O_3 concentrations over HGB. Such a relationship will serve as a policy-aiding analytical tool to understand the interannual variability of ozone nonattainment statistics over HGB attributable to that of large-scale circulations.

It is a known problem that the GEOS-Chem global chemical transport model (CTM), like many other global models, has a tendency to overestimate ozone at Gulf Coast sites in summer during onshore flow from the Gulf of Mexico (Li et al., 2002; Fiore et al., 2002; Reidmiller et al., 2009; Zhang et al., 2011; McDonald-Buller, 2011). Since the regulatory models of Texas Commission on Environmental Quality adopt boundary conditions from the GEOS-Chem global CTM, they are subject to the same deficiency. While inadequate marine boundary layer chemistry has been attributed as one possible explanation for the high bias in the global models, this bias can be also caused by insufficient representation of the dynamic linkage between BH and ozone inflow to HGB (Fiore et al., 2002). This project will develop the observation-derived, quantitative relationships between BH and HGB ozone which is then used as a mechanistic basis to design a bias correction scheme in the GEOS-Chem global CTM to improve its simulation of background O_3 associated with maritime inflow to HGB. The results will benefit the regulatory models of TCEQ through improved boundary conditions at the Gulf of Mexico model domain.

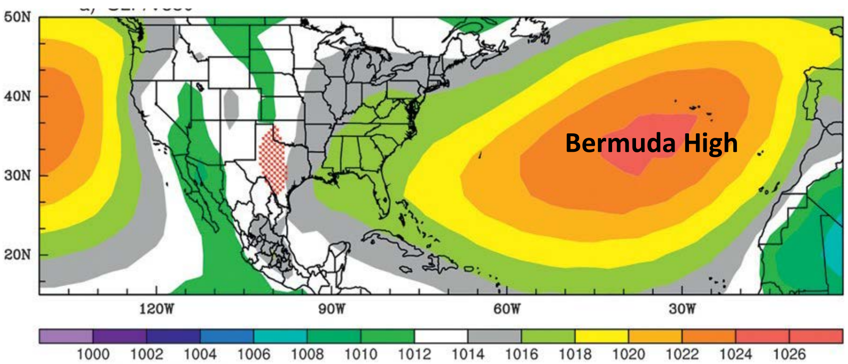

Figure 1. Climatological sea level pressure (SLP; hPa) with the center of the Bermuda High labeled (adopted and modified from Figure 1a of *Zhu and Liang*, 2013).

1.2 Project Objectives

The objectives of the project are: (1) to establish statistical relationships from historical observations to quantify the impact of the BH variations on the variability of MDA8 O_3 in HGB during the ozone seasons; (2) to apply the observation-derived relationship to improve the GEOS-Chem simulation of background ozone inflow from the Gulf of Mexico through development of a bias correction scheme.

To achieve the research objectives, we will conduct three tasks:

Task 1: Characterize the effects of BH on surface O_3 variations in HGB;
Task 2: Develop the statistical relationship between ozone and BH;
Task 3: Develop bias-correction scheme for background O_3 in GEOS-Chem.

2. ORGANIZATION AND RESPONSIBILITIES

2.1 Personnel and Responsibilities

The principal investigator (PI) of this project, Dr. Yuxuan Wang at Texas A&M University Galveston Campus (TAMUG), will have overall responsibility of the research and associated quality assurance. The PI will be supported by one graduate student (Jiaxi Hu) in the atmospheric science department at TAMU and one visiting scholar (Beixi Jia) in the marine science department at TAMUG. This project will be overseen by AQRP Project Manager Vincent Torres and TCEQ Project Liaison Mark Estes. Project participants and their responsibilities are listed in Table 1.

Table 1. Project participants and key responsibilities

Participant	Project Responsibility
Dr. Yuxuan Wang	Principal investigator (PI). Overseeing all aspects of this project and quality assurance; guiding a PhD graduate student and a research assistant to work on all the tasks; writing draft and final report.
Jiaxi Hu	PhD. student working with the PI to conduct data collection and analysis of surface ozone, meteorology, and GEOS-Chem model outputs.
Beixi Jia	Visiting scholar serving as research assistant to the PI to conduct the long-term GEOS-Chem simulations and to develop bias correction schemes in GEOS-Chem.

2.2 Schedule

The overall schedule of the project is presented in Table 2. The due day for each task is:

- April 15th 2015: Task 1 Characterize the effects of BH on surface O_3 variations in HGB
- June 30th 2015: Task 2 Develop the statistical relationship between ozone and BH
- Aug 30th 2015: Task 3 Develop bias-correction scheme for background O_3 in GEOS-Chem

Table 2. Schedule of project activities

Task **months in 2015**	1-2	3-4	5-6	7-8	9
Task 1. Characterize the effects of BH on surface O_3 variations in HGB	🟦	🟦			
Task 2. Develop the statistical relationship between ozone and BHI		🟦	🟦		
Task 3. Develop bias-correction scheme for marine background O_3 in GEOS-Chem			🟦	🟦	
Project Report and Presentation			🟦		🟦

3. SCIENTIFIC APPROACH

3.1 Task 1. Characterize the effects of BH on surface O_3 variations in HGB

We will analyze the more than decade-long observational record of surface O_3 and meteorology (1998 – 2013) during the ozone season (May 1 – October 31) to characterize the complex effects of the BH on surface O_3 variations in HGB. Surface ozone concentrations over HGB have been routinely monitored at continuous ambient monitoring stations (CAMS) maintained by TCEQ and the data will be downloaded through the TCEQ website (http://www.tceq.state.tx.us/agency/data/ozone_data.html). Figure 2 shows the distributions of these CAMS sites over HGB. We will obtain MDA8 O_3 at the individual sites for ozone season days (May – October) from 1998 to 2013, which will then be aggregated at the monthly, seasonal, and interannual time scales. The ozone nonattainment statistics under the 2008 NAAQS will be compiled at the monthly, seasonal, and interannual time scales by sites.

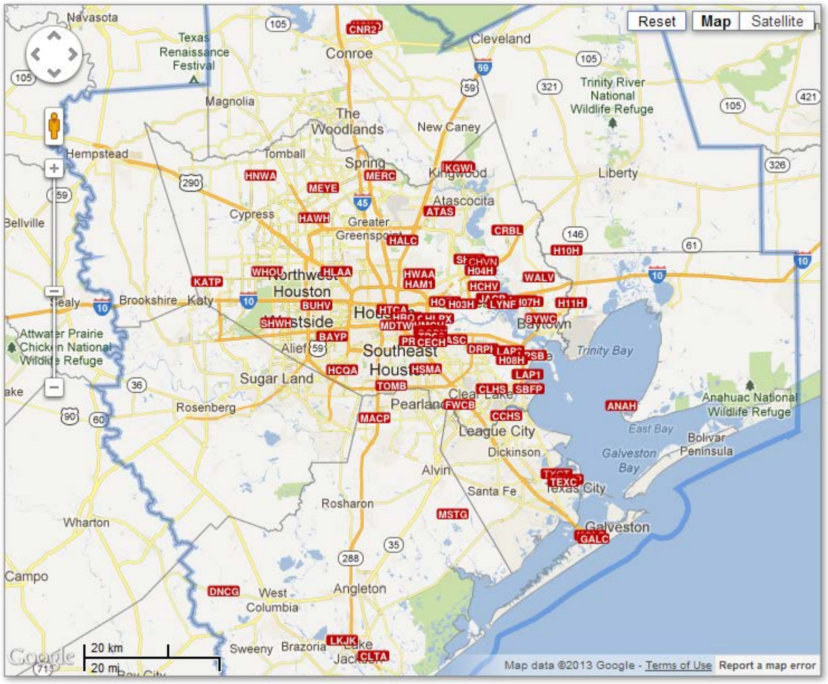

Figure 2. Locations of CAMS sites over HGB (sources: TCEQ).

We will analyze a variety of meteorological factors relating to large-scale atmospheric circulation patterns, including sea level pressure (SLP), winds, temperature, relative humidity (RH), precipitation, etc. These meteorological variables will be obtained from a number of reanalysis data and complemented by weather observation data from the Integrated Surface Database from the National Climatic Data Center (NCDC) (http://www.ncdc.noaa.gov/oa/climate/isd/). The reanalysis data include Modern Era Retospective-analysis for Research and Applications (MERRA), National Centers for Environmental Prediction/National Center for Atmospheric Research (NCEP/NCAR) Reanalysis 1, NCEP North America Regional Reanalysis, and European Centre for Medium Range Forecast Re-analysis Interim (ERA-Interim). Available datasets and references are summarized in Table 3. Because spatially extensive ozone observations have a shorter record than the meteorological data, the time period of analysis is from 1998 to 2013 and will be restricted to the ozone season days (May 1 to Oct 31) in each year.

Several indices have been used in the literature to define the intensity of the BH (Stahle and Cleaveland, 1992; Ortegren et al. 2011, Li et al. 2011; Zhu and Liang, 2013). The majority of the existing BH indices (BHI) are defined on the basis of SLP differences between two locations, one near New Orleans and the other near Bermuda, with their exact locations varying among studies. Zhu and Liang (2013) proposed a new BHI as the difference in regional-mean SLP between the Gulf of Mexico and the southern Great Plains. We will first adopt the existing BHIs in this project to test their utility.

Table 3. Selected datasets to be used in this project.

Data Type	**Dataset**	**Temporal coverage**	**Reference and additional notes**
Surface O_3 observations	TCEQ	1998-present	http://www.tceq.state.tx.us/agency/data/ozone_data.html temporal resolution: hourly and daily for MDA8
Meteorology observations	NOAA Global Historical Climatology Network (GHCN) daily products	1929-present	www.ncdc.noaa.gov/oa/climate/ghcn-daily temporal resolution: daily
	National Climatic Data Center (NCDC)	1929-present	http://www.ncdc.noaa.gov/oa/climate/isd/ temporal resolution: daily
Reanalysis products	MERRA reanalysis	1979-present	http://gmao.gsfc.nasa.gov/research/merra/ spatial resolution: 0.5° x 0.667°
	ERA-Interim reanalysis	1979-present	http://apps.ecmwf.int/datasets/ spatial resolution:0.5°x 0.5°
	NCEP North American Regional Reanalysis	1979 -present	http://rda.ucar.edu/datasets/ds608.0/ spatial resolution: ~32 km
	NCEP/NCAR Reanalysis I	1948-present	http://nomad3.ncep.noaa.gov/ncep_data/ spatial resolution: 2.5°x2.5°

Since the existing BHIs are not designed for the purpose of understanding the influence of BH on Texas air quality, we will propose new BHIs of better relevance to Texas air quality. The new BHIs will (1) use SLP in proximity to HGB as a reference point in calculating pressure difference, (2) incorporate a representation of the locations of the BH center and the west edge of the BH, and (3) consider the LLJ strength and location. As an example, Figure 3 shows June SLP and 10-m winds over the southern US and Gulf of Mexico for the long-term mean from 1998 to 2013 (3a) and two specific years: 2005 (3b), 2010 (3c). Data are from the MERRA reanalysis. Corresponding to the different location and strength of the BH between 2005 and 2010, there are significant differences between the two years in the location of the BH's west edge and center, onshore wind speeds and wind directions over HGB. All these factors will be considered in our proposed BHIs. Figure 4 compares the mean ozone concentrations at several sites over HGB between June of 2005 and 2010, which show significant differences between them.

For ozone, we will consider a number of metrics of MDA8 O_3 over HGB including but not limited to: mean, median, 5th-percentile, 95th-percentile, and nonattainment hours under the 2008 NAAQS standard (75 ppbv). These MDA8 metrics will be calculated on different time (monthly, seasonal, and interannual) and spatial scales (all sites, urban sites, rural sites, upwind and downwind sites of Houston). To remove the influence of trends in anthropogenic emissions over HGB on the interannual variability of ozone, the MDA8 O_3 metrics will be detrended and deseasonalized by subtracting the 30-day moving averages from the original daily data (Tai et al., 2010). We will test the correlations of individual BHIs or a subset of BHIs with different MDA8 O_3 metrics over HGB. The set of BHIs which show the strongest correlations to MDA8 metrics will be selected as the dependent variable to construct the statistical relationship to be accomplished in Task 2.

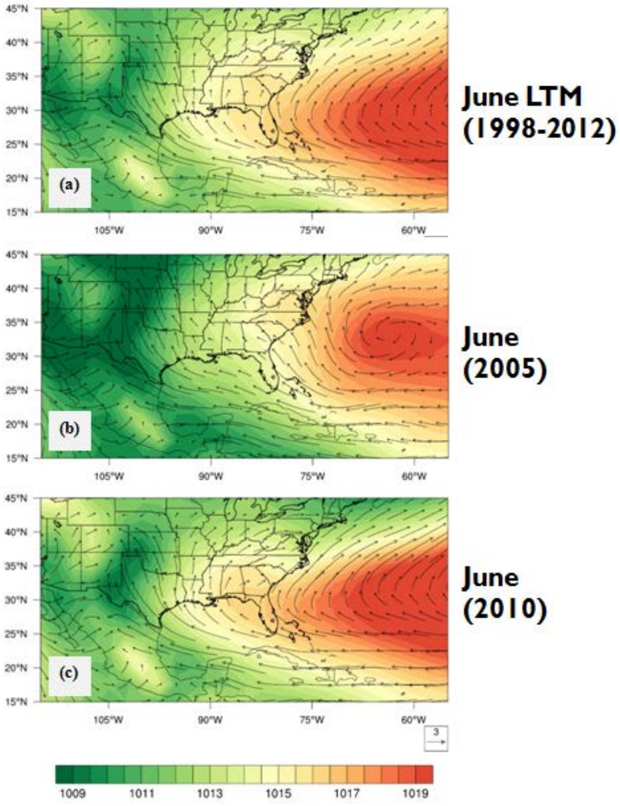

Figure 3. June SLP (hPa) and 10-m winds (m/s) for (a) the long-term mean, (b) 2005, and (c) 2010. Data are from MERRA reanalysis.

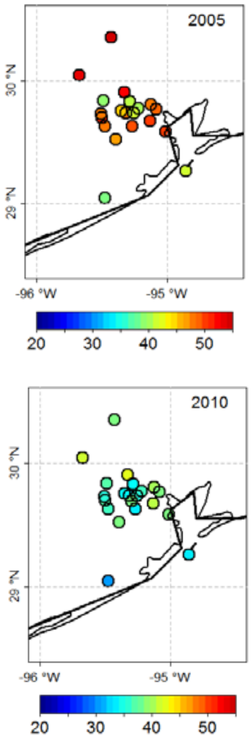

Figure 4. Surface ozone concentrations (ppbv) in June (a) 2005 and (b) 2010 at selected sites over HGB.

3.2 Task 2. Develop the statistical relationship between ozone and BH

We will apply a multiple linear regression (MLR) model (Kutner et al., 2004; Tai et al., 2010) to construct the statistical relationship between MDA8 and BHIs selected from Task 1 on the basis of the historical data compiled from Task 1. This relationship is referred to as O_3-BHI relationship in short. The MLR is a statistical technique that has been commonly used in air quality and climate studies. Since our focus is on synoptic-scale variability, all the MDA8 metrics, BHI, and other meteorological variables will be deseasonalized and detrended in the same way.

The model is of the form:

$$y = \beta_0 + \boldsymbol{\beta_{BH}} \boldsymbol{x_{BH}} + other\ meteorological\ variables + interaction\ terms \qquad (1)$$

where y is the deseasonalized and detrended MDA8 O_3 over HGB, $\boldsymbol{x_{BH}}$ is a set of BHIs representing the location, strength and other characters of the BH that are determined from Task 1 (deseasonalized and detrended), $\boldsymbol{\beta_{BH}}$ is the vector of the regression coefficients, and β_0 is the intercept. The other meteorological variables and interaction terms are added for the purpose of sensitivity tests (to be described below). The regression will be done stepwise to add and delete terms based on Akaike Information Criterion (AIC) statistics to obtain the best model fit (Venables and Ripley, 2003).

MLR will be employed to first estimate the effects of BHIs on MDA8 O_3 over HGB; that is, without the last two terms on the right-hand side of Equation 1. We will use regression splines (a non-linear smoother) to determine if the O_3-BHI associations are approximately linear or linear above a threshold. If exploratory analysis suggests reasonable linear associations, we will replace a smoother term by a linear term in the model; if exploratory analysis suggests reasonable linear associations above a threshold, we will determine the optimal threshold first by using AIC, a measure representing the goodness of model fitting, and then include a linear-threshold term in the model (Atkinson et al., 2012).

Sensitivity analyses will be conducted to evaluate whether the estimated effects of BHIs on MDA8 O_3 vary with the inclusion of other meteorological variables in Equation 1, such as temperature, RH, and precipitation (note that winds effect is incorporated in the design of BHIs; refer to Task 1). Given the known effect of temperature on ozone concentrations, the inclusion of a temperature term in Equation 1 may increase the predictability power of Equation 1 for MAD8. If this is the case, we will add another variable which is the interaction term between temperature and BHI to represent any indirect effect of BH on O3 through temperature. The same process will conduct for RH and precipitation. The interaction terms are up to third-order. The coefficient of determination (R^2), which quantifies the fraction of MAD8 variance that can be accounted for with the statistical model, will be used to rank the different varieties of the MLR model. A specific form of Equation 1 which exhibits the highest R^2 will be chosen to conduct further analysis of the O_3-BHI relationship and used in Task 3 to evaluate the GEOS-Chem model.

3.3 Task 3. Develop bias-correction scheme for background O_3 in GEOS-Chem

The observation-based O_3-BHI relationship obtained in Task 2 offers a test of the reliability of the GEOS-Chem global CTM in describing the response of surface ozone over HGB to the variability in BH. To derive the simulated O_3-BHI relationship for the same periods as observations, it is not practical to run the full-chemistry version of GEOS-Chem for the whole 15 years of the study period. Because our interest here is to correct for the high bias in the simulated background ozone associated with the large-scale maritime inflow, which is primarily a transport issue concerning ozone produced outside HGB, GEOS-Chem's representation of local-scale chemistry and emissions over HGB is not expected to play a significant role. In fact, the regulatory models at TCEQ have more advanced treatments on local-scale ozone chemistry and dynamics over HGB and as such they only require lateral boundary conditions from GEOS-Chem. Therefore, four sets of GEOS-Chem runs will be conducted, all at a spatial resolution of 2^o x 2.5^o: (Run 1) a full-chemistry simulation for the ozone season of one year with the weakest BH; (Run 2) same as run 1, but for another meteorological year with the strongest BH; (Run 3) a tagged-ozone simulation for a 15-year period (1998 to 2013) using time-varying meteorology from the MERRA reanalysis and archived ozone production and loss rate from run 1; and (Run 4) same as run 3, but with archived ozone production and loss rate from run 2. The two full-chemistry simulations (run 1 and run 2) will use the same anthropogenic emissions for the year of 2008 while allowing the natural emissions (i.e., soil NOx, lightning NOx, biogenic VOCs) to change with meteorology. This simple treatment of anthropogenic emissions is justifiable because the O_3-BHI relationship is constructed on the basis of deseasonalized and detrended

MDA8 and meteorology data and hence deliberately separates the impact of emission trends from that of meteorology. The tagged-ozone simulation is not only computationally efficient, but also provides a breakdown of total ozone at a given location to pre-defined analysis regions where ozone is produced (not where ozone precursors are emitted). The tagged-ozone simulation has been widely used in previous ozone source attribution studies (e.g., Fiore et al. 2002; Wang et al., 2011).

Given the known high bias of maritime background O_3 in GEOS-Chem, a mismatch between the observed and simulated O_3-BHI relationships is expected. We will investigate the model deficiencies in correlation coefficient, $\boldsymbol{\beta_{BH}}$ (the regression coefficient), and β_0 (the intercept) (c.f. Equation 1) to diagnose the causes. We will compare the O_3-BHI relationship from the two sets of tagged-ozone simulations with different ozone production/loss rate to examine the influence of chemistry.

The model-to-observation differences in the O_3-BHI relationship will be used as a basis to formulate a bias correction scheme in GEOS-Chem to link its deficiency in simulating background O_3 inflow from the Gulf of Mexico with the characteristics of BH. The proposed bias correction to GEOS-Chem will be designed to benefit the regulatory model at TCEQ through improving boundary conditions at the Gulf of Mexico model domain. To this end, we will calculate a correction function which will be applied to the tagged-ozone tracer from the Gulf of Mexico so as to minimize the differences between the observed and simulated O_3-BHI relationship.

The correction function is of the form:

$$C_{m,c} = C_{m,o} + \Delta\beta_0 + \Delta\beta_{BH}\, x_{BH} \qquad (2)$$

where $C_{m,c}$ is the maritime inflow of background O_3 after the correction, $C_{m,o}$ is the maritime inflow of background O_3 from the GEOS-Chem tagged-ozone run, $\boldsymbol{x_{BH}}$ is the set of BHIs as in Equation 1, $\Delta\beta_0$ is the difference in observed and simulated intercept (observed minus simulated) of the O_3-BHI relationship, and $\Delta\boldsymbol{\beta_{BH}}$ is the difference in observed and simulated coefficient (observed minus simulated) of the O_3-BHI relationship. Other terms as described in Equation 1 may be added in Equation 2 if they are determined useful from Task 2. Here we assume the GEOS-Chem model correctly simulates BH and the related BHIs, which is justifiable because the model is driven by the MERRA reanalysis meteorology.

A rearrangement of Equation 2 gives:

$$C_{m,c} - C_{m,o} = \Delta\beta_0 + \Delta\beta_{BH}\, x_{BH} \qquad (3)$$

where the left-hand side ($C_{m,c}$ - $C_{m,o}$) is the magnitude of the bias correction to GEOS-Chem ozone flowing in through the Gulf of Mexico. According to Equation 3, the bias correction has a time-varying component which depends on BHI ($\Delta\boldsymbol{\beta_{BH}}\,\boldsymbol{x_{BH}}$) and a time-independent component($\Delta\beta_0$). Because of the time-varying component, it fares better than the conventional method relying on a constant bias correction by adjusting to temporal changes of large-scale circulation patterns. Besides, the bias correction scheme has a mechanistic linkage to the BH characteristics. Given that we use 15-years' worth of observations and model runs to obtain the parameters in Equation 3, we anticipate the parameters to be robust and we will use statistical analysis to quantify their uncertainties. Furthermore, the bias correction scheme is simple to implement to correct for the boundary conditions used in the regulatory models of TCEQ.

Finally, we will collaborate with TCEQ in incorporating the bias-corrected GEOS-Chem boundary conditions into the regulatory model of CAMx and assess the impacts. We will run an episode with CAMx using the new bias correction applied to the boundary conditions from GEOS-Chem and compare the results from this model run to the results from the original model run. The impact of this approach on the model performance of surface ozone will be quantified and evaluated with ozone observations over HGB.

4. QUALITY METRICS

The project will derive a quantitative relationship between BH and HGB ozone from observations and apply that relationship to design an empirical bias correction scheme in the GEOS-Chem global CTM to improve its simulation of background O_3 associated with maritime inflow to HGB. Secondary data of surface ozone observations and meteorological reanalysis will be used in the Task 1 and Task 2 activities, while statistical modeling and GEOS-Chem modeling will be used in Task 2 and Task 3 activities. We will use the EPA quality assurance modeling document for guidance “EPA Requirements for Quality Assurance Project Plans EPA QA/R-5”. The quality assurance procedures will involve careful and detailed documentation as well as creation of appropriate metadata for all electronic databases used for inputs or generated as models’ outputs.

4.1 Quality of secondary data

A summary of the secondary data to be used in the project and their references is provided in Table 3. We will follow the quality assurance and quality control protocols of these data sources and document the data versions used in this project. Surface ozone concentrations over HGB will be downloaded through the TCEQ website (http://www.tceq.state.tx.us/agency/data/ozone_data.html). The distributions of the CAMS sites over HGB are shown in Figure 2. We will obtain MDA8 O_3 at the individual sites for ozone season days (May – October) from 1998 to 2013, which will then be aggregated at the monthly, seasonal, and interannual time scales. Meteorological data will be obtained from a number of reanalysis data (MERRA, NCEP, ERA-Interim) and weather observation data from the Integrated Surface Database from the National Climatic Data Center (NCDC) (http://www.ncdc.noaa.gov/oa/climate/isd/). Because spatially extensive ozone observations have a shorter record than the meteorological data, the time period of analysis is from 1998 to 2013 and will be restricted to the ozone season days (May 1 to Oct 31) in each year.

4.2 Quality of statistical modeling

The MLR model (Equation 1) to be used in Task 2 is a statistical technique that has been commonly used in air quality and climate studies. The independent variables used in the MLR model include the MDA8 O_3 metrics, BHI, and other meteorological variables which are obtained from surface observations and meteorology reanalysis (c.f. 4.1). To ensure quality, these input variables will be deseasonalized and detrended in the same way by subtracting the 30-day moving averages from the original daily data, following the method of Tai et al. (2010).

The regression will be done stepwise to add and delete terms based on Akaike Information Criterion (AIC) statistics to obtain the best model fit (Venables and Ripley, 2003). We will use regression splines (a non-linear smoother) to determine if the O_3-BHI associations are approximately linear or linear above a threshold. If exploratory analysis suggests reasonable linear associations, we will replace a smoother term by a linear term in the model; if exploratory analysis suggests reasonable linear associations above a threshold, we will determine the optimal threshold first by using AIC, a measure representing the goodness of model fitting, and then include a linear-threshold term in the model (Atkinson et al., 2012).

Sensitivity analyses will be conducted to evaluate whether the estimated effects of BHIs on MDA8 O_3 vary with the inclusion of other meteorological variables in Equation 1, such as temperature, RH, and precipitation. Given the known effect of temperature on ozone concentrations, the inclusion of a temperature term in Equation 1 may increase the predictability power of Equation 1 for MAD8. If this is the case, we will add another variable which is the interaction term between temperature and BHI to represent any indirect effect of BH on O3 through temperature. The same process will conduct for RH and precipitation. The interaction terms are up to third-order. The coefficient of determination (R^2), which quantifies the fraction of MAD8 variance that can be accounted for with the statistical model, will be used to rank the different varieties of the MLR model.

4.3 Quality of GEOS-Chem modeling

The GEOS-Chem global CTM has a standard benchmarking procedure for each major code release, using observations compiled from surface monitoring network, aircraft campaigns, and satellite retrievals around the globe. Building from these efforts, we will perform in-depth evaluation of the model’s performance in describing the response of surface ozone over HGB to the variability in BH. Four sets of GEOS-Chem runs will be conducted, all at a spatial resolution of 2^o x 2.5^o: (Run 1) a full-chemistry simulation for the ozone season of one year with the weakest BH; (Run 2) same as run 1, but for another meteorological year with the strongest BH; (Run 3) a tagged-ozone simulation for a 15-year period (1998 to 2013) using time-varying meteorology from the MERRA reanalysis and archived ozone production and loss rate from run 1; and (Run 4) same as run 3, but with archived ozone production and loss rate from run 2. The two full-chemistry simulations (run 1 and run 2) will use the same anthropogenic emissions for the year of 2008 while allowing the natural emissions (i.e., soil NOx, lightning NOx, biogenic VOCs) to change with meteorology. This simple treatment of anthropogenic emissions is justifiable because the O_3-BHI relationship is constructed on the basis of deseasonalized and detrended MDA8 and meteorology data and hence deliberately separates the impact of emission trends from that of meteorology. The MDA8 O_3 and BHIs will be compiled from the model results from run 3 and 4.

We will maintain documentation files for each model run that identifies model code versions, dates, analyst, and input and output files. Each input/output file used will be reviewed for quality assurance purposes using various visualization methods, including software animations and graphing, as well by quantitative filtering using selected filter criteria to identify anomalous data. The simulated O_3-BHI relationship will be compared with the observed relationship using the performance metrics listed in Table 4.

Table 4. Performance metrics of the GEOS-Chem model.

Mean Bias (MB)	$MB = 1/N\sum_{i=1}^{N}(M_i - O_i)$
Normalized Mean Bias (NMB)	$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N}O_i} \times 100\%$
Correlation Coefficient (Corr. R)	$Corr.R = \frac{\sum_{i=1}^{N}(M_i - \overline{M})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N}(M_i - \overline{M})^2}\sqrt{\sum_{i=1}^{N}(O_i - \overline{O})^2}}$
Root Mean Square Error (RMSE)	$RMSE = \sqrt{1/N\sum_{i=1}^{N}(M_i - O_i)^2}$

Note: M is the model output, O is the observation, N is the number of samples, and

$\overline{M} = 1/N\sum_{i=1}^{N}M_i$, $\overline{\mathrm{O}} = 1/N\sum_{i=1}^{N}O_i$.

5. DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

5.1 Data analysis and interpretation

For surface ozone observations, we will analyze a number of metrics of MDA8 O_3 over HGB including but not limited to: mean, median, 5th-percentile, 95th-percentile, and nonattainment hours under the 2008 NAAQS standard (75 ppbv). These MDA8 metrics will be calculated on different time (monthly, seasonal, and interannual) and spatial scales (all sites, urban sites, rural sites, upwind and downwind sites of Houston). To remove the influence of trends in anthropogenic emissions over HGB on the interannual variability of ozone, the MDA8 O_3 metrics will be detrended and deseasonalized. We will test the correlations of individual BHIs or a subset of BHIs with different MDA8 O_3 metrics over HGB. The set of BHIs which show the strongest correlations to MDA8 metrics will be selected as the dependent variable to construct the statistical relationship.

The GEOS-Chem model outputs will be analyzed according to Equation (2) and (3) to develop the bias correction scheme that is associated with the temporal changes of large-scale circulation patterns. Given that we use 15-years' worth of observations and model runs to obtain the parameters in Equation 3, we anticipate the parameters to be robust and we will use statistical analysis to quantify their uncertainties. Furthermore, the bias correction scheme is simple to implement to correct for the boundary conditions used in the regulatory models of TCEQ. We will collaborate with TCEQ in incorporating the bias correction scheme to the GEOS-Chem boundary conditions used in the regulatory models and to assess the impacts.

5.2 Audits of data quality

Secondary data: A member of the research team who did not develop or compile the secondary data (c.f. Table 3) will review at least 10% of the data for quality assurance purposes. We will also invite the Project Liaison at TCEQ to review at least 10% of surface ozone observations over HGB used in the project. The quality of the secondary data of meteorological observations and reanalysis will be reviewed by comparing descriptive statistics and summary graphs generated by the project with those from the original data's website or documentation.

Statistical modeling: A member of the research team who did not develop the statistical model or process its input data will review at least 10% of the results from the statistical modeling for quality assurance purposes. The results to be audited will include but not limited to: parameters generated by the statistical model, cross-validation results of the model, sensitivity test results of the model, and predicted correlations between the dependent and independent variables. We will also invite colleagues who have expertise in statistical modeling to review the statistical modeling outputs; potential peer reviewers are Dr. Kai Zhang at the University of Texas Health Science Center at Houston and Mr. Lu Shen at Harvard University.

GEOS-Chem modeling: A member of the research team who did not conduct the GEOS-Chem simulation or develop the bias correction scheme in GEOS-Chem will review at least 10% of the modeling results for quality assurance purposes. The results to be audited will include but not limited to: surface ozone simulated by the GEOS-Chem model prior to and after the bias correction scheme, implementation of the bias correction scheme, surface ozone simulated by CAMx prior to and after using the bias-corrected boundary conditions from GEOS-hem. We will also invite a few members from the GEOS-Chem development team and users' community to review at least 10% of the modeling results; potential peer reviewers are Dr. Daniel Jacob at Harvard University and Dr. Lin Zhang at Peking University.

5.3 Data management

The project will produce the statistical relationship, bias correction scheme, other electronic data generated from the statistical analysis, and GEOS-Chem model results. These data will be stored in the Storage Archive System of Texas A&M Supercomputing Facility and workstations managed by the PI. In addition, the data will be stored on redundant disk arrays and archived to hard media. The project will make available all data collected and produced for TCEQ and AQRP upon request or no later than 3 months after the data are collected or created. Transfer of data to TCEQ and AQRP will be facilitated through the internet (e.g., ftp exchange) or by mail of hard disks. The project data will be retained for no less than 3 years after the project has ended.

6. REPORTING

The project will deliver monthly, quarterly, and final reports according to AQRP requirements. The technical deliverables from each task will be incorporated in those regular reports when appropriate, and the electronic data generated from the project will be archived and made available for TCEQ and other AQRP researchers. A description of the specific reports to be submitted and their due dates are outlined below.

Executive Summary

At the beginning of the project, an Executive Summary will be submitted to the Project Manager for use on the AQRP website. The Executive Summary will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Due Date: Friday, January 9, 2015

Quarterly Reports

The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	January & February 2015	Friday, February 27, 2015
Quarterly Report #2	March, April, May 2015	Friday, May 29, 2015
Quarterly Report #3	June, July, August 2015	Monday, August 31, 2015
Quarterly Report #4	September, October, November 2015	Monday, November 30, 2015

Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY14-15 MTR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start – February 28, 2015	Monday, March 9, 2015
Technical Report #2	March 1 - 31, 2015	Wednesday, April 8, 2015
Technical Report #3	April 1 - 28, 2015	Friday, May 8, 2015
Technical Report #4	May 1 - 31, 2015	Monday, June 8, 2015
Technical Report #5	June 1 - 30, 2015	Wednesday, July 8, 2015
Technical Report #6	July 1 - 31, 2015	Monday, August 10, 2015
Technical Report #7	August 1 - 31, 2015	Tuesday, September 8, 2015

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY14-15 FSR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start – February 28, 2015	Monday, March 9, 2015
FSR #2	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #3	April 1 - 28, 2015	Friday, May 15, 2015
FSR #4	May 1 - 31, 2015	Monday, June 15, 2015
FSR #5	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #6	July 1 - 31, 2015	Monday, August 17, 2015
FSR #7	August 1 - 31, 2015	Tuesday, September 15, 2015
FSR #8	September 1 - 30, 2015	Thursday, October 15, 2015
FSR #9	Final FSR	Monday, November 16, 2015

Draft Final Report

A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Due Date: Tuesday, August 18, 2015

Final Report

A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Due Date: Wednesday, September 30, 2015

Project Data

All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information.

AQRP Workshop

A representative from the project will present at the AQRP Workshop in June 2015.

7. REFERENCES

Atkinson RW, Yu D, Armstrong BG, Pattenden S, Wilkinson P, Doherty RM, Heal MR, Anderson HR. 2012: Concentration–response function for ozone and daily mortality: results from five urban and five rural U.K. populations. Environ Health Perspect 120:1411–1417

Berlin SR, A.O. Langford, M. Estes, M. Dong, and D.D. Parrish. 2013: Magnitude, decadal changes, and impact of regional background ozone transported into the Greater Houston, Texas, area, Environ. Sci. Technol., 47, 13985−13992, dx.doi.org/10.1021/es4037644

Davis, R. E., B. P. Hayden, D. A. Gay, W. L. Phillips, and G. V. Jones, 1997: The North Atlantic subtropical anticyclone. J. Climate, 10, 728–744

Fiore, A.M., D.J. Jacob, I. Bey, R.M. Yantosca, B.D. Field, A.C. Fusco, 2002: Background ozone over the United States in summer: origin, trend, and contribution to pollution episodes. Journal of Geophysical Research 107 (D15). doi:10.1029/2001JD000982

Higgins, R. W.,Y. Yao, E. S. Yarosh, J. E. Janowiak, and K. C. Mo, 1997: Influence of the Great Plains low-level jet on summertime precipitation and moisture transport over the central United States. J. Climate, 10, 481–507

Kutner, M.H., Nachtsheim, C.J., Neter, J., Li, W., 2004. Applied Linear Statistical Models. McGraw-Hill/Irwin, New York, NY, USA.

Li, Q., D. J. Jacob, T. D. Fairlie, H. Liu, R. M. Yantosca, and R. V. Martin, 2002: Stratospheric versus pollution influences on ozone at Bermuda: Reconciling past analyses, J. Geophys. Res., 107, 10.1029/2002JD002138

Li, W., L. Li, R. Fu, Y. Deng, and H. Wang, 2011: Changes to the North Atlantic subtropical high and its role in the intensification of summer rainfall variability in the southeastern United States. J. Climate, 24, 1499–1506

McDonald-Buller, E. C.; D. T.Allen, N. Brown, D.J. Jacob, D. Jaffe, C.E. Kolb, A.S. Lefohn, S. Oltmans, D.D. Parrish, G. Yarwood, L. Zhang, 2011: Establishing Policy Relevant Background (PRB) Ozone Concentrations in the United States. Environ. Sci. Technol. 2011, 45, 9484−9497

Nielsen‐Gammon, J. W., J. Tobin, and A. McNeel, 2005b: A conceptual model for eight‐hour ozone exceedances in Houston, Texas, Part II: Eight‐hour ozone exceedances in the Houston‐Galveston metropolitan area, 79 pp., Houston Adv. Res. Cent., Houston, Tex.

Nielsen‐Gammon, J., J. Tobin, A. McNeel, and G. Li, 2005a: A conceptual model for eight‐hour ozone exceedances in Houston, Texas, Part I: Background ozone levels in eastern Texas, 52 pp., Houston Adv. Res. Cent., Houston, Tex.

Ortegren, J. T., P. A. Knapp, J. T. Maxwell, W. P. Tyminski, and P. T. Soule´, 2011: Ocean–atmosphere influences on low frequency warm-season drought variability in the Gulf Coast and southeastern United States. J. Appl. Meteor. Climatol., 50, 1177–1186.

Rappenglück, B., R. Perna, S. Zhong, and G. A. Morris, 2008: An analysis of the vertical structure of the atmosphere and the upper‐level meteorology and their impact on surface ozone levels in Houston, Texas, J. Geophys. Res., 113, D17315, doi:10.1029/2007JD009745

Reidmiller, D. R., A. M. Fiore, D.A. Jaffe, D. Bergmann, C. Cuvelier, F.J. Dentener, et al., 2009: The influence of foreign vs. North American emissions on surface ozone in the US. Atmos. Chem. Phys., 9, 5027–5042

Stahle, D. W., and M. K. Cleaveland, 1992: Reconstruction and analysis of spring rainfall over the southeastern U.S. for the past 1000 years. Bull. Amer. Meteor. Soc., 73, 1947–1961

Tai, A.P.K., L.J. Mickley, D.J. Jacob, 2010: Correlations between fine particulate matter ($PM_{2.5}$) and meteorological variables in the United States: Implications for the sensitivity of PM2.5 to climate change, Atmospheric Environment, 44, 3976-3984

Texas Commission on Environmental Quality (TCEQ), 2012: Houston-Galveston-Brazoria: Current attainment status; retrieved on November 16, 2014 from http://www.tceq.texas.gov/airquality/sip/hgb/hgb-status.

Tucker, S. C., R. M. Banta, A. O. Langford, C. J. Senff, W. A. Brewer, E. J. Williams, B. M. Lerner, H. Osthoff, and R. M. Hardesty, 2010: Relationships of coastal nocturnal boundary layer winds and turbulence to Houston ozone concentrations during TexAQS 2006, J. Geophys. Res., 115, D10304, doi:10.1029/2009JD013169

Wang, Y., Y.Q. Zhang, J.M. Hao and M. Luo, Seasonal and spatial variability of surface ozone over China, 2011: contributions from background and domestic pollution, Atmos. Chem. Phys.,11, 3511–3525

Zhang, L., D.J. Jacob, N.V. Smith-Downey, D.A. Wood, D. Blewitt, C.C. Carouge, A. van Donkelaar, D.B.A. Jones, L.T. Murray, and Y. Wang, 2011: Improved estimate of the policy-relevant background ozone in the United States using the GEOS-Chem global model with 1/2ox2/3o horizontal resolution over North America, Atmos. Environ., 45(37), 6769-6776, doi:10.1016/j.atmosenv.2011.07.054

Zhu, J., and X.-Z. Liang, 2013: Impacts of the Bermuda High on Regional Climate and Ozone over the United States, Journal of Climate, 26, 1018-1032, doi: 10.1175/JCLI-D-12-00168.1