Semiannual Progress Report on the Project:

"Modeling the Transport and Chemical Evolution of Onshore and Offshore Emissions and Their Impact on Local and Regional Air Quality Using a Variable-Grid-Resolution Air Quality Model"

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Abstract

This semiannual report summarizes the research performed from 17 April 2005 through 16 October 2005. Major portions of the research in several of the project's current eight tasks have been completed. We have successfully developed the meteorological inputs using the best possible modeling configurations, resulting in improved representation of atmospheric processes.

The development of the variable-grid-resolution emissions model, SMOKE-VGR, is also completed. The development of the MAQSIP-VGR has been completed and a test run was performed to ensure the functionality of this air quality model. We have started incorporating new emission data base to update the offshore emissions. However, we have faced some bottleneck problems in the testing the integrity of the new database. For this reason, we have asked for a no-cost extension of this project to tackle these scientific problems. Thus, the project is on a one-year delay schedule. During the upcoming reporting period, we expect to solve all problems related to the new emission database and perform the first MAQSIP-VGR simulations over the Houston-Galveston region to study the roles of the meteorology, offshore emissions, and chemistry-transport interactions that determine the temporal and spatial evolution of ozone and its precursors.

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Section 1: Experimental

1.1 Project Objectives

This research project has two primary objectives:

(1) to further develop and refine the Multiscale Air Quality Simulation Platform – Variable Grid Resolution (MAQSIP-VGR) model, an advanced variable-grid-resolution air quality model, to provide detailed, accurate representation of the dynamical and chemical processes governing the fate of anthropogenic emissions in coastal environments; and

(2) to improve current understanding of the potential impact of onshore and offshore oil and gas exploration and production (E&P) emissions on O_3 and particulate matter nonattainment in the Gulf of Mexico and surrounding states.

1.2 Task Descriptions

There are eight tasks to be completed during the first two years of the project and two tasks for the final year. This first semiannual report provides detailed descriptions of research work performed during the first six months of project year 1. The rest of this section provides brief descriptions of the first eight tasks. Section 2, "Results and Discussion," describes what has been completed in each of these tasks, Section 3 presents conclusions, and Section 4 presents a list of conference/workshop presentations and possible journal articles that may be developed during the course of this project.

1.2.1 Task 1: Develop Modeling Domains and Case Studies

The meteorological modeling domains will be configured with various horizontal grid resolutions. We propose to use grid resolutions of 36, 12, and 4 km. The 36-km resolution grid will cover a region extending west of the Atlantic Ocean westward to the Rockies; a grid at this coarse resolution will allow meteorological modeling simulations that are computationally inexpensive, and whose results will be used primarily to provide lateral boundary conditions to the nested grids. The 12-km grids will cover portions of Southern and Southeastern states. The 4-km grids will cover domains specific to addressing air pollution issues proposed in this study.

Selection of the time periods simulated for the case studies will be based on analysis of measurement data and the availability of offshore emissions activity data. The choice will also consider other current and prior modeling efforts (e.g., the Gulf Coast ozone study); simulating similar time periods will allow us to cross-compare and evaluate our modeling results against others available for the region.

The MAQSIP-VGR simulation domain will cover the Gulf of Mexico and some inland parts of surrounding states. Our air quality modeling analyses will focus on two geographical regions of

the Gulf Coast. The variable-grid mesh for these regions will consist of grid resolutions ranging from 400 m to 4 km, while the grid resolution for the areas beyond these two regions of interest will have grid resolutions ranging from 4 km to 12 km. The time-dependent lateral boundary conditions for this grid-mesh configuration will be obtained from regional uniform grid simulations of the MAQSIP-VGR.

1.2.2 Task 2: Improve the Representation of Boundary Layer Processes

Emissions of NO_x, VOC, and SO_2 from point and other (ships, helicopters) sources released over the outer continental shelf regions can be transported by land and sea breezes, leading to increased pollutant concentrations in coastal and inland regions surrounding the Gulf of Mexico. Because marine boundary layer processes are controlled mostly by weak forcing mainly due to shear production and in part by weak buoyancy production of turbulence, it is critical to study the benefits of using a turbulent kinetic energy-based scheme (TKE scheme) in the MM5 compared to a traditional eddy diffusivity-based first-order atmospheric boundary layer (ABL) scheme. We will perform MM5 simulations using a TKE-based scheme and an eddy diffusivity-based scheme and evaluated them rigorously in their ability to realistically simulate marine and coastal circulations**.**

1.2.3 Task 3: Assimilation of Surface Observations to Improve MM5 Simulations

At least, two types of surface observations are available for use in the MM5 simulations: traditionally available measurements from routine land-based measurements (at 2 m and 10 m AGL), and remotely sensed satellite-based observations. To a larger extent, both of these observations are mainly used for model evaluation rather than for improving model simulations.

1.2.3.1 Land-Based Observations

Since uncertainty in the specification of vegetation and soil parameters and other modeling assumptions and descritizations leads to modeling errors, particularly near the surface, we will use the Flux-Adjusting Surface Data Assimilation System (FASDAS) developed and tested by Alapaty et al. (2001a,b,c) to reduce these errors. In this continuous surface data assimilation technique, abundant land-based surface measurements of temperature and relative humidity (dew-point temperature) are used to nudge a 1-D model's lowest-layer air temperature and moisture along with the ground/skin temperature. To do this, surface-layer temperature and water vapor mixing ratio are directly assimilated by using the analyzed surface data, while ground/skin temperature and soil moisture are indirectly assimilated, thereby maintaining greater consistency between the soil temperature and moisture fields and the surface-layer mass-field variables. The FASDAS then uses the differences between the observations and model predictions to estimate adjustments to the surface fluxes of sensible and latent heat. These adjustment fluxes are then applied in calculating a new estimate of the soil/ground temperature and soil moisture for each soil layer using a land surface model (Chen and Dudhia, 2001), thereby affecting the predicted surface fluxes in the subsequent time step. This indirect data assimilation is applied simultaneously with the direct assimilation of surface data in the model's lowest layer, thereby maintaining greater consistency between the ground temperature and the surface layer mass-field variables. Usage of this technique is critical for minimizing errors in the ground temperature and

temperature gradients across coastal regions for realistic simulation of land-sea breeze circulations.

1.2.3.2 Satellite-Based Observations

To successfully simulate land-sea breeze circulations, improved predictions of the ground/soil temperature alone are not sufficient. One also needs to improve the representation of temperature gradients across the water-land continuum, resulting in more accurate representation of sea surface temperatures (SSTs). For this purpose, we have acquired satellite measurements from NOAA at very high spatial (1 km) and temporal (1 h) resolutions (http://www.mslabs.noaa.gov/cwatch/) over the Gulf of Mexico region. These satellite observations are ingested into the MM5 inputs in place of analyzed SSTs obtained at 40-km resolution. Preliminary results obtained from the MM5 simulations using the 40-km resolution analyzed SSTs and the satellite-based SSTs are presented in the Section 2.

1.2.4 Task 4: Simulate Mesoscale Circulations Using the MM5

In the next six-month period, we will perform and analyze MM5 simulations at various grid resolutions (i.e., 36, 12, and 4 km) under Tasks 2 and 3. We will then perform rigorous evaluations of the MM5 simulations. Finally, we will reconfigure the MM5 using the combination of schemes/methods that produces the best representation of atmospheric circulations in various domains. At that point, we will be ready to perform the final MM5 simulations using grid resolutions of 36, 12, and 4 km, which will be used to drive the MAQSIP-VGR for the time periods selected in Task 1. Results obtained from this comprehensive evaluation of MM5 simulations will be documented in our first annual report.

1.2.5 Task 5: Develop Emission Estimates

A variety of recent emission inventories and activity data will be used to prepare updated emissions inputs that are compatible with the MAQSIP-VGR. Existing emissions estimates from offshore area sources, consisting of commercial marine vessels and helicopter flights throughout the Gulf of Mexico, will be included in runs performed with our emissions modeling system, the Sparse Matrix Operator Kernel Emssions (SMOKE) system. We will also include the newest yearly emissions inventory being prepared by the Minerals Management Service (MMS), data from the Gulf wide Offshore Activities Data System (GOADS), and data that were collected in the Breton Offshore Activities Data System (BOADS). Processed emissions will be quality assured for correctness and accuracy, using various tools we have developed for this process; for example, we will compare “before” and “after” emissions totals against inventory data, and will examine temporal profiles to check their correctness. In addition, we will adapt SMOKE to accommodate the varying horizontal resolution of the MAQSIP-VGR grids.

1.2.6 Task 6: Enhance Representation of Cloud Processes in the MAQSIP-VGR

There are four primary processes by which clouds modify atmospheric chemical composition and distribution: (1) subgrid-scale vertical turbulent redistribution of mass; (2) aqueous chemical effects, including dissolution, dissociation, and kinetic reactions; (3) rainout and wet removal due to precipitation; and (4) modification of solar actinic flux and hence the rate of photolytic

reactions. The current representation of cloud effects in the MAQSIP-VGR accounts only for attenuation of photolysis rates due to the presence of clouds and is based on the cloud fields specified by the driving meteorological fields. In Task 6 we will extend the model representation of cloud processes to include the other affects discussed above by adapting the mesoscale and urban-scale cloud modules available in the regular grid version of the MAQSIP model. This includes representation of shallow convection, deep convection, resolved-scale clouds, and subgrid-scale layer clouds (McHenry and Binkowski, 1996; McHenry et al., 1996).

1.2.7 Task 7: Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain

During the project year 2, we will use the MAQSIP-VGR to simulate the two 5-day periods chosen in Task 1 (during August-September 2000) over the Houston-Galveston domain. The availability of specialized measurements from the Texas 2000 air quality study provides a unique opportunity not only to conduct a detailed evaluation of the model but also to use both the model and the measurements in a complementary manner to improve our understanding of the complex coupling between dynamical and chemical processes that lead to rapid O_3 formation in the region. In the upcoming months we will also study how land-sea breeze circulations shape the distributions of primary and secondary species. Model simulations will focus on assessing the impact of onshore emissions from petrochemical industries on air quality in the region. Of particular interest is investigating the suitability of current emission inventories for representing emissions variability from these onshore facilities and consequently their potential impact on O_3 distributions.

1.2.8 Task 8: Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain

During the second year of the project, we will perform MAQSIP-VGR simulations for selected periods during 1998 and/or 2000 over the northeast Gulf domain (the D04 southern Louisiana region in Figure 1). Model simulations will focus on assessing the impact of offshore emissions from oil and gas E&P facilities on local and regional air quality in the southern states. Model simulations of ozone will be compared to available measurements from the Aerometric Information Retrieval System (AIRS) (US EPA;http://www.epa.gov/air/data/index.html) database.

Section 2: Results and Discussion

During second year of our project, we completed portions of the research outlined in Section 1. The results obtained are presented below.

2.1 Develop Modeling Domains and Case Studies (Task 1)

As a starting point for our research, we developed four domains for use in performing numerical simulations with a meteorological model, the Mesoscale Model Version 5 (MM5) (Grell et al.,

1994), to generate meteorological inputs to the MAQSIP-VGR. These meteorological modeling domains (Figure 1) are configured with different horizontal grid resolutions: 36, 12, and 4 km. In order to specifically study the effects of onshore and offshore emissions on the coastal environments, we developed two different 4-km grid resolution domains for performing air quality modeling studies: one over the Houston-Galveston region and the other over southern Louisiana.

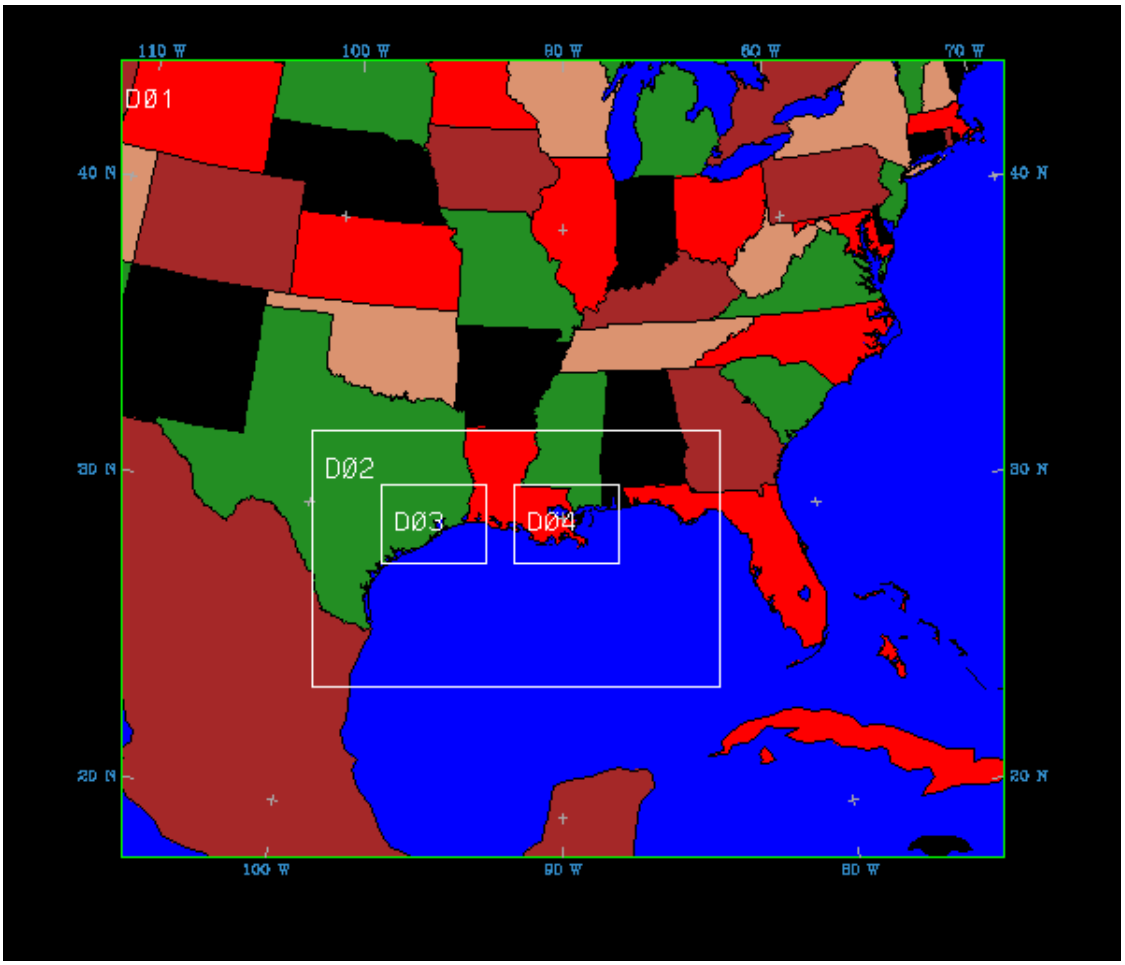

Figure 1. Simulation domains for the MM5 simulations. Domains D01 and D02 use 36- and 12-km grids, respectively, while domains D03 and D04 use 4-km grids located over the Houston-Galveston region and southern Louisiana.

We selected an initial time period of 23 August to 2 September 2000 for our numerical simulation case study over the Houston-Galveston region. These dates were chosen because a severe air pollution episode occurred over the region at that time. In Task 7, MAQSIP-VGR simulations will be performed to study the effects of various onshore and offshore emissions on the air quality of the coastal environment. To provide meteorological inputs to the MAQSIP-VGR for this purpose, we performed MM5 simulations for 11 days starting from August 23 using the 36-km, 12-km, and 4-km grids (domains D01, D02, and D03). We used 28 vertical

layers to represent atmospheric processes in the vertical, consistent with the literature (e.g., Neilson-Gammon, 2002).

For the southern Louisiana region, we will select a time period pertinent for simulating ozone and aerosol concentrations during the third year of the project.

2.2 Improve the Representation of Boundary Layer Processes (Task 2)

This task was completed during the last reporting period. Model simulations using a TKE scheme were referred to as “Eta” and those obtained using a K-profile approach as “Mrf”. It was found that, in general, the temperature and wind speed simulations in “Eta” compare slightly better with observations, while the mixing ratio and wind directions simulated by “Mrf” compare well with observations. However, precipitation was overestimated in “Eta” while slightly underestimated in “Mrf”. For these reasons, we strongly believe that the “Mrf” simulations, in general, are usable to drive the air quality model. We will therefore utilize the “Mrf” simulations as meteorological inputs to drive the MAQSIP-VGR.

2.3 Assimilation of Surface Observations to Improve MM5 Simulations (Task 3)

2.3.1 Assimilation of Land-based Surface Observations using the FASDAS

This subtask was completed during the last reporting period. Model simulations using the base configuration structure were referred to as “Base” and those obtained using the Flux-Adjusting Surface Data Assimilation System (FASDAS) as “Fasdas”. In general, there are several improvements derived from using “Fasdas” compared to using “Base” in the 36- and 12-km grids. Hence, the “Fasdas” results will be used in creating final meteorological fields in the final modeling configuration.

2.3.2 Ingestion of Satellite-Measured Sea Surface Temperatures into the MM5

This subtask was completed during the last reporting period. Model simulations using the base configuration structure were referred to as “Base” and those obtained using the satellite-derived SSTs as “Sat”. Considering all of the results, we found that, in general, the “Sat” case seems to perform better than the “Base” case, although we saw that the differences between the two types of simulations are very small for the parameters for which measurements are available. Note that the diagnostic analysis indicated the presence of larger differences between the “Base” and “Sat” cases. One of the main hindrances in analyzing 4-km grid simulations is the lack of statistically significant numbers of measurements that could allow a stronger conclusion showing the superiority of the “Sat” over the “Base”. To that end, we will acquire special measurements that were collected during the Texas 2000 Air Quality Study to further evaluate these two cases. These results will be reported in a journal article and in the next progress report.

2.4 Simulate Mesoscale Circulations Using the MM5 (Task 4)

We performed a comprehensive analysis and evaluation of the results obtained using the final modeling configuration in the MM5. In general, model simulations for the final modeling configuration case compare favorably with observations, indicating overall improvements compared with the "Base" simulations. Now, we are in the process of generating variable-grid-resolution meteorological fields for use in by SMOKE-VGR and the MAQSIP-VGR.

2.5 Develop Emission Estimates (Task 5)

There are two important issues to be addressed when developing emissions estimates for the MAQSIP-VGR: (1) enhancing the SMOKE configurations to handle the variable grids in the MAQSIP-VGR, and (2) acquiring offshore-point-sources data and using them to update our emission inventory for the proposed MAQSIP-VGR simulations. The status of these two subtasks is given below.

2.5.1 Enhancing the SMOKE Configuration

The development of the SMOKE-VGR is completed except testing and evaluation that is progressing during the final year of our project. We anticipate that the SMOKE-VGR will fully be developed and tested in the next couple of months.

2.5.2 Updating the Emissions Inventory

We have enhanced our emission database using the National Emissions Inventory (NEI) 1999 Version 3 becomes. This covers updates to area, non-road, and point sources. For updating mobile sources, we used MOBILE6 with updated vehicle miles traveled (VMT) data from the Texas Commission on Environmental Quality (TCEQ). Other databases available from the TCEQ are a 1999 area/non-road inventory and a 1997 Galveston Bay shipping inventory. Further, TCEQ has an offshore point- and area-source inventory that we have used in the past; we will contact TCEQ for any updates. We will also use BELD3 land use data to approximate the biogenic emissions (down to 1-km resolution). For the Mexican region, we will use the 1999 BRAVO Mexican inventory. Emissions data for the Outer Continental Shelf in the Gulf of Mexico available from the MMS will also be included in updating our emissions database. After completing this task, we will use SMOKE to prepare emissions estimates for use in the MAQSIP-VGR.

2.6 Enhance Representation of Cloud Processes in the MAQSIP-VGR (Task 6)

During the second year of our project we completed the testing (in a 1-D model) and implementation of the cloud processor for use in the MAQSIP-VGR. We plan to turn on the cloud processes when performing the MAQSIP-VGR simulations over the Houston-Galveston region.

2.7 Perform Simulations and Evaluation of the MAQSIP-VGR over the Houston-Galveston Domain (Task 7)

The meteorological inputs on the variable-grid format are being produced and will be completed in the next couple of months. At the same time, we expect that the SMOKE-VGR testing will be completed, enabling us to generate emissions inputs on the variable grid. After completing this step, we will use the MAQSIP-VGR to perform a few 10-day simulations (23 August through 2 September) that focus on the Houston-Galveston region. This will be done during the upcoming reporting period.

We will perform two simulations with two different model configurations. In the first configuration, a variable-grid domain over the Houston-Galveston region and offshore will have a high horizontal resolution (~1 km), gradually changing to a coarse resolution of about 12 km at the lateral boundaries of the domain. The second simulation will be for a similar but smaller domain but with a very high-resolution grid ranging from 400 m to 4 km. These simulations will also be completed during the upcoming reporting period.

2.8 Perform Simulations and Evaluation of the MAQSIP-VGR over the Northeast Gulf Domain (Task 8)

After successfully completing the MAQSIP-VGR simulations and evaluations over the Houston-Galveston region, we will perform similar simulations with a focus on the southern Louisiana region (i.e., Domain D04 in Figure 1) if the project resources allows for it. Details of this work will be presented in upcoming reports.

Section 3: Conclusion

Major portions of this project were completed successfully during the past two years. A comprehensive evaluation of various cases has been completed, and we have generated the meteorological inputs for 36-, 12-, and 4-km grids using a carefully selected final modeling configuration. The variable-grid-resolution meteorology is being generated to drive the MAQSIP-VGR. We have also completed the development of the emissions model, SMOKE-VGR. The development of the MAQSIP-VGR has also been completed. Thus, during the upcoming reporting period, we expect to rigorously test the new emission inventory that included new offshore emissions. We also expect to perform the MAQSIP-VGR simulations and complete evaluations of various scenarios to study the high ozone episodes over the Houston-Galveston region.

To perform quality control and analysis of our research results on the VGR domains, we have configured the National Center for Atmospheric Research visualization package, NCL. This task has been a bottle neck issue since the beginning of this project and we are glad that we now have the NCL meeting our needs for this project. One of the project scientist will attend a NCL training session during the upcoming report period to develop a tailored visualization package for our project.

Section 4: Publications

The following conference/workshop presentations will be made during the project's final year:

1. Preliminary Results on the Testing of a Variable-Grid-Resolution Air Quality Model. For Presentation at the *Models-3 Users' Workshop*, October 24-27, 2005, Chapel Hill, NC.
2. Simulation and Evaluation of the Year 2000 Ozone Episode over the Houston-Galveston Region using a Variable-Grid-Resolution Air Quality Model. Annual 2006 AMS meeting, Atlanta, GA.

The work we are completing on several of the project tasks may result in publication of the following journal articles during the first two years of this project (the titles shown are tentative).

1. Development of a Variable-Grid-Resolution Air Quality Model

2. Development of the Flux-Adjusting Surface Data Assimilation System (FASDAS) for Applications in Mesoscale Models (in preparation for submission to JGR)

3. The Effects of Using Satellite-derived Sea Surface Temperatures on Mesoscale Circulations over a Coastal Region and Their Impacts on Air Quality Simulations

We plan to submit these manuscripts for publication in reputable scientific journals.

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