Oil & Natural Gas Technology

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Progress Report
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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

By the end of this project reporting period, we had completed most of the tasks that were originally planned. We identified modeling domains and case studies to perform meteorological and air quality model simulations. We evaluated the performance of two different atmospheric boundary layer schemes, and identified the best-performing scheme for simulating mesoscale circulations for different grid resolutions. Use of a newly developed surface data assimilation scheme has resulted in improved meteorological model simulations. We have also successfully ingested satellite-derived sea surface temperatures into the meteorological model simulations, leading to further improvement of simulated wind, temperature, and moisture fields. We believe that these improved meteorological fields will lead to improved simulations from our variable-grid-resolution air quality model. Also, we have updated our emissions database to include the newly released off-shore and on-shore emission estimates over the Gulf of Mexico. We are working on an issue with the variable-grid version of SMOKE, our emissions processing model; we are currently performing further testing and evaluation of this new emissions modeling tool. We have completed the development of our variable-grid-resolution air quality model (MAQSIP-VGR) and performed various diagnostic tests. We have started the test runs for MAQSIP-VGR for the Houston-Galveston domain. These runs will be finalized as soon as the SMOKE-VGR issue has been resolved. The results and analyses based on the Houston-Galveston case will be presented in the American Meteorological Society annual meeting (January 2008)

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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.

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

2. Task Descriptions and Progress

Out of the eight tasks proposed under this project at its inception, Tasks 5, 7, and 8 were to be completed in the final year of the original three-year project. We have requested and been granted an extension to October 2007. The eight subsections below summarize the status of each of the tasks and describe any planned work needed to finish up the project.

2.1 Task 1: Develop Modeling Domains and Case Studies

This task is complete (please refer to our revised annual progress report (4/17/06 to 4/16/07) submitted September 19, 2007).

2.2 Task 2: Improve the Representation of Boundary Layer Processes

This task is complete (please refer to our revised annual progress report (4/17/06 to 4/16/07) submitted September 19, 2007).

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

This task is complete (please refer to our revised annual progress report (4/17/06 to 4/16/07) submitted on September 19, 2007).

2.4 Task 4: Simulate Mesoscale Circulations Using the MM5

This task is complete (please refer to our revised annual progress report (4/17/06 to 4/16/07) submitted on September 19, 2007).

2.5 Task 5: Develop Emission Estimates

We are using the National Emissions Inventory (NEI) 1999 Version 3. Updates in this NEI version include revisions to area, nonroad, and point sources. For updating mobile sources, we will use 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/nonroad inventory and a 1997 Galveston Bay shipping inventory. Further, TCEQ has an off-shore 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 cover data (available at 1-km resolution) to estimate biogenic emissions. For the Mexico region, we will use the 1999 BRAVO Mexican inventory. Emissions data for the Outer Continental Shelf in the Gulf of Mexico that are available from MM5 will also be included in updating our emissions database.

As we mentioned in the revised annual progress report (4/17/06 to 4/16/07) submitted on September 19, 2007, we are working on an issue in the variable-grid SMOKE code and expect it to be resolved shortly. We are meeting with some of the SMOKE developers this week to investigate the possible causes.

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

We analyzed the results of a 1-D cloud model to examine the effect of the fine-resolution configuration of the variable-grid model on the cloud processes, which in turn affect the pollutant formation and deposition.

There are four primary processes by which clouds modify atmospheric chemical composition and distribution: (1) sub-grid-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. We will perform some sensitivity modeling analysis to examine the effect of extending the model representation of cloud processes to include the other effects discussed above by adapting the mesoscale and urban-scale cloud modules available in the uniform grid version of the MAQSIP model. This includes representation of shallow convection, deep convection, resolved-scale clouds, and sub-grid-scale layer clouds**.**

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

Figure 1 shows a flow diagram of the variable-grid modeling components. MM5 simulations using a uniform grid provide the file MMOUT, which includes the meteorological simulations for specific episodes. The meteorological outputs are processed through the Meteorology-Chemistry Interface Processor (MCIP) for the same uniform grids. The variable-grid horizontal grid structure is introduced through the grid definition file ("S-Grid" in Figure 1), which

provides grid information to allocate all data onto the variable grid, to process emissions through the SMOKE-VGR and to process chemistry through the MAQSIP-VGR.

Meteorological data as an output from MM5 are available from previous runs of the model on a uniform grid at horizontal resolutions of 36 km, 12 km, and 4 km (domains D01, D02 and D03, shown in Figure 2).

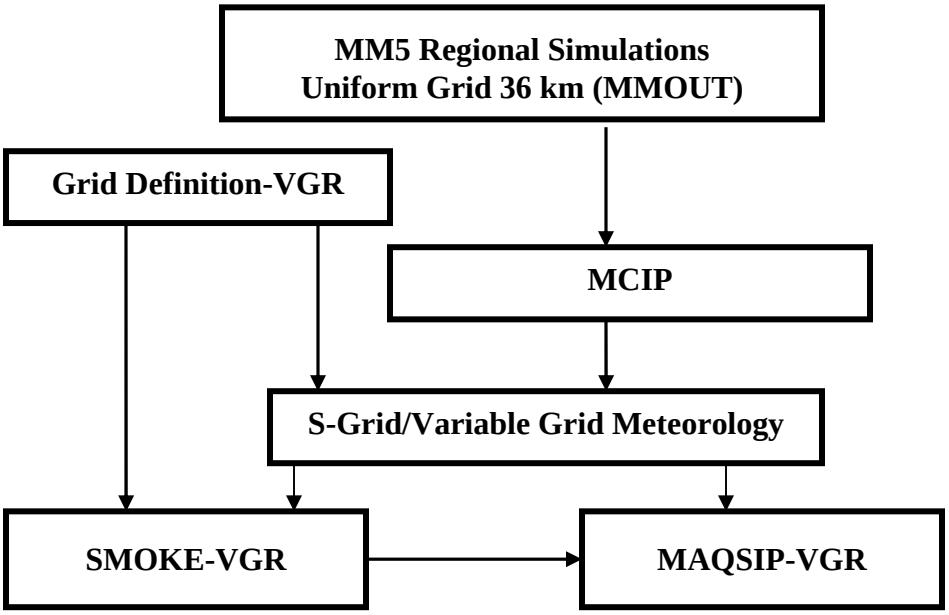

Figure 1: Flow diagram of the variable-grid modeling components.

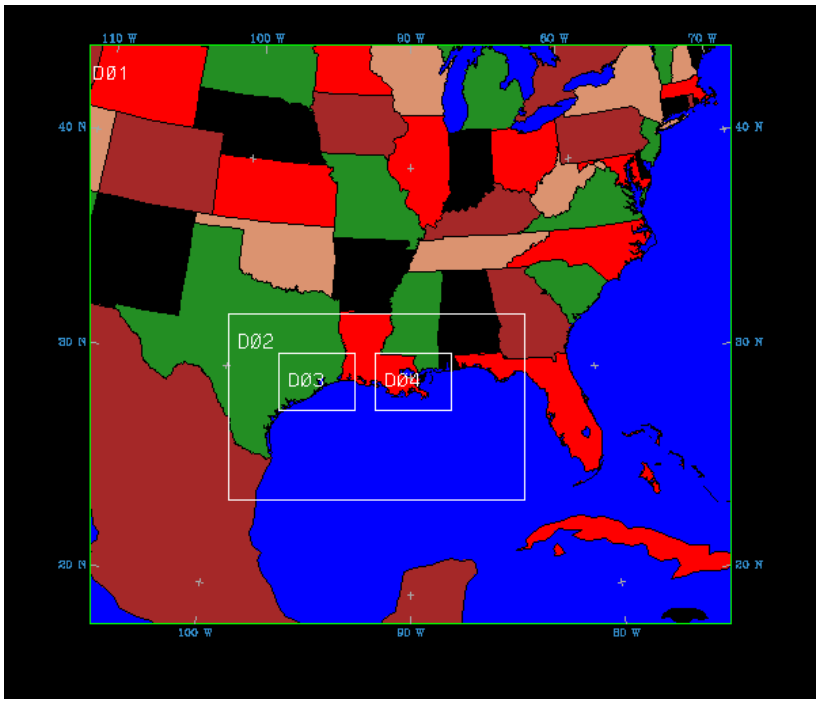

Figure 2. Simulation domains for the MM5 simulations. Domains D01 and D02 use 36- and 12-km grids, respectively, while domains D03 and D04 use 4-km grids located over the Houston-Galveston region and southern Louisiana.

We are currently processing the data needed to generate the meteorological variable-grid inputs for the Houston-Galveston domain. The Houston case will use the meteorological inputs of the 10-day summer episode noted earlier (August 23 through September 2, 2000) to demonstrate the variable-grid modeling concept. As described above and shown in Figure 1, the meteorological output data from MM5 and MCIP will be processed to prepare variable-grid meteorology data that feed into the SMOKE-VGR to prepare variable-grid emissions. The meteorological and emissions data on the variable grid are the two main inputs to MAQSIP-VGR.

The results and analyses of the MAQSIP-VGR simulations, for the Houston-Galveston area, will be presented in the upcoming American Meteorological Society annual meeting (January 2008). The results and analyses will also be posted on the project's web site.

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

Following the completion of MAQSIP-VGR simulations over the Houston-Galveston region, 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 2). Model simulations will focus on assessing the impact of off-shore 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 EPA Air Quality System (AQS) database (U.S. EPA; http://www.epa.gov/air/data/index.html).

3. Project Publications

1) A presentation and review of the project's tasks and results were presented during

DOE/PERF Air Program Review, August 22-23, 2007, Annapolis, MD. Hosted by Argonne National Laboratory. (Please see our revised annual progress report (4/17/06 to 4/16/07) submitted on September 19, 2007 for a copy of this presentation)

2) An abstract has been accepted for presentation at the American Meteorological Society annual meeting in January 2008:

"Application of a Variable-Grid Air Quality Model to Simulate On-shore/Off-shore Emissions near Coastal Areas" – Hanna, Alapaty, Mathur, Arunachalam, Xiu, and Shankar

3) Following the completion and analysis of all the variable-grid simulations, a journal article will be prepared (Dr. Alapaty will be the lead author) to document the methodology and results in a scientific journal.

4) A project web site has been prepared to display the results of the project (at this time it is password protected). Web site URL:

http://www.ie.unc.edu/cempd/projects/variable_grid/index.cfm

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