April-October 2006 Semiannual Report:

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

Prepared for the Department of Energy
National Energy and Technology Laboratory

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* DOE has approved Dr. Hanna to be the project's PI due to the departure of Dr. Alapaty to accept a position at DOE

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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.

Progress

At the end of this reporting period of the project, we have completed all of the tasks as 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 in 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. We are close to completing the development of a variable-grid version of SMOKE, our emissions processing model; we are currently performing further testing and evaluation of this new emissions modeling tool. Also, we have updated our emissions database to include the newly released offshore and onshore emission estimates over the Gulf of Mexico. Further, we have completed the development of our variable-grid-resolution air quality model (MAQSIP-VGR) and performed various diagnostic tests.

Plan

We are currently developing final inputs to the MAQSIP-VGR for the Houston case study. The next stage is to perform initial simulations of ozone and its precursors using the MAQSIP-VGR..

In addition we plan to transfer the variable grid resolution (VGR) schemes and approaches, some of them have been tested in MAQSIP, to the Community Multi-scale Air Quality Model (CMAQ) and to demonstrate the CMAQ-VGR application in the Houston area within a larger

The work is divided between three main components:

1) Preparation of the VGR meteorology for the Houston Case Study

Meteorological data as an output from the Mesoscale Meteorology Model (MM5) are available from previous runs of the model on a regular grid horizontal resolutions of 36km, 12km, and 4km. The data will be used to generate the meteorological variable grid inputs for the Houston case study.. Similar to the prototype modeling application using MAQSIP-VGR (the North Carolina case study), the Houston case will use the metrological inputs of a ten-day episode during the summer of 2000 to demonstrate the MAQSIP-VGR.

2) Prepare the emissions processor SMOKE for VGR applications:

The metrological processing described above generates a grid-2d file which provides meteorological parameters at the VGR locations. These data will be used by SMOKE to prepare the emissions for the modeling domain. This is the first time SMOKE will run on a variable grid.

3) Prepare a CMAQ-VGR

For the CMAQ application, we will develop a modified version of MCIP (this processor utilizes the MM5 outputs in the format and parameters needed as an input to CMAQ) that handles variable grid resolutions. A grid generation subroutine will be executed to initiate the variable grid coordinates needed for the MCIP-VGR.

Specific processors, in CMAQ, that are directly related to horizontal scales and gridding need to be modified. These are horizontal and vertical advection, horizontal diffusion, deposition, and cloud processes.

Publications

Following the completion and analyses 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

ARAROLINA ENVIRONMENTAL PROGRAM
ACCOUNT: 5-35995-0-110-3118
BUDGET PERIOD: 04/17/03-04/16/07

PI: ALAPATHY, K
TITLE: MODELING TRANSPORT & CHEMICAL EVOLUTION ONSHORE /OFFSHORE EMISSIONS & IMPACT
SPONSOR: DEPT OF ENERGY

Object		Original Budget	Revised Budget	Fiscal Year-To-Date Actual	Encumb.	Available as of 10/31/06
1001	PERSONNEL	$377,107.00	$136,327.51	$0.00		
1112	EPA NON TEACH		$240,779.49	$240,779.49		
1117	STU/OTHER		$0.00	$0.00		
1421			$0.00	$0.00		
TOTALS		$377,107.00	$377,107.00	$240,779.49		$136,327.51
1800	STAFF BENEFITS	$73,889.00	$40,427.33			
1812	SOCIAL SECURITY		$12,503.24	$12,503.24		
1813	SOC SECUR-HOSP		$2,968.75	$2,968.75		
1822	STATE RETIRE		$7,512.19	$7,512.19		
1832	MEDICAL INSUR		$5,111.95	$5,111.95		
1836	MEDICAL INS GRAD		$2,247.08	$2,247.08		
1872	TIAA RETIREMENT		$164.16	$164.16		
1873	TIAA HEALTH		$2,235.16	$2,235.16		
1892	COMPOSITE BENEFIT		$719.14	$719.14		
TOTAL		$73,889.00	$73,889.00	$33,461.67	$0.00	$40,427.33
1920	PROF CONSULT	$14,245.00	($180.00)	$0.00		
		$14,245.00	($180.00)	$0.00	$0.00	($180.00)
2000	SUPPLIES/MATER	$5,652.00	$5,107.77			
2311	EDUC SUPP		$544.23	$544.23		
2611				$2,178.98	$0.00	
		$5,652.00	$5,652.00	$2,723.21	$0.00	$2,928.79
3100	TRAVEL	$4,320.00	$18,745.00	$3,972.34	$0.00	
TOTAL		$4,320.00	$18,745.00	$3,972.34	$0.00	$14,772.66
3200	COMMUNICATION	$4,000.00	$3,934.85			
3211	POSTAGE		$65.15	$65.15	$0.00	
TOTAL		$4,000.00	$4,000.00	$65.15	$0.00	$3,934.85
3914	Transit Fee			$267.99		
TOTAL		$300.00	$300.00	$267.99		$32.01
6571	Trainee Stip	$12,129.00	$12,129.00			
6577	GRAD ASST TUITION			$8,629.00		
TOTAL		$12,129.00	$12,129.00	$8,629.00	$0.00	$3,500.00
8982	RESTRICT FUND	$0.00	$0.00		$0.00	
Direct Cost		$491,642.00	$491,642.00	$289,898.85	$0.00	$201,743.15
8983		$218,178.00	$90,200.20	$127,977.80	90,200.20	
			$127,977.80			
Indirect		$218,178.00	$218,178.00	$127,977.80	$90,200.20	$0.00
Total		$709,820.00	$709,820.00	$417,876.65	$90,200.20	$201,743.15