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MODELING SULFUR OXIDE CONCENTRATIONS IN THE EASTERN UNITED STATES: MODEL SENSITIVITY, VERIFICATION AND APPLICATIONS

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1. INTRODUCTION

This paper briefly reports on results from the BNL Long and Short Range Air Quality Model. The model calculates the transport, transformation and resulting pollutant concentrations for given SO_x emission inventories. Some details and results of the model in earlier stages are reported elsewhere (Meyers and Cederwall, 1975a; Meyers, et al., 1978a).

2. MODEL METHODOLOGY

Horizontal trajectories of pollution from each source are calculated using observed upper-air winds averaged in the vertical through the mixing layer. Horizontal diffusion along the trajectory is parameterized as Gaussian about the center of mass. Vertical diffusion is calculated using eddy diffusivity or "K" theory, and is solved semi-implicitly with a fast tri-diagonal sparse matrix method; the chemistry is solved explicitly. The derivative boundary condition at the surface allows for removal by dry deposition; removal by wet deposition is calculated at each level. Concentrations at variable levels in the vertical up to the mixing height are calculated using a variable grid, modified Crank-Nickelson finite-difference method. For this study, concentrations were calculated at twelve levels and values at the breathing level (2 meters) were projected onto a horizontal grid of approximately 32 kilometer resolution.

3. SENSITIVITY ANALYSES

Sensitivity analyses were performed on the model calculations. All critical parameters in the model were varied systematically; this included chemical conversion rates, deposition velocities, release heights, mixing heights and seasons of the year. A reference case was run for 284 large power plants in the East, representing 98% of the SO_2 emissions from eastern power plants. Reference case values for the critical parameters were selected based on the literature and current studies. These values included: 0.005 per hour conversion rate from SO_2 to $SO_4^=$, 0.02 in-stack conversion (by mole) of SO_2 to $SO_4^=$ (primary sulfate), 3.0 cm/sec deposition velocity for SO_2, 0.3 cm/sec deposition velocity for $SO_4^=$, a release height (stack height plus plume rise) of 200 meters, a mixing height of 1000 meters and wind data in the mixed layer for the month of July 1974. The reference case gave population-weighted concentrations of 7.40 $\mu g/m^3$ for SO_2 and 5.47 $\mu g/m^3$ for $SO_4^=$ for the East. For each critical parameter, runs were made with values varying about the reference value while other critical parameters remained at their reference values. The change in population-weighted concentrations of SO_2 and $SO_4^=$ are given in Table 1.

TABLE 1.
Sensitivity Analyses for Model Parameters

Parameter	Reference Value[1]	Value in this run	Change* in SO_2	Change* in $SO_4^=$
1. SO_2 to $SO_4^=$ conversion rate	0.005/hr	0.001/hr	+5%	-59%
	0.005/hr	0.01/hr	-6%	+65%
2. SO_2 to $SO_4^=$ in-stack conversion	0.02[2]	0.06	-4%	+25%
3. SO_2 deposition velocity	3.0 cm/sec	1.0 cm/sec	+132%	+41%
	3.0 cm/sec	10.0 cm/sec	-66%	-21%
4. $SO_4^=$ deposition velocity	0.3 cm/sec	1.0 cm/sec	0%	-48%
5. Release Height	200 meters	400 meters	-9%	+9%
6. Mixing Height	1000[3] meters	500 meters	-5%	+6%
7. Wind Data (season)	July 74	Jan. 74	+36%	+24%
	July 74	Apr. 73	-15%	-31%
	July 74	Oct. 74	-10%	-10%

Notes:
[1] Sensitivity analyses for parameters 1,3,4 & 5 used July 1975 winds and 255 power plant locations.
[2] Sensitivity analysis used 0.01/hr for parameter 1.
[3] Sensitivity analysis used January 1974 winds.
* Per cent change of population-weighted concentrations from reference case.

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DISCLAIMER

4. MODEL VERIFICATION

The most complete SO_2 emission inventory available for the United States sources east of the Mississippi River was used in a verification study. This amounted to 89% of the total SO_2 emissions in the East and included 98% of the power plant emissions, 73% of the industrial plant emissions and 67% of the area source emissions. Reference case values for the critical parameters were used. The months of January, April, July and October were run and the results compared with NASN and EPRI SO_2 and $SO_4^=$ data for the same periods. Using time averaged spatial values for the four months, the calculated SO_2 concentrations had greater than 0.7 correlation with observed SO_2, and calculated $SO_4^=$ had greater than 0.6 correlation with observed $SO_4^=$. Improvements in the model have resulted in correlations greater than 0.8 for $SO_4^=$ for single months.

"Priori" and "posterior" analyses were performed on the uncertainty of the calculation. That is, reference cases were calculated and the uncertainty in the calculations was documented based on the uncertainty of critical parameter values (prior analysis). The reference cases were compared with data and conditioned (posterior analysis) values of the critical parameters were formed to minimize the error between calculated and observed population-weighted concentrations. It was found that comparison of model results with data in this manner reduces the uncertainty in the relative values of the critical model parameters.

5. MODEL APPLICATION

The model has recently been applied to assessing environmental impacts to air pollution from fossil fuel (coal) energy generation in the United States for future years (Meyers, et al., 1978b). As an example, continental concentration patterns for SO_2 and $SO_4^=$ are shown in Figures 1 and 2, respectively. Projected 1985 SO_2 emissions for 1088 coal-burning utility and industrial sources were used in the simulation (see Fig. 3). The projected emissions totaled 21.855×10^6 tons SO_2/year for the contiguous United States; the 1973 SO_2 emissions total for all fossil-fuel burning utility and industrial sources was 22.875×10^6 tons/year. The concentration patterns highlight the predominance of high SO_x levels in the East. The heterogeneous or spiked nature of the SO_2 pattern is indicative of the "local" character of the SO_2 concentrations, while the more homogeneous or smoothed nature of the $SO_4^=$ pattern reflects the "regional" character of the $SO_4^=$ concentrations due to long-range transport and diffusion. Considering the high population in the East, Figure 4, this leads to predominately higher population-weighted concentrations and population exposure. Comparing these concentration patterns with current air quality observations (NASN and EPRI) gave correlations of approximately 0.6 for SO_2 and 0.8 for $SO_4^=$. The high $SO_4^=$ correlation is due in part to the noticeable trend in concentrations from west to east which is reflected in both the calculated and observed patterns.

The model is particularly useful in supplying air quality input to assessments of health and environmental effects of various energy strategies. In addition to this input to energy planning activities, the model has provided insight into the scales of transport for SO_2 and $SO_4^=$ from large point sources; this is valuable input to planning regional pollution measurement programs. The model has also been used to address contribution of SO_x from energy generation to the acid rain problem in the East (Meyers and Cederwall, 1975b). Some initial work is in progress with the model to address transport and transformation of fine particulates and NO_x and to relate this, along with SO_x, to visibility reduction. Work is also progressing, under the DOE MAP3S program, in the development of a 3-D national scale model to address problems of nonlinear chemical transformations, advection and diffusion.

6. ACKNOWLEDGEMENTS

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CALCULATED SO 2

SCENARIO 1985 NCUA UTILITY (MIDDLE) AND INDUSTRIAL

(MEYERS, CEDERWALL, KLEINMAN. BROOKHAVEN NATIONAL LABORATORY. 9/78)

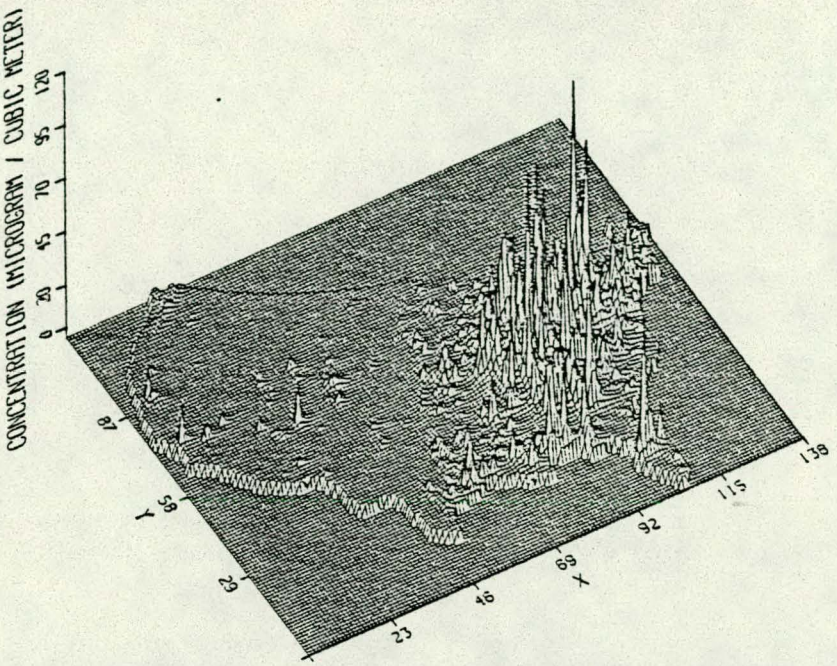

Figure 1. Calculated concentrations of SO_2 ($\mu g/m^3$) for the contiguous U.S.

CALCULATED SO 4

SCENARIO 1985 NCUA UTILITY (MIDDLE) AND INDUSTRIAL

(MEYERS, CEDERWALL, KLEINMAN. BROOKHAVEN NATIONAL LABORATORY. 9/78)

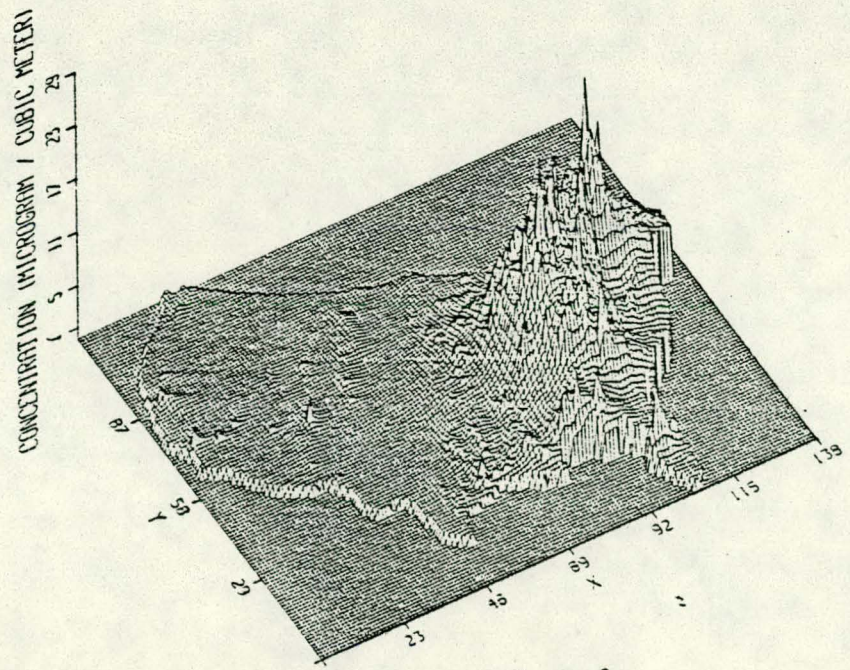

Figure 2. Calculated concentrations of $SO_4^=$ ($\mu g/m^3$) for the contiguous U.S.

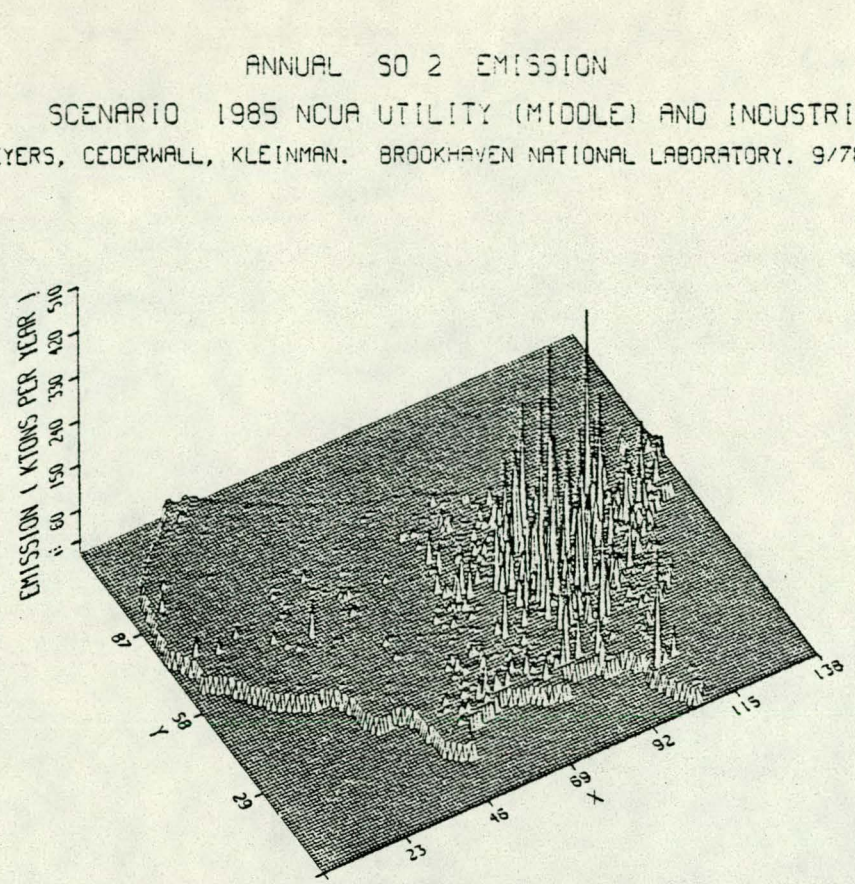

Figure 3. Projected 1985 SO_2 emissions (ktons/year) for 1088 coal-burning sources for the contiguous U.S.

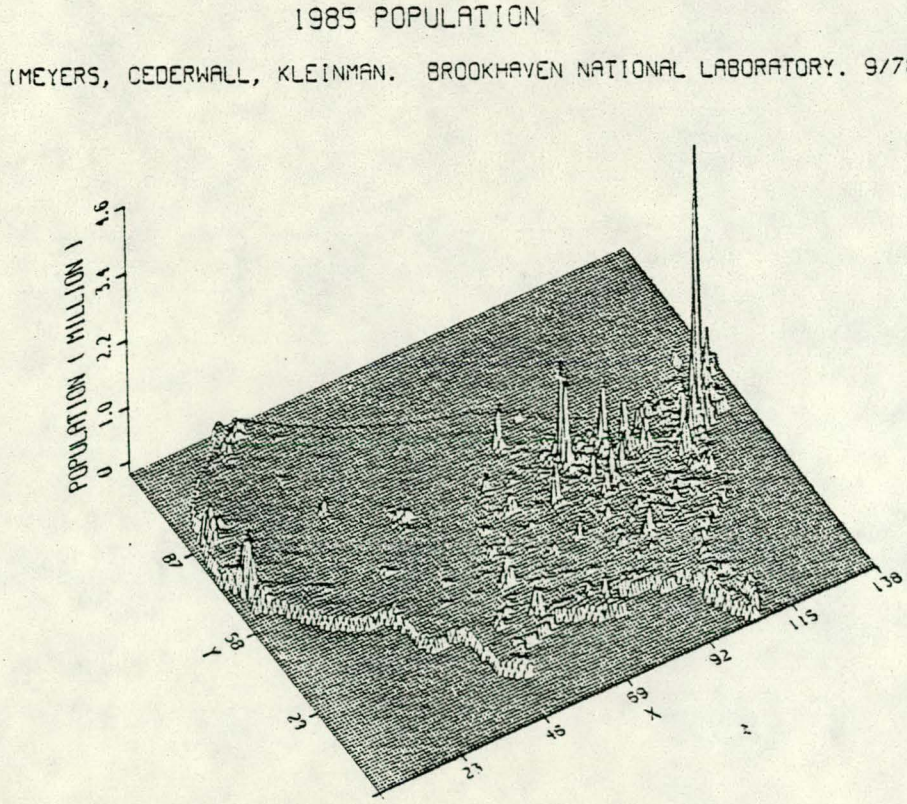

Figure 4. Projected 1985 population for the contiguous U.S.