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Project Summary

The ENAMAP-2 Air Pollution Model for Long-Range Transport of Sulfur and Nitrogen Compounds

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This report describes the Eastern North American Model for Air Pollution (ENAMAP-2), which simulates long-range air pollution transport over eastern North America. The ENAMAP-2S version of the model uses SOx emissions data inventories and standard daily weather reports to compute the airborne concentrations of SO_2 and sulfate and their deposition on the earth's surface. ENAMAP-2S operates in a Lagrangian manner by tracking pollution puffs emitted periodically over the grid domain. As each puff travels with the winds, chemical processes occur, and the puff loses pollutant mass through dry and wet deposition processes. For each grid cell, the deposition amounts and airborne pollution concentrations are summarized for periods generally taken as one month.

The newest form of the model includes the influences of smoothed terrain on the winds and divides the atmospheric boundary layer into three parts, allowing pollution emissions to be partitioned among the layers. Vertical mixing is controlled by diffusion coefficients computed from fields of wind shear, stability, and mixing depth. The transformation and wet and dry deposition rates are based on recent information. However, there are still substantial uncertainties about them.

This Project Summary was developed by EPA's Environmental Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

SRI International (SRI) has developed a numerical model for calculating the ambient concentrations and depositions of pollutants. This research was sponsored by Umweltbundesamt of the Federal Republic of Germany for application in Europe and by the U.S. Environmental Protection Agency for application in North America. During the two phases of model development, SRI has replaced the simplistic parameterizations in the North American version (ENAMAP-1) with more complex parameterizations expressed in terms of known or theoretical physical relationships.

The final version of the North American model (ENAMAP-2) includes transformation rates dependent on solar insolation, dry deposition rates dependent on surface characteristics, stability, and time of day, and wet deposition rates dependent on rain type. In addition, ENAMAP-2 divides the planetary boundary layer into three layers. This version of the model accounts for diurnally changing mixing depths and the vertical mixing of pollutants based on vertical mixing coefficients expressed in terms of atmospheric stability.

The ENAMAP-2S model, which pertains to sulfur compounds, was applied to simulate wet and dry depositions and monthly average ambient concentrations of SO_2 and sulfate for January and August 1977. These model results were compared to those generated earlier by the more simplistic one-layer version. In addition, a model sensitivity study was conducted. The ENAMAP-2N version was applied to simulate wet and dry depositions and average ambient concentrations of NO, NO_2, NO_3^-, HNO_3, and PAN.

ENAMAP-2S Applications

The sulfur budgets of the emissions from Ohio, Indiana, and Illinois were computed from the January and August 1977 ENAMAP-2S and ENAMAP-1 applications to assess the resultant effects of the model modifications. The January and August sulfur budgets are presented in Tables 1 and 2, respectively. The two models did not differ significantly for the ambient SO_2 or sulfate concentrations. However, the budget comparisons showed a significant increase of dry sulfate deposition for ENAMAP-2S. This was due to the replacement of the low nocturnal dry deposition rates with the higher rates used for the daytime. On the other hand, the sulfate wet deposition showed a decrease for ENAMAP-2S. Total deposition of sulfate computed by ENAMAP-2S was approximately 90% greater than that calculated by its predecessor for January and only 8% greater for August.

After ENAMAP-2S was applied for the entire model domain using emissions from all states and provinces within the domain for January and August 1977, the monthly average SO_2 and sulfate concentrations and SO_2 wet and dry depositions did not differ significantly from those computed from ENAMAP-1. The significant differences in the sulfate wet and dry depositions resulted from the higher nocturnal sulfate dry deposition rates used in ENAMAP-2S.

The effects of the greater complexities in ENAMAP-2S seemed to have been smoothed over the month simulation period. One could have expected the three-layer model to compute lower ambient concentrations in Layer 1, close to the surface, since this version of the model considers nocturnal mixing heights. However, due to the exaggerated nocturnal mixing heights used in these applications, pollutants from Layer 2 were mixed to the surface throughout the night.

ENAMAP-2S Sensitivity Tests

In order to minimize the costs of sensitivity testing, ambient concentrations and depositions were calculated across the entire model grid using only the emissions from Ohio (which was near the center of the grid) for August 1977. The baseline or nominal case used the model input parameter values applied in previous model runs. The parameters that were adjusted during this sensitivity analysis included:

1) transformation rate

2) SO_2 and sulfate wet and dry deposition rates

3) proportion of nocturnal emissions injected into Layer 1, and

4) vertical diffusion coefficients.

When compared to air quality measurements, the ENAMAP-2S ambient sulfate concentrations appeared to be significantly higher. On the other hand, the SO_2 concentrations showed no consistent bias. The results of the sensitivity analysis indicated that a combination of 1) reducing the homogeneous transformation rate by 25%, 2) increasing the wet and dry depositions by 25%, and 3) partitioning the nocturnal pollution injections 25% in Layer 1 and 75% in Layer 2 yielded results which compared well with measurements.

ENAMAP-2N Description and Applications

A major portion of this phase of the project was devoted to the adaptation of the sulfur version of ENAMAP-2 to a version designed to simulate, in a linear fashion, the depositions and complex non-linear chemical transformations of nitrogen compounds. In ENAMAP-2N, the primary gaseous pollutants, NO and NO_2, form an initial puff over each emitter cell. The concentrations of the two are calculated and equilibrated with a diurnally varying equilibrium constant. The

Table 1. *Comparison of ENAMAP-1 and ENAMAP-2S Budgets for Illinois, Indiana, and Ohio Emissions (kton) for January 1977*

Process	*ENAMAP-1*	*ENAMAP-2S*
SO_2		
Total emitted	*645.1*	*645.1*
Wet deposition	*-7.2*	*-7.5*
Dry deposition	*-213.5*	*-242.6*
*Flux**	*-165.4*	*-126.7*
Transformation ($SO_2 \rightarrow SO_4^=$)	*-259.0*	*-268.4*
$SO_4^=$		
Emitted	*15.3*	*15.3*
Total emitted and transformed	*403.8*	*417.9*
Wet deposition	*-11.7*	*-8.6*
Dry deposition	*-131.7*	*-262.6*
*Flux**	*-260.4*	*-146.7*

**Flux is the amount of SO_2 or $SO_4^=$ that was transported out of the model domain by the wind.*

Table 2. *Comparison of ENAMAP-1 and ENAMAP-2S Budgets for Illinois, Indiana, and Ohio Emissions (kton) for August 1977*

Process	*ENAMAP-1*	*ENAMAP-2S*
SO_2		
Total emitted	*582.9*	*582.9*
Wet deposition	*-164.7*	*-153.9*
Dry deposition	*-68.1*	*-88.7*
*Flux**	*-7.5*	*-1.7*
Transformation ($SO_2 \rightarrow SO_4^=$)	*-342.3*	*-338.5*
$SO_4^=$		
Emitted	*12.4*	*12.4*
Total emitted and transformed	*525.9*	*520.3*
Wet deposition	*-305.7*	*-238.4*
Dry deposition	*-170.7*	*-273.4*
*Flux**	*-49.5*	*-8.5*

**Flux is the amount of SO_2 or $SO_4^=$ that was transported out of the model domain by the wind.*

NO_2 can react to form PAN, HNO_3, and NO_3^-, with the products formed in a 5:4:1 molar ratio. The reaction rate of NO_2 varies dirunally.

The dry and wet deposition rates of the nitrogen compounds are defined according to Tables 3 and 4, respectively. Wet deposition rates for the nitrogen compounds are expressed as fractions of those for the sulfur compounds used in ENAMAP-2S.

Concentration and wet and dry deposition patterns and source/receptor relationships for the months of January and August 1977 for all five nitrogen compounds were determined during this project. In general, these simulated patterns seem quite reasonable in terms of what one would expect for regionally averaged concentrations. Unfortunately, no air quality measurements existed for 1977 to evaluate the model.

Table 3. *Dry Deposition Velocities for Atmospheric Nitrogen Compounds*

Compound	*V_d (cm s^{-1})* Day	Night
NO_2, NO	0.2	0.07
HNO_3	1 0	0 07
PAN	0.25	0.07
NO_3^- (aerosol)	0.6	0.6

Table 4. *Wet Deposition Rates for Atmospheric Nitrogen Compounds Expressed as Fraction of Rates (α) for SO_x*

Compound	*Relative Rate*
NO_2, NO	$0.25 \times \alpha SO_2$
HNO_3	$0.50 \times \alpha H_2SO_4$
PAN	$0.50 \times \alpha SO_2$
NO_3^- (aerosol)	αH_2SO_2

Conclusions

The ENAMAP-2S ambient SO_2 concentrations compared favorably with measurements, but the calculated ambient sulfate concentrations were significantly greater. The ENAMAP-2S/ENAMAP-1 comparisons showed that the concentration fields differed insignificantly, thus the testing of ENAMAP-2 indicated that the resultant effects of the more complicated parameterizations of ENAMAP-2S were smoothed over the month simulation periods. However, the exaggerated nocturnal mixing heights used in the ENAMAP-2S applications could have been responsible for the fact that these differences were insignificant. The dry deposition of sulfate did vary significantly, because the nocturnal dry deposition rates were significantly increased in ENAMAP-2S applications.

The sensitivity testing of ENAMAP-2 indicated that the resultant effect of reducing the transformation rate, increasing the wet and dry deposition rates, and apportioning some of the nocturnal emissions into Layer 1 yielded results that compared well with measurements. Further model evaluations using these new values and several months of meteorological data are required before solid conclusions can be drawn.

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The complete report, entitled "The ENAMAP-2 Air Pollution Model for Long-Range Transport of Sulfur and Nitrogen Compounds," (Order No. PB 84-120 930; Cost: $22.50, subject to change) will be available only from:
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