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Project Summary

Intermediate-Range Grid Model and User's Guide for Atmospheric Sulfur Dioxide and Sulfate Concentrations and Depositions: Wisconsin Power Plant Impact Study

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A three-dimensional time-dependent grid type model for two chemically reacting species that undergo atmospheric transport, diffusion, and wet and dry deposition in the atmosphere boundary layer is described. The model is useful for assessing a single source or a group of sources on a scale of 10s to 100s of kilometers. The equations are solved by an implicit finite-difference scheme. The model is shown to accurately treat advection, diffusion, time step, and grid size. The sensitivity of the model to chemical reaction rate, surface dry deposition rate, surface roughness, horizontal diffusivity, pH of the rain and emissions rate is demonstrated. The model is applied to sulfur dioxide and sulfate deposition in the Rainy Lake Watershed using the available emissions and meteorological data. Model calculations are compared to NADP wet deposition data and snow core data. Model calculations for the Atikokan, Ontario power plant are also presented.

This Project Summary was developed by EPA's Environmental Research Laboratory, Duluth, MN, 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

Much attention is currently being given to acid impacts of substances carried by and transformed in the atmosphere. Many models and methods have been proposed and tested. The computer model herein described addresses sulfur dioxide and sulfate deposition (wet and dry) and the chemical transformation of sulfur dioxide to sulfate. The sulfur depositions as they alter the pH of the soil and water are not a part of the model. Nitrogen compounds also produce acidification, but these are not yet incorporated into the model. Hence, the sulfur loadings simulated by the model can only be taken as indicators of potential acidification.

Atmospheric deposition models may be divided into two major classes: (1) long-range transport models, where the region of interest extends over thousands of kilometers (i.e., the eastern half of the U.S.); and (2) mesoscale models in which analysis extends over hundreds of kilometers (i.e., the state of Wisconsin). Some advantages of mesoscale over macroscale models are: providing higher resolution and more detailed simulation of meteorological conditions; focusing on smaller geographical entities (watersheds, lakes, sensitive biological regions, etc.); and predicting the relative influence specific emission sources on nearby receptors. The main disadvantage of a mesoscale model is that it is not possible to predict absolute depositions within the region due to omission of extra-regional emission sources and transport.

This report describes a mesoscale (10s-100s kilometer scale) computer model for two chemically reacting species which

undergo atmospheric transport, diffusion, and dry and wet deposition. Application of the model to sulfur dioxide and sulfate deposition in the Rainy Lake Watershed in northern Minnesota and western Ontario is presented. The model is a three-dimensional, time-dependent grid which uses an implicit finite-difference numerical scheme to solve two coupled species conservation of mass equations in the atmospheric boundary layer.

The primary purpose for developing the model was to be able to estimate sulfur dioxide and sulfate deposition from the atmosphere to the ground over a medium size (10^3 to 10^5 km^2) geographical region. One of the central questions which such a model can answer is how much in-region sulfur emissions are deposited locally and how much leave region boundaries. Other questions which such a model can answer are: What is the relative deposition contribution of single sources to a particular receptor location? How might one best locate monitoring stations given the deposition distribution pattern predicted by the model? What is the deposition impact on any given subregion (i.e., a watershed) within the larger region?

Description of UWATM-SOX Model

In this section the salient features and operational aspects of the model are described.

Summary of Model Features

The UWATM-SOX model is a time-dependent, cell-type model. At its heart is the numerical solution of coupled SO_2 and SO_4 conservation of mass equations described in an Eulerian (fixed) frame of reference for a dilute species in the atmospheric boundary layer. Included are the processes of wind transport, turbulent diffusion, chemical reactions, source input and dry and wet deposition. The numerical solution is a first-order, fully implicit scheme.

The model inputs emissions once at the beginning of the simulation and new meteorological data every hour. It performs calculations every 20 minutes within 1 h. (The time-step is variable and can be altered if necessary.) As long as data are available, any time period for simulation can be chosen. The model has been run for time periods up to 1 yr.

The model region is divided into a uniform, horizontal, two-dimensional grid network. The rectangular grid size depends on the extent of the region, the desired cost/efficiency of the computer runs and the desired accuracy of analysis. Above the grids are stacked a specified number of vertical cells from the ground level to an upper limit called the mixing height. At present the model uses six vertical cells — three lower fixed-height (50 m) and three upper variable-height cells. (This arrangement can be altered.) Therefore, the space enclosing the region of study is partitioned completely by a three-dimensional cell structure. The single 3D cell is the basic unit within which the model calculations are performed.

The model can handle point, line and area emission sources. The sources are assigned within one of the grids. All sources are treated simultaneously, therefore, a specific source-to-concentration/deposition value cannot be determined unless the single source is run separately. The emissions data are obtained from outside organizations (usually government control agencies). For point sources a plume rise is calculated using one of a set of five equations. The resulting "effective stack height" is placed within the appropriate vertical cell. The meteorological condition known as lofting (effective stack height above mixing height) is accounted for. This is an important condition affecting long-range pollutant transport.

The meteorological data are obtained on tapes from the National Climatic Center (NCC) in Asheville, NC. The tapes required are: hourly surface observations, twice daily mixing heights and hourly precipitation. An integrating program (METDATA) converts the data to the hourly format required by the model.

The atmospheric boundary layer is characterized by a set of wind speed and eddy diffusivity profile equations which are calculated from ground level to the top of the mixing layer. The profiles describe the transport and diffusion behavior of the pollutants. They are vertically variable but horizontally uniform and constant across the region of study over a 1 h period. The profiles are dependent on the stability of the atmosphere.

The boundary layer has been subdivided into a surface layer and a second layer up to the mixing height. Therefore, each profile has two forms, one above and one below the surface layer. The surface layer equations are based on the Monin-Obukov similarity theory. In the upper layer the wind profile is a form of the power-law and the diffusivity is assumed constant. The profiles are calculated from a knowledge of the geostrophic wind speed, net heat flux to the ground and surface roughness. The geostrophic wind is calculated from a knowledge of the surface wind speed and height at which it is measured using a modified Regula Falsi iteration scheme. The net heat flux is calculated by first using the NCC surface observations data and the Pasquill-Turner method of stability classification to determine the stability class. Then a heat flux value is assigned to each class. A single surface roughness value is chosen to characterize the entire region.

The chemical conversion from SO_2 to SO_4 is assumed to be first order. At present two reaction rates are used — a day value and a night value — although hourly changes are possible if the data is available.

The dry deposition is handled by means of a deposition velocity which is calculated as a function of terrain and meteorological conditions. The deposition velocity changes hourly, but is uniform across the region. It is determined from an aerodynamic resistance which depends on the meteorological conditions close to the ground, and a surface resistance which depends on the pollutant species and nature of the surface (snow, water, vegetation, etc.). The surface resistances are input by the user and aerodynamic resistance is internally calculated from wind profile information.

The wet deposition scheme is based primarily on a model developed by Scott (1978). It assumes all precipitation forms according to the Bergeron or cold cloud process. Ice crystals form in the upper portion of the cloud and as they sweep downward through the cloud they capture cloud droplets containing SO_4 and dissolved SO_2. The S eventually incorporated into the precipitation is assumed to be drawn in through the cloud base. A set of three equations for the wet deposition removal rate are used; one for rain or snow removal of SO_4, and one each for rain and snow removal of SO_2.

Unlike dry deposition, the wet removal of SO_2 and SO_4 is calculated separately from the numerical solution of the atmospheric dispersion equation because it must consider an entire column of cells from ground level to mixing height, as opposed to single cells. Precipitation is assumed to occur uniformly across the region.

A significant feature of the model is a complete set of regional mass summations within the main program. Their purpose is to continually double-check to ensure mass is conserved at all stages during the internal calculations and to provide the basis for deriving a regional atmospheric S budget for the modeled emissions sources within the region.

There are several computer techniques worth noting. First, to handle the numerical calculations for arbitrary wind directions a dual grid system is used, one fixed in position and one which overlaps the fixed system and rotates with the wind angle. Transfers of concentrations are performed back and forth between the two systems as the wind direction shifts. Second, the main program has a "stop-start" capability so that progress can be stopped anywhere in the stream of

calculation and started exactly where it left off with no outside intervention other than re-starting the run. Third, extensive use has been made of common blocks and the "FORTRAN Procedure (PROC)" statement to eliminate unnecessary interprogram storage locating calls and to make it easier to make internal changes which affect many programs at once. Fourth, a very complete record of the values of all significant variables is stored on tape hourly for future analysis. The saved information includes the date, ground level concentration and deposition arrays, and certain meteorological, emissions and regional mass balance data. All this is compactly stored for each hour as a record of a tape file. The file covers the entire time period of simulation.

The model results include 3-h, 24-h, seasonal and annual average ground level concentrations, and dry, wet and total depositions of SO_2 and SO_4. (These are the standard averaging periods but the model is capable of averaging upper level concentrations or using other time periods.) The results also include pH of the precipitation during a storm event, and the values and dates of the 3-h and 24-h maximum concentrations. All of the above results are printed grid by grid in an array format and can be isopleth computer plotted. The results include — a frequency distribution of concentrations/deposition values for any selected grid, and a regional atmospheric S budget which analyzes, by total mass and percentage of S input, the flow of S (SO_2 and SO_4) through the various physical and chemical processes into, out of or within the region.

The model is written in ASCII Fortran and has been run on the Madison Academic Computing Center's SPERRY UNIVAC 1100/82 series computer. In an application of the model to the BWCA wilderness area in northern Minnesota in which a cell structure of 11 x 13 x 6 was used with hourly changes in meteorological data and calculations carried out every 20 min, the main program required 50K core space, and a 1 yr simulation cost $200 (at the cheapest computer rate) and took 6 hr of CPU time. A 1 day calculation at the "normal" rate (10 x the cheapest) can be done for $7 and takes 1 min CPU time.

A complete description of the model and how to use it is contained in Wilkening and Ragland (1982) and summarized in Ragland and Wilkening (1983).

Overview of Modeling Operation

This section is an examination of the total modeling operation: programs, subroutines, input data and output results, the sequence of program execution, and storage modes and formats. A flow chart of the modeling operation is shown in Figure 1 with the model features shown in Table 1.

There are five major components to the modeling effort:

1) Development of emissions inventory
2) Development of meteorological data-base
3) Simulation of atmospheric transport, diffusion, chemical reactions and deposition
4) Processing of hour-by-hour concentration and deposition output
5) Isopleth computer plotting

In all there is a collection of 11 programs, 11 subroutines, and one FORTRAN PROC used. They are stored in a program file called UWATM*ACIDRAIN. Each of the above tasks are briefly discussed to give the user an overview of the entire sequence of model operation.

Emissions Inventory

The model is capable of handling point, line, and area sources. A detailed methodology for converting agency inventories to a model form has been worked out for point sources. Line and area source emissions are grid apportioned. For each point source the model requires a set of six variables: location, stack height, stack diameter, gas temperature, gas flow rate and emission rate. Five steps involved in converting outside inventory data to usable form are:

1) Obtain complete inventories from outside organizations
2) Select largest sources
3) Combine sources
4) Locate sources within grid network
5) Convert data to model format

Carrying out these steps involves compiling four tables and executing two programs. The first two tables are a record of what data was selected for use from the original inventories and a record of all alterations (and reasons for) made in the process of selection. For each of the selected sources a "potential plume rise" is calculated (using a program called PLUMEPOT) and this value is used as the basis of combining sources to reduce the inventory to manageable size (if necessary). The second two tables are a record of the combined sources and a record of all alterations (and reasons for) made in the process of combining. After compiling these tables, the only remaining task is to grid locate the source. This is done by hand, using U.S. Geological Survey maps. The resulting grid ID numbers are recorded on the combined sources table. Finally, a program called MODEL-EMISS takes the combined sources data and changes units and places the final model emissions inventory on a mass storage file which is directly accessed by the model.

Meteorological Data-Base

The model requires a set of seven hourly meteorological variables: stability, heat flux, wind speed, wind direction, air temperature, mixing height, and precipitation. All are directly or indirectly obtained from a set of three NCC tapes. There are three steps involved in converting the original NCC tape data to the model usable form:

1) Purchase hourly surface observations, twice daily mixing height, and hourly precipitation tapes from NCC for a given meteorological station and given year.
2) Pre-process data with set of three UDH programs.
3) Execute METDATA program.

Each of the NCC tapes are run through a separate Unified Data Handler (UDH) program (called SFCOBSDATA, MIXINGHTDATA, PRECIPDATA), which together extract the hourly wind speed, wind direction, air temperature, cloud cover, ceiling height, precipitation, and afternoon mixing height data. The data is stored as three files on another user-supplied tape which is accessed by the METDATA program. This program performs several jobs: 1) uses the Pasquill-Turner stability class model to determine the hourly stability, 2) uses the basic earth-sun angular equations to calculate sunrise and sunset times and solar altitude (which are used both in the stability and mixing height determinations), 3) uses a linear interpolation scheme to estimate hourly mixing height values, 4) determines precipitation type (rain or snow), 5) assigns hourly heat flux values on the basis of wind speed and stability information, 6) converts the units of wind speed, direction and air temperature, and finally, 7) stores all the hourly values for an entire year on a mass storage file which is directly accessed by the model.

Atmospheric Transport, Diffusion, Chemical Reaction, and Deposition Simulation

This component is "the model." It consists of one main program and 10 subroutines. These contain the computer code equivalent of the mathematical equations expressing the wind transport, turbulent diffusion, chemical transformation and dry and wet deposition processes affecting SO_2 and SO_4. The central equation is a pair of coupled continuity equations for dilute pollutant species in the atmospheric boundary layer described in an Eulerian (or fixed) reference system. The simulation technique is a first-order, fully implicit solution of the finite difference form of the coupled equations and are described completely in Ragland and Wilkening (1983).

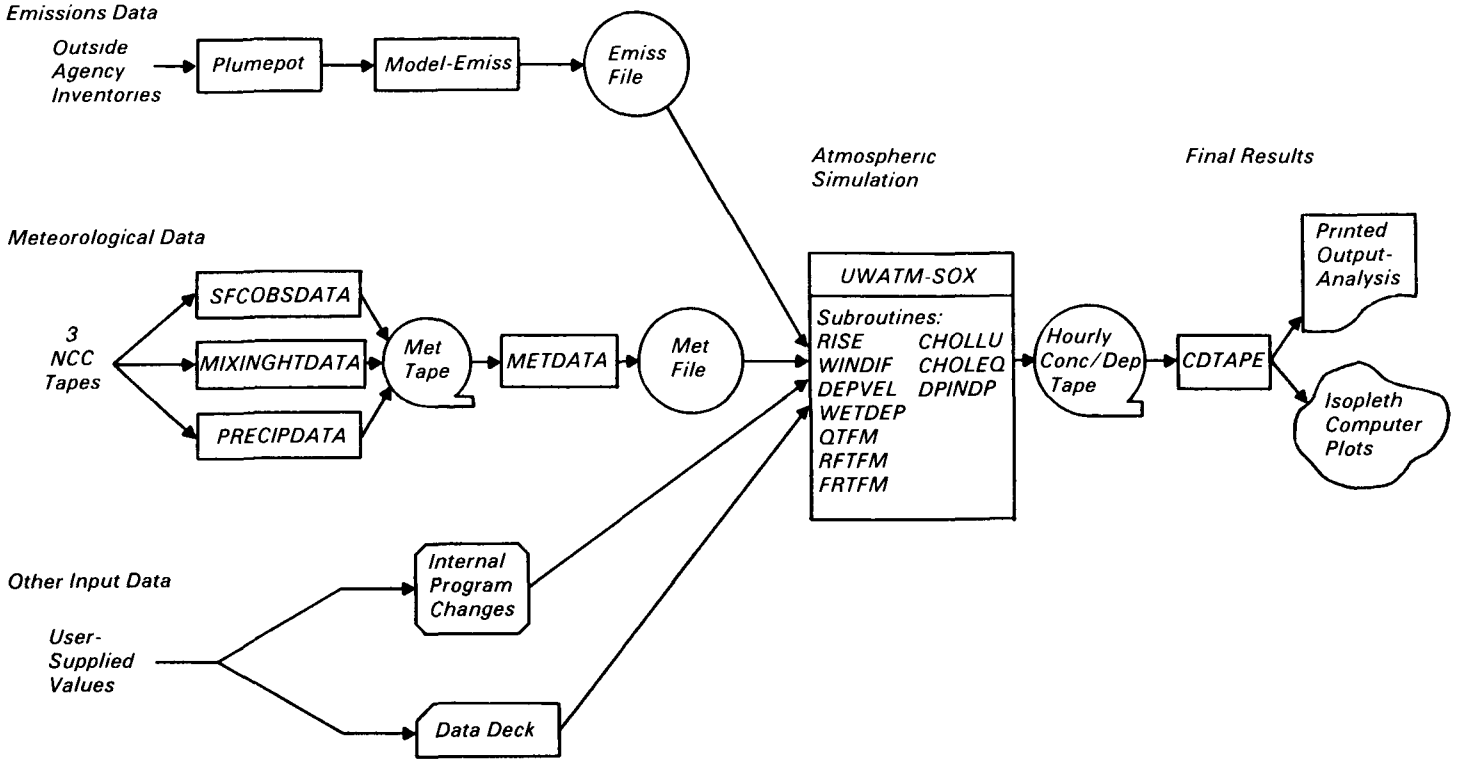

Figure 1. *Schematic of entire modeling operation.*

Table 1. *Summary of Model Features*

Feature	Description
General	— *Cell-type model* — *Time-dependent (hourly)* — *Mesoscale analysis (10s to 100s km)* — *Run in batch mode* — *Numerically solves coupled SO_2 and SO_4 conservation of mass equations for a dilute species in the atmospheric boundary layer described in an Eulerian frame of reference* — *Includes physical processes of:* *wind transport* *turbulent diffusion* *chemical reactions* *source input* *dry deposition* *wet (rain or snow) deposition* — *Uses 2D uniform horizontal grid network over region of study, Uses set of 6 (3 fixed at 50 m and 3 variable) 3D cells in the vertical height from ground to mixing height* — *Emission data is input once, meteorological data is input hourly, model calculates at 20 min intervals within 1 h* — *Numerical solution is of first-order fully implicit type*
Emissions	— *Can handle point, line, area sources* — *Treats all emission sources simultaneously* — *For point sources — calculates a plume rise (using 1 of a set of 5 Briggs or Moses-Carsons equations)* *— accounts for lofting condition* *— SO_4 stack emissions X% of SO_2 (where X is supplied by user)*
Meteorological Data	— *Uses data tapes from National Climatic Center (NCC)* — *Fully computerized processing of tapes to convert data to hourly format required by model*

For a region which has been partitioned by a 3D cell structure, the equations are solved in a downwind-step (x-step) and time-step (t-step) fashion. They are solved for one complete block of cells in the yz-plane and within the block they are solved for each t-step for the specified number of steps (currently three, thus calculating at 20-min intervals). This procedure is repeated block by block from the upwind edge to the downwind edge of the region. The matrix solution for one x-step and one t-step can be symbolized as:

$$[C] = [A]^{-1}\,[D]$$

where

[C] contains the unknown concentrations,

[A] the known meteorological, chemical and deposition data, and

[D] the known concentrations from the previous x-step and t-step.

This matrix equation is solved for each x-step and each t-step in the whole region for a 1-h period, then repeated with new input data. The whole process is repeated hourly until the end of the simulation period. All these calculations are performed in the main program (UWATM-SOX) with the help of three matrix handling subroutines (CHOLLU, CHOLEQ, DPINDP).

To arrive at the solution, numerous subsidiary calculations (mainly carried out by the

Table 1. *(Continued)*

Feature	Description
Atmospheric Boundary Layer	— *Characterized by set of wind speed and turbulent eddy diffusivity profiles, assumed vertically variable but horizontally uniform and constant within region over 1 h period* — *Theory uses concepts of stability, geostrophic wind, surface roughness and mixing height* — *Layer divided into two regions — surface layer and layer between top of surface layer and mixing height* — *Profile equations for surface layer based on the 1954 Monin-Obukov similarity theory, equations for upper region based on a form of wind speed power-law and on assumed constant diffusivity* — *Profiles function of stability (stable, neutral, unstable); stability determined using the 1961 Pasquill-Turner model* — *Profiles function of geostrophic wind; geostrophic wind determined solely from knowledge of surface wind and the height at which it is measured using a Modified Regula Falsi iteration scheme* — *Profiles function of surface roughness; single user-supplied roughness value assumed to be constant and uniform over region* — *Profiles function of mixing height; hourly mixing height determined from NCC Twice Daily Mixing Height tape using linear interpolation scheme* — *Diffusivity profile based on Mixing-Length Model*
Chemical Reactions	— *Linear and homogeneous* — *Uses two conversion rates (based on work by Husar) — 2%/hr (day), 0.5%/hr (night)*
Dry Deposition	— *Uses deposition velocity of form* $V_D = \frac{1}{r_a + r_s}$, *where* r_a *accounts for atmospheric conditions and* r_s *for terrain* — V_D *assumed uniform and constant over region*
Wet Deposition	— *Based on model by Scott (1978)* — *Assumes only Bergeron or cold cloud precipitation development process* — *Assumes removal over entire vertical column from ground to mixing height at once (so calculation is separate from cell-by-cell finite difference calculations)* — *Set of 3 wet removal equations developed:* 1. SO_4 *rain or snow* 2. SO_2 *snow* 3. SO_2 *rain* — *Precipitation is assumed to occur uniformly across the region and uniformly over a 1-h period*
Computer Techniques	— *Written in ASCII FORTRAN* — *Uses complex set of internal total mass summations as basis for* 1. *continual internal conservation of mass check* 2. *basis of regional total atmosphere S budget* — *Employs dual-grid system to handle arbitrary wind directions* — *Employs stop-start capability* — *Employs extensive use of COMMON'S and the FORTRAN Procedure (PROC)* — *Stores compactly on tape complete set of hourly calculations*
Output Results	— *Ground level concentration* *Dry deposition* *Wet deposition* *Total deposition* SO_2 *and* SO_4 *3-h* *24-h* *Seasonal* *Annual* *Averages* — *Ground level concentration* *Dry deposition* *Dates* SO_2 *and* SO_4 *Maximum 3-h* *and Values* *Wet deposition* *Total deposition* *Maximum 24-h* *(All the above are printed on a grid array basis and can be isopleth computer plotted)* — *Concentration frequency distribution for any selected grid point* — *pH of precipitation* — *Total atmospheric* SO_2/SO_4 *budget for in-region emission sources*

subroutines) must be performed. These include:

1) For point sources, calculate a plume rise and determine if lofting occurs (RISE subroutine).
2) Calculate the wind and diffusivity profiles (WINDIF subroutine).
3) Calculate the deposition velocity (DEPVEL subroutine).
4) Calculate the wet deposition removal (WETDEP subroutine).
5) Shift emission source coordinates as wind direction changes (QTFM subroutine).
6) Transfer concentrations between the dual fixed and rotating cell systems as wind direction changes (FIXROT and ROTFIX subroutines).

Output Processing

Hourly the main program outputs ground level concentration arrays, dry and wet deposition arrays, certain meteorological data, the wind and diffusivity profiles, certain emissions data and certain total regional mass calculations. A program called CDTAPE (for concentration/deposition tape processor) does all the summing, averaging and other manipulations of the hourly output. The program is complex but highly flexible. Besides printing the results, CDTAPE stores them on tape in a format suitable for computer isopleth plotting.

Computer Plotting

Our group uses the WISMAP2 computer graphics package developed by the University of Wisconsin Cartography Laboratory. To use this package it is first required that an outline map of the region of study be "digitized." Once this is done, a wide variety of plotting techniques are available through WISMAP2. The plotting process will not be explained in detail because it is assumed users will have other similar plotting packages at their disposal.

Accuracy and Sensitivity Analysis

In this section *accuracy* refers to how the model conforms to expected and known results when given "ideal," i.e., artificial and highly restrictive, input data. *Sensitivity* refers to the model's relative response to changes made in important parameters. Accuracy and sensitivity analysis together with comparison of model predictions to monitoring results provide a basis for judging the model's reliability and usefulness.

The *accuracy* of the model was tested in five simple cases:

1) Pure Advection — The simplest case is to consider a single steady source under constant meteorological conditions in

Table 1. *(Continued)*

Feature	*Description*
Cost/Time of Application	*— For 11 x 13 x 6 cells, hourly meteorological and emission input, 3 time-steps/h, 50K computer core, a run on SPERRY UNIVAC 1100/82 series computer,* *One year simulation:* *Cost = $200 (cheapest rate)* *CPU Time = 6 h* *One day simulation:* *Cost = $7 (normal rate, 10x cheapest)* *CPU Time = 1 min*

which only a constant steady wind transports the pollutants.

2) Advection with Diffusion — The next simplest case to test is that of a single source under constant meteorological conditions with a constant steady wind and constant lateral diffusivity.
3) Time Step and Grid Size — The time step size was halved (from a 20-min to a 10-min interval). The conclusion is that increasing the number of calculations above three does not affect the accuracy of the results.
4) Grid Subdivision — The model uses a double grid system to handle arbitrary wind direction. One grid is assumed fixed in position and the other rotates with changing wind directions.

To investigate the *sensitivity* of the model, six parameters ranging from doubling reaction and emission rates to defaulting pH values by increasing one unit were tested. Results are indicated in Table 2.

Case Study — Rainy Lake Watershed

To investigate acid rain effects on a sensitive wilderness area the UWATM-SOX model was applied to the Rainy Lake Watershed.

Questions to be answered are: How much of the regional S emissions are deposited within the region? How much leaves the region? How does this compare to the available monitoring data in an annual, seasonal and weekly basis? The years 1976 and 1978 were chosen for the case study because 1976 was the year of the first comprehensive emissions inventory, and 1978 was the most recent meteorological data set available as well as the start of the National Atmospheric Deposition Program data at Marcell, Minnesota.

Description of Region and Data Input

The Rainy Lake Watershed is located in northeastern Minnesota and western Ontario. It includes the Quetico Provincial Park, the Boundary Waters Canoe Area and Voyageurs National Park. This area lies within two days travel of 50 million people and yet contains extensive prime wilderness areas. The modeling area is the 330 by 390 km region of the Rainy Lake Watershed where the major emission sources are in Duluth, the Missabe Iron Range, International Falls and Atikokan, Ontario (Ragland and Wilkening, 1983).

The total emissions of SO_2 due to point sources in the region in 1976 were 3,232 g/s or 112,000 tons/year. In 1978 the SO_2 emissions were 3,139 gs or 109,000 tons/year. The area source emissions of SO_2 due to space heating and small industrial and commercial sources were not available, but are believed to be small in this region. Direct SO_4 emissions were assumed to be 3% of the SO_2 emissions by weight, which is a generally observed result from stack sampling. The regional SO_2 emissions of 112,000 tons/year may be compared to the Minnesota statewide total of 521,000 tons/year, Wisconsin 937,000 tons/year and Illnois 2,344,000 tons/year.

The meteorological data were obtained from the NCC for International Falls, Minnesota, for the years 1976 and 1978. The other data input parameters used were the same as the base case in the previous section.

The annual average SO_2 concentrations away from any sources were calculated to be about 0.5 $\mu g/m^3$, while the ambient SO_4 concentrations were about 10 times smaller. The 24-h worst-case SO_2 concentrations away from any sources were 5 $\mu g/m^3$ and the 24-h worst-case SO_4 concentrations also were 5 $\mu g/m^3$. These levels are reasonable in view of the relatively few sources in the region. Monitoring at the remote Fernburg site in the region showed essentially no readings above the 5 $\mu g/m^3$ threshold of the instrument.

Annual and Seasonal Deposition

The (1976) annual wet plus dry deposition isopleths resulting from 35 emission sources within the region are shown in Figure 2. The areas of largest annual deposition center around the Clay Boswell power plant, Calland and Steep Rock mines, Taconite Harbor and Duluth.

The regional mass balance, presented in Table 3 for 1976, shows that 17% of the S emissions were deposited in the region due to dry deposition and 0.3% was retained due to wet deposition. Whereas 82% of the S emissions were transported out of the region on an annual basis. Of the S deposited in the region 8.5 x 10^9 g out of 9.4 x 10^9 g were deposited by dry deposition SO_2. The regional mass balance for 1978 was similar.

Table 2. *Summary of Sensitivity Analyses*

	Average Concentration		*3-h Maximum Concentration*		*Dry Deposition*		*Wet Deposition*	
Cases	SO_2	SO_4	SO_2	SO_4	SO_2	SO_4	SO_2	SO_4
Double reaction rate	*0.93*	*1.68*	*0.89*	*1.74*	*0.96*	*1.64*	*0.94*	*1.66*
Double sulfate surface resistance	*1.00*	*1.07*	*1.00*	*1.09*	*1.00*	*0.55*	*1.00*	*1.02*
Reduce surface roughness by 1/2	*1.06*	*1.16*	*1.18*	*1.23*	*1.25*	*1.18*	*1.25*	*1.24*
Reduce horizontal diffusivity by 1/2	*0.99*	*1.00*	*1.00*	*1.01*	*1.01*	*1.01*	*1.01*	*1.00*
Set default pH to 5.8	*0.93*	*0.97*	*0.98*	*0.98*	*0.93*	*0.98*	*2.30*	*0.96*
Double emissions	*1.99*	*1.97*	*1.99*	*1.98*	*1.97*	*1.94*	*1.98*	*2.01*

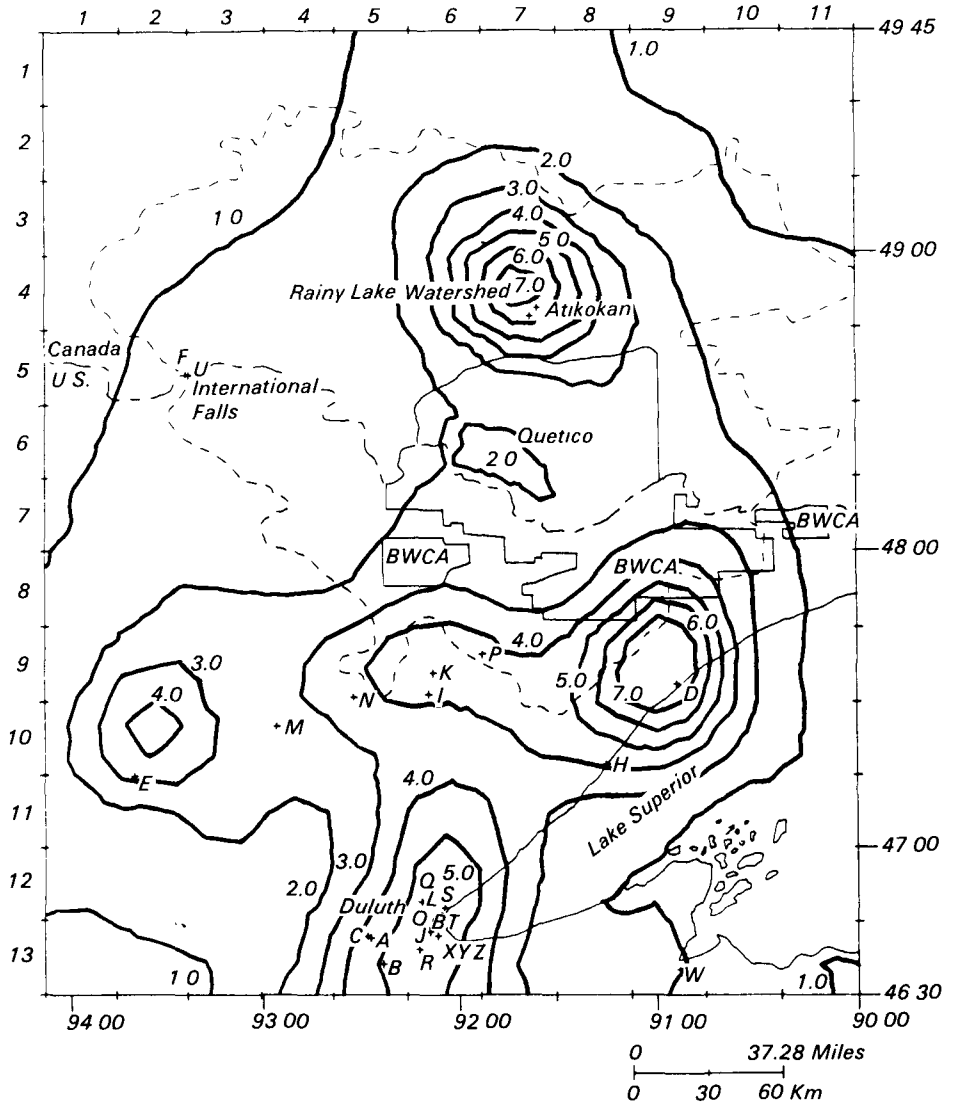

Figure 2. *Map of the study region where 35 emission sources result in the computed annual (1976) wet plus dry deposition of $SO_4^=$ as kg SO_4/ha. The SO_2 depositions have been multiplied by 1.5 (the ratio of molecular weights) and combined with the $SO_4^=$ values to represent the total loading from regional sources.*

Table 3. *Regional Mass Balance for 1976*

	SO_2 (10^9 g/yr)	SO_4 (10^9 g/yr)	S (10^9 g/yr)
Emissions	102	3.1	52.3
Chemical reaction	6	9.8	—
Dry deposition	17	0.6	8.7
Wet deposition	1	0.5	0.7
Transport out of region	78	11.8	42.9

It is of interest to compare the deposition during the snow season (November-April) with the non-snow season (May-October). The calculations are summarized for grid (2, 9) the Marcell, Minnesota NADP monitoring site, in Table 4. The greatest percentage of S deposition occurs by dry deposition of SO_2 during the summer. Wet deposition of SO_4 is comparable in winter and summer, although total wet deposition is greater in the summer. It is believed that the reason wet deposition of SO_4 is similar in winter and summer is that there are more hours of precipitation in winter than in summer although the total amount of precipitation is greater in the summer. The wet deposition in 1978 is nearly twice as great as 1976 because of increased precipitation.

Comparison With Monitoring Data — NADP and Snow Cores

The National Atmospheric Deposition Program located a site in the region at Marcell, Minnesota, starting in July 1978. The NADP site measures wet SO_4 deposition on a weekly basis from inter- and intraregional transport. Total wet SO_4 deposition monitored at the site was considerably more than that calculated for the site, mainly due to transport of SO_4 from outside the region. Dry deposition is not measured reliably at the NADP site and hence cannot be compared.

Sixty-five snow cores taken in April 1979 in the BWCA provide valuable information on wet plus dry deposition. They yielded SO_4 depositions mostly in the range of 1 to 2 kg/ha, whereas the regional model predicted 0.5 kg/ha. The NADP site at Marcell measured 1.6 kg/ha SO_4 wet deposition during the 1978 to 1979 snow season.

Extreme-Case Weeks

The calculated wet and dry deposition fluxes also may be compared on a weekly basis for several extreme case weeks. The weekly SO_4 wet deposition data at the Marcell NADP site show that a few big events account for much of the annual SO_4 wet deposition. The wet SO_4 deposition is clearly dominated by long-distance transport of SO_4 during the worst-case weekly events.

Single Source

The model was also run for a new single source to be located at Atikokan, Ontario (Ragland and Wilkening, 1983). The emissions were 70.5 x 10^9 g/yr of SO_2 and 2.1 x 10^9 g/yr of SO_4. The stack height was 200 m and the plume rise was typical of a coal-fired power plant. The model also was run with the stack height reduced to 100 m. Overall, 18.6% of the S remained in the region compared to 15% at full stack height. Table 5 gives the results of the predicted mass balance for sulfur emissions.

References

Ragland, K.W. and K.E. Wilkening. 1983. Intermediate-Range Grid Model for Atmospheric Sulfur Dioxide and Sulfate Concentrations and Depositions. Atmos. Environ. 17: 935-947.

Scott, B.C. 1978. Parameterization of Sulfate Removal by Precipitation. J. Appl. Meteorol. 17: 1375-1389.

Wilkening, K.E. and K.W. Ragland. 1982. A User's Guide to the University of Wiscon-

Table 4. *Calculated Regional Deposition at the Marcell, Minnesota Site*

	Dry		Wet		Wet and Dry	
S Deposition (kg/ha)	1976	1978	1976	1978	1976	1978
Winter SO_2 deposition	0.24	0.21	0.01	0.02	0.25	0.23
Summer SO_2 deposition	1.23	1.13	0.10	0.19	1.33	1.32
Winter SO_4 deposition	0.02	0.02	0.03	0.03	0.05	0.05
Summer SO_4 deposition	0.02	0.02	0.03	0.06	0.05	0.08
Winter deposition as SO_4	0.36	0.34	0.06	0.05	0.41	0.39
Summer deposition as SO_4	1.86	1.72	0.18	0.35	2.04	2.07
Annual deposition as SO_4	2.22	2.06	0.23	0.40	2.45	2.46

Table 5. *Mass Balance Due to Single Source at Atikokan*[a]

	SO_2 (10^9 g/yr)	SO_4 (10^9 g/yr)	S (10^9 g/yr)
Emissions	70.5	2.1	35.9
Chemical reactions	4.7	7.1	—
Dry deposition	10.0 (12.4)	0.3 (0.5)	5.1 (6.4)
Wet deposition	0.4 (0.4)	0.4 (0.4)	0.3 (0.3)
Transport out of region	55.4 (52.9)	8.4 (8.4)	30.5 (29.2)

[a]*Note: Numbers in parentheses represent a stack height of 100 m instead of 200 m.*

sin Atmospheric SO_2/SO_4 Air Pollution Computer Model (UWATM-SOX). U.S. Environmental Protection Agency, Cincinnati, Ohio. (Available from NTIS.)

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The complete report, entitled "Intermediate-Range Grid Model and User's Guide for Atmospheric Sulfur Dioxide and Sulfate Concentrations and Depositions: Wisconsin Power Plant Impact Study," (Order No. PB 84-189 257; Cost: $13.00, subject to change) will be available only from:
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