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ON THE USE OF AUTOMATIC DIFFERENTIATION FOR SENSITIVITY ANALYSIS IN EMISSION CONTROL PROCESS

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1. INTRODUCTION

Air quality models simulate the fate of atmospheric pollutants using a set of algebraic and differential equations based upon the physical laws of science. Air quality models require meteorological inputs, emission inputs, and initial and boundary condition concentration fields. Theoretically, if all the inputs are completely specified, the governing set of equations allows us to predict the details of air flow and chemical transformations. However, it is impossible in practice to describe all the inputs and model parameters precisely because they have to be estimated from stochastic atmospheric motions. Model performance is inevitably influenced by errors and uncertainties introduced into the model by the parameterization schemes and the input data. Among all input data and parameters, emissions have received great attention because of their critical role in the decision making process.

Knowledge of the complex chemical interactions characterizing the photochemistry of tropospheric ozone production has significantly increased in the past but there exists no clear scientific consensus on the best strategy for reducing ozone. The role of volatile organic compounds and oxides of nitrogen in the production of tropospheric ozone has long been recognized. Elevated tropospheric ozone levels have proven to be much more difficult to control than other pollutants that have shared the focus of recent control efforts. A fundamental complicating factor relates to the fact that ozone is not directly emitted, but formed in the atmosphere by reactions involving reactive hydrocarbons and nitrogen oxides. Because of the nonlinearities in the relationships between ozone and its precursor species, it is not at all simple to prescribe the requisite precursor emission reductions necessary to reduce ozone concentrations to a given level. Sensitivity analysis of emitted species will provide important insights for emission control strategies for reducing ozone. We will present a preliminary result of sensitivity analysis in the emission control process by using an automatic differentiation technique.

2. METHOD

We will use an automatic differentiation technique, ADIFOR, (Automatic DIfferentiation in FORtran) (Bischof et al. 1992) in this work. ADIFOR is based on a source translator paradigm and was designed from the outset with large-scale codes in mind. ADIFOR provides automatic differentiation for programs written in FORTRAN-77. To apply ADIFOR to a given code, the user need only specify which variables correspond to independent and dependent variables with respect to differentiation. ADIFOR then generates new FORTRAN-77 code for the computation of the original function evaluation as well as the associated derivatives. This technique has been demonstrated to be applicable and efficient for sensitivity analysis in air quality models (Hwang and Byun, 1995).

A 3-dimensional model with only vertical diffusion, emission, and deposition processes is used for this study:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}(k\frac{\partial C}{\partial z}) + \alpha E + D \qquad (1)$$

where C is the concentration field, k is the diffusivity coefficient, E is the emission input, D is the deposition, $\alpha(x,y,z,t)$ is the emission control factor and z is the vertical coordinate variable. Based on the value of emissions, two levels of control are set up. Strong control, α_1, is set on locations with high emissions and weak or no control, α_2, on locations with low emission: $\alpha = \alpha_1$ if $E \geq h$, $\alpha = \alpha_2$ if $h > E \geq l$ and $\alpha = 1$ if $E < l$ for high emission level h and low level l. Note that there will be no control if

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$\alpha_1 = \alpha_2 = 1$ and this will become uniform control if $h = l = 0$. We will calculate the sensitivity of model output to emission control factor, $\partial C / \partial \alpha$.

3. RESULT

We applied the sensitivity model of the diffusion-emission process for a two-day period, 00GMT, September 7 to 00 GMT, September 9, 1983 on northeastern United States. We have run four test cases among which three of them are uniform control cases and the last one is a nonuniform control case. The emission control parameters used for the four cases are; (A) (α_1, α_2)= (1, 1), (B) (α_1, α_2)= (0.75, 0.75), (C) (α_1, α_2)= (0.5, 0.5), and (D) (α_1, α_2)= (0.5, 0.75) for (h, l)= (5000 g/sec, 3000 g/sec). As an example, we show the sensitivity analysis results for species SO_2. The sensitivity ($\partial C / \partial \alpha$) of case A is given in Figure 1 and the differences of sensitivity of case A and case D is given in Figure 2. Figure 1 shows that the cells potentially sensitive to an emission control coincide with the high SO_2 emission cells. Figure 2 shows cells that are more susceptible to change to the specific emissions control strategy, case D.

The peak values of sensitivity and concentrations all occur at cell (19, 30) and are summarized in Table 1. It shows that the sensitivities of uniform control cases change linearly with the control factor changes and the concentrations are proportional to the emissions input. The nonuniform control case shows sensitivity and concentration values in between those of cases B and C as expected.

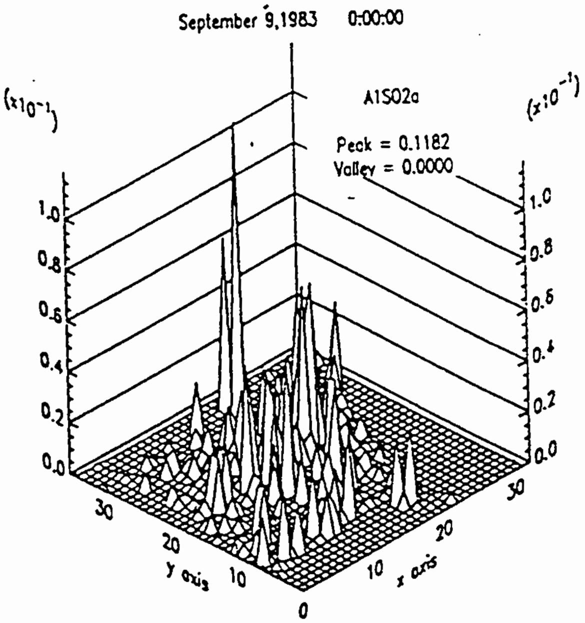

Figure 1: Sensitivity of concentration to control factor in case A, (α_1, α_2)=(1, 1), after 48 hours simulation.

Table 1: Peak values of sensitivity of concentration to control factor after 48 hours simulation.

Case	$\partial C / \partial \alpha$ (ppm)	Concentrations (ppm)
A	0.1182	0.1260
B	0.0887	0.0964
C	0.0591	0.0669
D	0.0631	0.0709

DISCLAIMER

This paper has been reviewed in accordance with the U.S. Environmental Protection Agency's peer and administrative review policies and approved for presentation and publication. It has also been approved for publication by MCNC. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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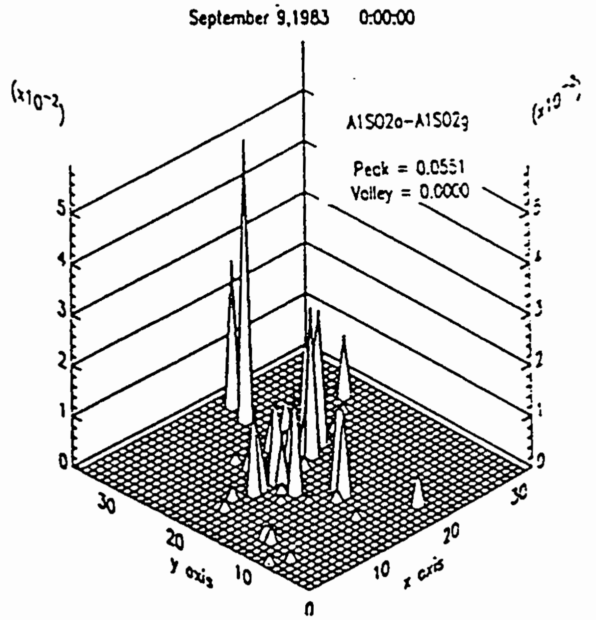

Figure 2: Differences of sensitivity of concentration to control factor in case A, (α_1, α_2)=(1, 1) and case D, (α_1, α_2)=(0.5, 0.75) after 48 hours simulation.

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

Knowledge of the complex chemical interactions characterizing the photochemistry of tropospheric ozone production has significantly increased in the past but there exists no clear scientific consensus on the best strategy for reducing ozone. The role of volatile organic compounds and oxides of nitrogen in the production of tropospheric ozone has long been recognized. Elevated tropospheric ozone levels have proven to be much more difficult to control than other pollutants that have shared the focus of recent control efforts. A fundamental complicating factor relates to the fact that ozone is not directly emitted, but formed in the atmosphere by reactions involving reactive hydrocarbons and nitrogen oxides. Because of the nonlinearities in the relationships between ozone and its precursor species, it is not at all simple to prescribe the requisite precursor emission reductions necessary to reduce ozone concentrations to a given level. Sensitivity analysis of emitted species will provide important insights for emission control strategies for reducing ozone. We will present a preliminary result of sensitivity analysis in the emission control process by using an automatic differentiation technique.

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