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Project Summary

Plume Concentration Algorithms with Deposition, Sedimentation, and Chemical Transformation

K. Shankar Rao

The basic assumptions underlying a gradient-transfer model for the atmospheric transport, diffusion, deposition, and first-order chemical transformation of gaseous and particulate pollutants emitted from an elevated continuous point source are presented. This analytical plume model treats gravitational settling and dry deposition in a physically realistic and straightforward manner. For practical application of the model, the eddy diffusivity coefficients in the analytical solutions are expressed in terms of the widely used Gaussian plume dispersion parameters. The Gaussian parameters latter can be specified as functions of the downwind distance and the atmospheric stability class within the framework of the standard turbulence-typing schemes.

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

Pollutant gases and suspended particles released into the atmosphere are transported by the wind, diffused and diluted by turbulence, and removed by several other natural processes. Depletion of airborne pollutant material by these natural processes affects pollutant concentrations and residence times in the atmosphere. One important pollutant removal mechanism is dry deposition on the earth's surface by gravitational settling, eddy impaction, chemical absorption, and other processes. Surface deposition of acidic and toxic pollutants may adversely affect local ecology, human health, biological life, structures, and ancient monuments. Another significant removal mechanism is chemical transformation in the atmosphere. The product of a chemical reaction may be the pollutant of primary concern, the reactant itself. Furthermore, large concentrations of particulate products resulting from chemical reactions may lead to significant deterioration of atmospheric visibility. It is important, therefore, to obtain reliable estimates of the effects of dry deposition and chemical transformation of pollutants.

This Summary describes an analytical plume model based on gradient transfer (K-theory) for diffusion, dry deposition, and first-order chemical transformation of gaseous or particulate pollutants released from an elevated continuous point source. The model solves the atmospheric advection-diffusion equation subject to a deposition boundary condition. The model includes similar and complementary sets of equations for the primary (reactant) and the secondary (product) pollutants. The complete Project Report (see ordering information at back) includes a brief review of the literature on gradient-transfer models that incorporate chemical transformation. Details of the mathematical formulations and analytical solutions of the present model with deposition, sedimentation, and chemical transformation are given, and the parameterized concentration algorithms for the primary and the secondary pollutants are listed. Calculated variations of the ground-level concentrations and results of a sensitivity analysis are presented and discussed. Some guidance is provided for the specification of the settling and deposition velocities in the model.

Theoretical Basis

Two chemically coupled gaseous or particulate pollutant species are considered in this model. The primary (species-1 or reactant) pollutant is assumed to transform into the secondary (species-2 or reaction product) pollutant at a known constant rate. In general, the two species are assumed to have known nonequal deposition and settling velocities. As a first step, analytical solutions for concentrations of the two pollutant species emitted from an elevated continuous point source are derived. The K-coefficients in these solutions are expressed in terms of the widely used Gaussian plume dispersion parameters. The resulting expressions are parameterized, simplified, and presented as extensions of the Gaussian plume algorithms currently used in EPA air quality models for various atmospheric stability and mixing conditions. Further simplifications of the new algorithms are indicated for gaseous or fine suspended particulate pollutants with negligible settling and for ground-level sources and/or receptors. Limiting expressions of the algorithms are derived for large particles for which gravitational settling is the dominant deposition mechanism. Finally, using an innovative approach based on mass balance considerations, these new point source concentration algorithms are used to derive expressions for the concentrations of the two species emitted from an area source. In the limit when deposition and settling velocities and the chemical transformation rate are zero, the analytical plume algorithms for the primary and the secondary pollutants reduce to the well-known Gaussian plume diffusion algorithms presently used in EPA dispersion models for assessment of air quality. Thus, model described here retains the ease of application associated with Gaussian plume models and is subject to the same basic assumptions and limitations that apply to the Gaussian models.

A new mathematical approach, based on mass budgets of the species, is outlined to derive simple expressions for ground-level concentrations of the primary and secondary pollutants resulting from distributed area-source emissions. These expressions, which involve only the point-source algorithms for the well mixed region, permit use of the same program subroutines for both point and area sources. Thus, the area-source concentration equations developed in this project are simple, efficient, and accurate.

Input Assumptions

No assumptions are made in this model regarding the nature of the pollutant species. The formulations and the solutions are, therefore, general enough to be applicable to any two gaseous or particulate pollutants that are coupled through a first-order chemical transformation. Either of the two species may be a gas or may be particulate matter of known average size. Molecular weights of the two species are assumed to be known. Direct emission of the secondary pollutant from both point and area sources is permitted. A direct emission of the secondary pollutant can contribute to its concentration significantly more than does the chemical transformation. In the absence of a chemical coupling, expressions for concentrations of two chemically independent pollutants, each subject to deposition and/or sedimentation, can be obtained as degenerate cases of the concentration algorithms for the general case.

Conclusions

A gradient-transfer model that accounts for the atmospheric diffusion and deposition of two gaseous or particulate pollutant species coupled through a first-order chemical transformation has been formulated. This model, which includes a deposition boundary condition for each species, treats the pollutant removal mechanisms in a physically realistic and straightforward manner. The exact analytical solutions for concentrations of the two pollutants released from an elevated continuous point source have been derived. For practical application of the model to a variety of atmospheric stability conditions, the eddy diffusivity coefficients in the analytical solutions have been expressed in terms of the widely used Gaussian plume dispersion parameters, which are functions of downwind distance and stability class.

In order to facilitate comparison with the Gaussian plume dispersion algorithms, the new diffusion-deposition-transformation algorithms for various stability and mixing conditions have been parameterized and presented as analytical extensions of the Gaussian algorithms presently used in EPA air quality models. In the limit when the deposition and settling velocities and the chemical transformation rate are zero, the new algorithms reduce to the standard Gaussian plume equations. Thus, the model outlined here retains the ease of application—and is subject to the same basic assumptions and limitations-associated with Gaussian plume type models.

The point- and area-source concentration algorithms developed in this project may have wide applicability in practical rural and urban air pollution and particulate models. In separate work associated with this project, the algorithms were incorporated into an existing air quality model and a user's guide for the model was written.

K. Shankar Rao is with the National Oceanic and Atmospheric Administration, Oak Ridge, TN 37830.
***Jack H. Shreffler** is the EPA Project Officer (see below).*
The complete report, entitled "Plume Concentration Algorithms with Deposition, Sedimentation, and Chemical Transformation," (Order No. PB 84-138 742; Cost: $11.50, subject to change) will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
The EPA Project Officer can be contacted at:
Environmental Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

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