SOME NEED BASED MATHEMATICAL DISPERSION MODELS FOR AIR POLLUTION STUDIES WITH SPECIAL REFERENCE TO SCAVENGING MODELS

by

SATYAJIT GHOSH

Submitted in fulfilment of the requirements
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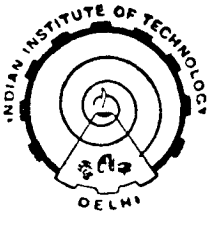
DOCTOR OF PHILOSOPHY



Centre for Atmospheric and Fluids Sciences
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CERTIFICATE

This is to certify that the thesis entitled 'SOME NEED BASED MATHEMATICAL DISPERSION MODELS FOR AIR POLLUTION STUDIES - WITH SPECIAL REFERENCE TO SCAVENGING MODELS' being submitted by SATYAJIT GHOSH for the award of the degree of DOCTOR OF PHILOSOPHY, is a record of the original bonafide research work carried out by him. He has worked under our joint guidance and supervision and has fulfilled the requirements for the submission of this thesis. The results presented in this thesis have not been submitted in part or full to any other University or Institute for award of any degree/diploma.

Prof. M.P. SINGH
Head: Centre for Atmospheric Sciences
Indian Institute of Technology, Delhi
New Delhi.

Dr. O.P. SHARMA
Senior Scientific Officer-I
Centre for Atmospheric Sciences
Indian Institute of Technology, Delhi
New Delhi

Dr. V.K.SRIVASTAVA
Assistant Professor
Department of Chemical Engineering
Indian Institute of Technology, Delhi
New Delhi

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(SATYAJIT GHOSH)

ABSTRACT

In the wake of rapid industrialisation air pollution problems in India is progressively increasing. The threat to our air quality is not new. It is in fact complementary to industrial progress. Since industrial development has to continue one must take sufficient safety measures to ensure that our air quality is not impaired. Mathematical models are thus being developed the world over for predicting pollutant concentrations in the atmosphere.

Owing to a substantial rise in fossil fuel combustion, today, the world faces a serious environmental hazard - The Acid Rain Problem. Eventhough rain water acidity in India has not yet reached alarming levels at most places, in the immediate vicinity of factories there still is an acid rain threat.

The primary objective of this thesis is two fold. Firstly, to simulate mathematically the processes of advection, diffusion and washout of air pollutants released into the atmosphere and secondly to estimate the extent of precipitation contamination by means of appropriate formulation of scavenging models. The latter aspect is all the more relevant considering the fact that India is a country lashed by intense monsoonal rains.

Chapter I is an introductory chapter and gives a brief review of the acid rain problem.

Chapter II deals with a detailed survey of rain water acidity measurements in India and also summarises various available models and their relative merits and demerits.

The central theme of Chapter III is model formulation and it also sets out the general framework of the assumptions for the formulation of the scavenging model. First the formulation of a 2D model is presented, where an atmospheric washout and transport model is presented for pollutants released from elevated sources over flat terrain.

In Chapter IV a 3D model is presented for analysis around a large coal fired power plant in New Delhi. The efficacy of the south-west monsoonal rains to scavenge a soluble pollutant like SO_2 from an urban environment is also discussed.

In Chapter V, first the 3D model described in Chapter IV is further generalised for the case when the ground is covered with water, as is very often the case during the monsoons. The second part of this chapter deals with a study of SO_2 emissions over Delhi and its correlation with the corresponding trends in precipitation chemistry.

In Chapter VI a Lennard-Jones 6-12 potential model was used to calculate the molecular diffusivity of SO_2 in air. A profile of molecular diffusivity of SO_2 in air from the ground level to the PBL is obtained. Results indicate a change of about 17.5% between the diffusivity values at the ground and at the PBL top. The possible changes that could result in scavenging calculations due to this change in diffusion coefficient are also illustrated. This is perhaps the first work of its kind wherein a systematic theoretical procedure is developed to estimate the molecular diffusivity of pollutant gases in the PBL.

In Chapter VII, numerical models are presented to study the concentration of SO_2 outside a falling rain drop and also the concentration of $SO_3^=$ undergoing oxidation inside the drop.

In Chapter VIII, a more general model is developed where the flow fields outside and inside are coupled together. The aqueous phase chemistry of the SO_2-H_2O system is treated in detail. The concentration of SO_2 outside the drop and the concentration of H_2SO_3, HSO_3^-, $SO_3^=$ and H^+ inside the drop are obtained.

In Chapter IX, an analytic dispersion model based on the solution of the unsteady state atmospheric advection-diffusion equation is presented to study the dispersion of methyl isocyanate released during the Bhopal Gas Tragedy.

The reaction of MIC with a humid atmosphere is also featured. Apart from the chemical conversion of MIC to Methylamine, dry deposition effects are also considered.

Chapter X is the concluding chapter of the thesis. It points out the main achievements and also sets out various suggestions for improvement and future work.

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