CALIFORNIA INSTITUTE OF TECHNOLOGY

PASADENA, CALIFORNIA 91125

ENVIRONMENTAL QUALITY LABORATORY

Department of Energy
Institutional Grant to the
California Institute of Technology
Environmental Quality Laboratory Block

Progress Report on Project Element No. 6

December 1, 1978 - November 30, 1979

RELATION OF EMISSIONS TO AIR QUALITY FOR PHOTOCHEMICAL SMOG

John H. Seinfeld

Principal Investigator

EQL Open File Report No. 80-6

April 1980

Relation of Emissions to Air Quality for Photochemical Smog

INVESTIGATORS: J. H. Seinfeld, Professor and Executive Officer of Chemical Engineering
G. J. McRae, Graduate Student, Environmental Engineering Science
J. W. Tilden, Senior Research Engineer, Environmental Quality Laboratory
W. R. Goodin, Research Fellow, Environmental Engineering Science*

Effective evaluation of air pollution control strategies requires the use of validated and reliable mathemtical models that can relate pollutant emissions to atmospheric air quality. The primary objective of this research program has been to develop a fundamental capability to assess the effectiveness of air pollution control measures in reducing photochemical air pollution. An important aspect of the development has been to simplify the preparation of input data and operational use of the resulting model. The system has been designed to be used by air pollution agencies with relatively little experience in atmospheric physics and chemistry. The assumptions commonly employed in model formulations have been evaluated to ensure a valid representation of the physical and chemical processes in the atmosphere.

In the most recent phase of this research the comprehensive photochemical airshed model has been evaluated against data available in the South Coast Air Basin of Southern California. This task was undertaken in collaboration with the California Air Resources Board, Air Quality Modeling Section. A statistical analysis package has been used to evaluate the correspondence of predicted and observed concentrations for the days on which the model was evaluated. An assessment of the EPA ozone isopleth modeling technique has been initiated.

One objective of the current work is to develop a general framework for assessing quantitatively the accuracy and validity of physico-chemical air quality models. As desccribed above, a consistent

*Former investigator who has left Caltech.

and general framework for evaluating the performance of models with respect to the degree to which their predictions match ambient pollutant concentration data has been accomplished. Also, a general technique for executing sensitivity/uncertainty analysis has been developed and employed to study the sensitivity and uncertainty of complex kinetic mechanisms for photochemical smog. The proposed future program is devoted to an expansion of sensitivity and uncertainty analysis of photochemical air quality simulation models. The major elements of uncertainty in simulation of urban air pollution are associated with the cemical mechanisms, the source emission inventory and the treatment of meteorology. It is proposed that additional studies involving uncertainty associated with chemical kinetic mechanisms be undertaken, particularly with simultaneous diffusion and source emissions.

Although the model application has been site specific, there will be important research results applicable for other air pollution problems especially those involving reacting species. In fact, it is impossible to make practical progress in air pollution modeling without being site specific because it is necessary to learn how to cope with such real world problems as inadequate or inconsistent input data. Partial sponsorship by DOE and interactions with DOE personnel will assist in the dissemination and exchange of necessary modeling skills. An adequate ability to predict regional air quality consequences is, of course, an important part of assessing the environmental impact of various energy supply strategies.

PUBLICATIONS FROM PROJECT ELEMENT NO. 6

6a. A. H. Falls, G. J. McRae and J. H. Seinfeld, "Sensitivity and Uncertainty of Reaction Mechanisms for Photochemical Air Pollution," International Journal of Chemical Kinetics, in press, 1979.

6b. W. R. Goodin, G. J. McRae and J. H. Seinfeld, "A Comparison of Interpolation Methods for Sparse Data: Application to wind and Concentration Fields," Journal of Applied Meteorology, vol. 18, no. 6, pp. 761-771, 1979.

6c. W. R. Goodin, G. J. McRae and J. H. Seinfeld, "An Objective analysis Technique for Constructing Three-Dimensional, Urban-Scale Wind Fields," Journal of Applied Meteorology, in press, 1979.

6d. M. Koda, G. J. McRae and J. H. Seinfeld, "Automatic Sensitivity Analysis of Reaction Mechanism," International Journal of Chemical Kinetics, vol. 11, pp. 427-444, 1979.

6e. G. J. McRae, W. R. Goodin and J. H. Seinfeld, "Development of a second Generation Mathematical Model of Photochemical Air Pollution," Final Report to California Air Resources Board Under Contract No. A5-046-87, 1979.

6f. G. J. McRae, W. R. Gooding and J. H. Seinfeld, "A Second Generation Mathematical Model of Photochemical Air Pollution," American Meteorological Society, Fourth Symposium on Atmospheric Turbulence, Diffusion, and Air Quality, January 1979.

6g. G. J. McRae, "Mathematical Modeling of Photochemical Air Pollution," Proceedings AIAA Symposium on Society and Aerospace Technology, Los Angeles, November 15, 1979.

6h. J. H. Seinfeld and G. J. McRae, "Use of Models to Establish Source-Receptor Relationships and Relative Source Contributions of NO_x to Air Qualtiy," Proceedings EPA Symposium on Implications of a Low NO_x Vehicle Emission Standard, Washington, D. C., May 4, 1979.