Meetings

Modeling of Photochemical Smog

Presently an intense effort is under way to develop a photochemical model capable of predicting air quality. One important input to such a model is the set of kinetic equations describing the chemistry of atmospheric transformation processes. Before the full potential of modeling can be achieved, the mechanism and rates of reaction of photochemical smog processes must be better defined. In an effort to determine what research should be undertaken to acquire this information, the Chemistry and Physics Laboratory of the Environmental Protection Agency (EPA) sponsored a workshop on photochemical modeling on 30–31 October 1972, at the National Environmental Research Center in Research Triangle Park, North Carolina. In addition to developing future directions for the laboratory, this workshop was held to establish better lines of communication between experimentalists and modelers. Among the topics discussed were elementary rate constants, reaction mechanisms, smog chamber research, and atmospheric measurements that are needed for model verification.

In introductory remarks M. C. Dodge (EPA) described the research activities of the Chemistry and Physics Laboratory in elucidating atmospheric transformation processes. A survey was presented of the smog chamber studies, field studies, and the program of instrumental methods in progress to develop new capabilities for detecting pollutants. The current laboratory activity in the modeling program was discussed along with plans that are being formulated to acquire further data for modeling.

An overview of the state of the art of photochemical modeling was given by P. M. Roth (Systems Applications, Inc.). He discussed potential uses of models as predictive tools to assess the effects of alternative control strategies, determine the impact of projected sources, plan effective least-cost, long-term control strategy, and enable real-time prediction to prevent impending air pollution episodes. Also discussed were the types of models that have been formulated in an attempt to fulfill these needs. Emphasis was placed on the grid and trajectory models that are currently under development. These approaches are based on the solution of the equations of continuity. These equations include terms to describe the transport of pollutants, source and sink terms to describe the influx and removal of pollutants, and chemical reaction terms. The many uncertainties associated with these various inputs were discussed. Such factors as imprecisely known emission rates and inadequate meteorological and air quality data were mentioned. Emphasis was placed on the uncertainties associated with the chemistry and the difficulties encountered in trying to extrapolate smog chamber studies to atmospheric processes. A description of the various types of mechanisms that have been postulated to explain atmospheric chemistry were also discussed.

T. A. Hecht (California Institute of Technology) distributed a list of some 40 reactions that are either known, or suspected to be, important in explaining photochemical smog formation. He discussed these reactions, emphasizing the uncertainties associated with each. Those reactions for which the rate constants are either unknown or are highly suspect were pointed out. Reactions for which the intermediates and products of reaction are unknown were also discussed.

An open discussion was conducted on each of the reactions in Hecht's list. The following is a summary of some of the recommendations offered during this discussion:

1) The first-order dissociation constant for NO_2 should be better determined.

2) The effects of surface-to-volume ratios on the rates of formation of HNO_3 and HONO should be determined.

3) Rate constants for the reactions of alkoxy radicals should be measured.

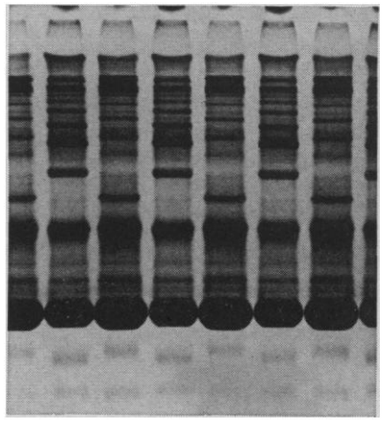
4) The products of the reactions of olefins with O_3, O atoms, and OH radicals under atmospheric conditions should be determined.

5) The quantum yields of the photolysis of aldehydes as a function of wavelength need to be better determined.

On the second day, a session was held on the role of smog chamber experiments in model validation. A. Eschenroeder (General Research Corporation) suggested that reactants and products should be analyzed in situ, and that controlled investigations of the effects of aerosols should be carried out. In addition, Eschenroeder suggested that nitrogen balances should be achieved in order that wall effects may be ascertained and, if possible, measurements of free radicals should be made. To this list Hecht added the need for careful control of light intensity, relative humidity, temperature, and the initial NO_2 concentration. Hecht also recommended that the precision and accuracy of all measurements should be reported and more complete product identification and analysis should be carried out. L. G. Wayne (Pacific Environmental Services) stated that, if the model is to meet functional criteria, it should be detailed enough to permit extrapolation with reasonable confidence to ambient air quality concentrations. To achieve this, appreciable amounts of experimental data should be collected for these low concentration ranges.

H. Jeffries (University of North Carolina) discussed a novel type of chamber study soon to be initiated. This chamber facility is being constructed out-of-doors in a rural community. The structure consists of an A-frame, covered with transparent Teflon film, that is divided into two halves. Each half of the chamber will be filled with relatively clean rural air. The chambers will then be charged with varying amounts of hydrocarbons and NO_x. Irradiations will be carried out under conditions of natural sunlight, temperature, and humidity. The experiments to be conducted in this chamber are designed to furnish information on the effects a reduction in ambient hydrocarbon concentrations will have on air quality.

A. Levy (Battelle Memorial Institute) discussed plans for conducting studies to furnish information on the role of aerosols in photochemical smog formation. This research is designed to provide information on such factors as



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the effect of mechanical stirring on aerosol formation in chambers, the inhibition of aerosol formation that occurs with certain hydrocarbon mixtures, and the effect of primary aerosols on the formation of secondary aerosols.

The final session of the workshop was concerned with the role of atmospheric measurements in modeling. Eschenroeder discussed the type of field measurements required for model verification. He recommended that vertical profiles of temperature and pollutant concentrations be obtained and that more numerous hydrocarbon measurements be taken. He also suggested that atmospheric removal processes for NO_x should be identified and the influence of concentration inhomogeneities upon atmospheric reaction rates should be determined.

W. A. Perkins (Metronics Associates, Inc.) discussed the measurement program planned for the Los Angeles Basin during the 1973 smog season. The objective of this program is to provide a data base suitable for developing and testing photochemical models. In this study a block of air will be followed by ground and air mobile units as it traverses an area. Aerometric measurements will be made of the pollutants in this air mass. By following an air parcel, rather than sampling from ground stations, one can observe directly changes in the nature of the pollutants as they undergo reaction.

R. C. Sklarew (EPA) ended the session with a discussion of some of the difficulties that the Meteorology Laboratory must solve before the full potential of photochemical models can be realized. One of the problems of current concern is the incorporation of chemistry into the models. Chemical reactions can be handled with relative ease by utilization of the trajectory approach. However, errors in following the chemistry can result if the grid approach is used. Another difficulty that must be resolved is that the effects of local point sources are presently handled by smearing the emissions over a wide area, giving poor resolution to the models. The efforts presently being made to resolve these difficulties were discussed.

The proceedings of this workshop, including presentations and discussions, are available upon request.

MARCIA C. DODGE
Environmental Protection Agency, Research Triangle Park, North Carolina

BOOKS RECEIVED

(Continued from page 1229)

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Health Hazards of the Human Environment. World Health Organization, Geneva, 1972 (U.S. distributor, American Public Health Association, Washington, D.C.). 388 pp. Paper, $11.

A Historical Introduction to the Philosophy of Science. John Losee. Oxford University Press, New York, 1972. 218 pp., illus. Paper, $3.50.

Human Nutrition. Its Physiological, Medical and Social Aspects. A Series of Eighty-Two Essays. Jean Mayer. Thomas, Springfield, Ill., 1972. xvi, 272 pp. $12.95.

Immune Complexes and the Pathogenesis of Various Diseases. Papers by Margherita Branca and others. MSS Information Corp., New York, 1973. 240 pp., illus. $15.

Introduction to Marine Environments. Robert Zottoli. Mosby, Saint Louis, 1973. xii, 125 pp., illus. Paper, $4.95.

An Introduction to Respiratory Physiology. Frederick F. Kao. Excerpta Medica, Amsterdam, and Elsevier, New York, 1972. xii, 332 pp., illus. $20.

The Isoquinoline Alkaloids. Chemistry and Pharmacology. Maurice Shamma. Academic Press, New York, and Verlag Chemie, Weinheim, Germany, 1972. xviii, 596 pp., illus. $35. Organic Chemistry, vol. 25.

Katamnesen bei kastrierten Sittlichkeitsdelinquenten aus forensisch-psychiatrischer Sicht. F. Cornu. Karger, Basel, 1973 (U.S. distributor, Phiebig, White Plains, N.Y.). viii, 132 pp., illus. Paper, $15.40.

Laboratory Embryology of the Chick. Lloyd E. Downs. Brown, Dubuque, Iowa, ed. 2, 1972. x, 96 pp., illus. Spiral bound, $2.95.

Laboratory Methods in Infrared Spectroscopy. R. G. J. Miller and B. C. Stace, Eds. Heyden, New York, ed. 2, 1972. xxii, 376 pp., illus. $18.

Life Between Tidemarks on Rocky Shores. T. A. Stephenson and Anne Stephenson. Freeman, San Francisco, 1972. xiv, 426 pp., illus. Cloth, $15; paper, $6.95.

A Life of One's Own. Three Gifted Women and the Men They Married. Joan Dash. Harper and Row, New York, 1973. xx, 388 pp., illus. $10.

Linnaeus. Heinz Georke. Translated from the German edition (Stuttgart, 1966) by Denver Lindley. Scribner, New York, 1973. xii, 178 pp., illus. $9.95.

Lipide während der Schwangerschaft und Niederkunft. Franz Jaisle. Karger, Basel, 1972 (U.S. distributor, Phiebig, White Plains, N.Y.). vi, 184 pp., illus. $16.80. Fortschritte der Geburtshilfe und Gynäkologie, vol. 48.

The Living Oceans. Alec Laurie. Doubleday, Garden City, N.Y., 1973. 188 pp., illus. $6.95. Nature and Science Library.

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