UNIVERSITY OF CALIFORNIA

Los Angeles

Simple Computer Simulation Model of Photochemical Air Pollution

A thesis submitted in partial satisfaction of the requirement for the degree Master of Science in Chemistry

by

Chung Shing Liu

1976

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1976

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ABSTRACT OF THE THESIS

Simple Computer Simulation Model

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Professor Christopher S. Foote, Chairman

An attempt has been made to develop a simple computer simulation model to describe photochemical smog formation in the ambient atmosphere. A 7-step chemical kinetic mechanism has been proposed, based on the nature of known chemical reaction rates and experimental smog chamber data. The chemical equations have been recast as differental equations and the integration routine has been programmed in DYNAMO, a convenient computer simulation language. The related rate constants and reaction parameters have been adjusted to simulate the available data results. Some statistical methods are used to generalize the kinetics of the model by fitting two parameters which are functions of initial concentrations of HC and NO_x to rectangular hyperbolas. The simulation

capability of this model has been checked against concentration-time relationships with the experimental data and gives excellent fits for a wide range of initial concentrations.