

AN ABSTRACT OF A THESIS

MODELING PHOTOCHEMICAL SMOG USING THE ADVANCED CONTINUOUS SIMULATION LANGUAGE

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Master of Science in Chemical Engineering

The Advanced Continuous Simulation Language (ACSL) has been used to model the production of photochemical smog. Two categories of models were developed: laboratory smog chamber models and the box model for predicting the concentration of air pollutants in urban airsheds. Nine smog chamber models and four box models were developed. Testing the use of the Pseudo-Steady State Approximation (PSSA) was done. It has been concluded that since ACSL readily solves simultaneous differential equations, the use of PSSA should be used only if stiff differential equations are encountered.

The models that have been developed include the following chemical species: oxides of nitrogen, ozone, hydroxide, alkanes, alkenes, diolefins, aldehydes, and aromatics.

The amount of code the user must write using ACSL to simulate smog production is much less than that of Fortran. The models developed required from 45 to 249 lines of code.

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