PREDICTION OF RATE CONSTANTS IN THE CH_2Cl_2 REACTION SET

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Abstract

The serious problems concerning hazardous waste disposal have prompted recent studies in incineration, since this disposal strategy represents one of growing application. Clearly, there remain a number of unanswered questions relating to this waste control option. Several practical questions of interest include how to predict incinerator efficiencies, how to determine optimal operating conditions, how to design optimal future generation units, and how to predict off-design operation. Modeling strategies, at various levels, will play an important part in answering these and other pertinent questions. Any realistic modeling activity in the incineration area must include the flame-mode chemistry involved. Unfortunately, for many of the compounds of interest, flame-mode chemical kinetic data are not available for use in incinerator models. The work to be presented in this poster session has focussed upon obtaining this chemical kinetic information for a select group of hazardous wastes.

A method for predicting reaction rate constants for the oxidation of chlorinated methanes will be presented, with emphasis on the dichloromethane (CH_2Cl_2) set. These reactions are then used to simulate two premixed CH_2Cl_2/CH_4/air flat flames at a Cl/H ratio of 0.33. Simulations are made for a fuel rich flame ($\varnothing = 1.10$), and a fuel lean flame ($\varnothing = 0.77$). The model uses a reaction set with 347 reactions and 71 species, and includes chemistry for hydrocarbons and chlorinated hydrocarbons up to the C_2's.

The calculated species profiles are given for each flame, and are then compared to experimental results. These profiles include the major species and ten important stable intermediates, including the chlorinated methanes. A reaction rate analysis is performed for each flame. This allows for the identification of the important reactions in the destruction of the chlorinated species, and provides insight into the role of chlorine in hydrocarbon flames. The important reaction pathways for the CH_2Cl_2/CH_4/air flames will also be shown.