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Chemical Kinetics Computer Program
for Static and Flow Reactions

A general chemical kinetics computer program for complex gas mixtures has been developed. This program can be used for any homogeneous reaction in either one dimensional flow or a static system. It is flexible, accurate, and easy to use. It can be used for any chemical system for which species' thermodynamic data and reaction rate constant data are known. The program handles several types of reaction: biomolecular exchange reactions, unimolecular decompositions, bimolecular decompositions, and the reverse recombination processes.

An implicit numerical integration method is used for the solution of the differential equations that describe a complex reaction. A new step size optimization procedure has been developed to make this technique work efficiently for a wide range of conditions. This includes the extremes of very slow and very fast reactions.

The program can be used to compute: (1) chemical reaction behind a shock wave, (2) ignition and combustion in a flowing or static system, (3) ignition, combustion, and nozzle expansion in supersonic flow, (4) chemical reaction in any flowing gas mixture whose velocity does not reach the speed of sound, (5) chemical reaction in any static system, and (6) constant temperature and/or constant volume reactions.

Notes:
1. This program is written in FORTRAN IV, Version 13, for use on an IBM 7044-7094/Direct Couple System.
2. Inquiries concerning this program should be directed to:

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       112 Barrow Hall
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       Reference: LEW-11467

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