

PACKAGE ID - 000188GENWS00 CHEMKIN III

KWIC TITLE - The CHEMKIN-III COLLECTION

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LIMITATION CODE -COPY **AUDIENCE CODE** - LIM

COMPLETION DATE - 06/01/9619 **PUBLICATION DATE** - 06/01/1996

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DESCRIPTION - An integrated set of Fortran 77 codes, example problems in the form of unix scripts, and input data for use as a tool in modeling a variety of gas and multi phase chemical kinetics problems; included are equilibrium and sensitivity analysis programs, and modeling codes for a shock tube, premixed flame, gas/gas-surface/plasma flow in a stirred reactor, gas/gas-surface plug flow, deposition on a rotating disk and in cylindrical or planar channels.

PACKAGE CONTENTS - Media Directory; Software Abstract; SAND96-8216; SAND96-8217; Media Includes Source Code, Auxiliary Material, Compilation Instructions, Linking Instructions Sample Problem Input Data;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

METHOD OF SOLUTION - ODE's boundary value solvers, iterative methods.

COMPUTER - WORK STATION

OPERATING SYSTEMS - Machine dependent

PROGRAMMING LANGUAGES - FORTRAN 77

SOFTWARE LIMITATIONS - Explicit dimensions for data storage have been given default values which the user may need to increase/decrease for a particular problem: the maximum number of mesh points, atoms, molecules, or chemical reactions depends on the user's needs, and the limits of such data storage is defined by the user's computing environment.

SOURCE CODE AVAILABLE (Y/N) - Y

RELATED SOFTWARE - The CHEMKIN III Collection is a significant upgrade to the earlier set of chemical kinetics software, CHEMKIN II; it maintains backward compatibility for solving the CHEMKIN II problems, while adding capabilities for multi-phase kinetics and plasma flow. It is a highly-integrated suite of codes and data, with no superfluous elements. Some public-domain mathematical and ODE solver software is included for convenience.

HARDWARE REQS - The CHEMKIN III Collection requires approx, 5Mb disk space to store the entire suite of codes and data, however, the requirements for using an application code to solve any one particular problem will need only a few of the files, and to generate the objects, executables, and output for a problem requires minimal computer resources.

TIME REQUIREMENTS - The CHEMKIN III Collection provides example problems which would require less than 3 min on most platforms.

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TIME REQUIREMENTS - (CONT)

REFERENCES - Michael E Coltrin, Robert J Kee, Fran M Rupley, and Ellen Meeks, Surface CHEMKIN-III: A Fortran Package for Analyzing Heterogenous Chemical Kinetics at a Solid-Surface - Gas-Phase Interface, SAND96-8217, May 1996; Robert J Kee, Fran M Rupley, Ellen Meeks, and James A Miller, CHEMKIN-III: A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical and Plasma Kinetics, SAND96-8216, May 1996.

ABSTRACT STATUS - Released AS-IS 4/30/1998.

SUBJECT CLASS CODE - U

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
C CODES
REACTOR KINETICS
REACTORS
COMPUTERIZED SIMULATION
THERMODYNAMICS
FLUID FLOW
HEAT TRANSFER
REACTIVITY
POLLUTION CONTROL
PLASMA
CHEMICAL ANALYSIS

EDB SUBJECT CATEGORIES -

990200

SPONSOR - DOE/ER

PACKAGE TYPE - AS - IS