PACKAGE ID - 001170MLTPL00 ICRKFLO

KWIC TITLE - Two-Dimensional Integral Reacting Computer Code for Multiple Phase Flows

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

COMPLETION DATE - 05/01/1994 **PUBLICATION DATE -** 05/01/1994

DESCRIPTION - ICRKFLO solves conservation equations for gaseous species, droplets, and solid particles of various sizes. General conservation laws, expressed by ellipitic-type partial differential equations, are used in conjunction with rate equations governing the mass, momentum, enthalpy, species, turbulent kinetic energy and dissipation for a three-phase reacting flow. Associated sub-models include integral combustion, two-parameter turbulence, particle melting and evaporation, droplet evaporation, and interfacial submodels. An evolving integral reaction submodel, originally designed for ICOMFLO2 to solve numerical stability problems associated with Arrhenius type differential reaction submodels, was expanded and enhanced to handle petroleum cracking applications. A two-parameter turbulence submodel accounts for droplet and particle dispersion by gas phase turbulence with feedback effects on the gas phase. The evaporation submodel treats not only particle evaporation but the droplet size distribution shift caused by evaporation. Interfacial submodels correlate momentum and energy transfer between phases.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Includes Source Code, Sample Problem Input and Output, User's Documentation, Programmer Documentation;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - The ellipitic-type partial differential equation solver relies on a control volume approach, while a modified SIMPLER numerical algorithm is used for the conservation of mass, energy, momentum, and species calculations for the gas, liquid, and particle phases.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - An operating system with an ANSI FORTRAN compiler capable of compiling and linking large programs that may require a sizable amount of data storage for intermediate results (6 Mbytes

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OPERATING SYSTEMS -(CONT) or more depending on grid size and number of condensed phase size r

PROGRAMMING LANGUAGES - FORTRAN

SOFTWARE LIMITATIONS - The grid size and number of condensed phase size groups can be limited by the memory space available. Double-precison calculations are recommended on computers with fewer than 14 significant digit floating-point number representation. Either the FORTRAN compiler must have an include capability to bring in COMMON blocks stored in a seperate file or the operating system must have a preprocessor with that capability.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Integral reaction submodels which enhance numerical stability and convergence and enlarge the class of chemically-reacting flow problems which can be solved. A coke formation submodel which allows coke deposition on particle surface. Droplet evaporation submodel which permits mass transfer between droplets and gas. A two-parameter turbulence submodel with condensed phase treatment. Due to its compact size and efficient equation solvers, the code runs well on most 486 class or better personal computers. A Eulerian method is applied for both the gas and condensed phase computation. The ellipitic-type partial differential equation solver achieves conservation of flow properties independent of the grid size by use of a control volume approach.

HARDWARE REQS - A computer system with a minimum of 6 Mbytes RAM and file storage capacity of at least 10 Mbyte. A 386/25 MHz class personal computer with math coprocessor is the minimum machine considered for acceptable run times.

TIME REQUIREMENTS - Given a grid with 3000 nodes and a single particle-size group, a steady-state computation takes about 15 minutes of Cray/YMP CPU time for 300 iterations. On a 386/25 PC with 80387 math processor, the same problem takes roughly 2 minutes CPU time for iteration using double-precision calculations. The CPU time drops to about 10 seconds per iteration with a 90 MHz Pentium CPU.

ABSTRACT STATUS - Submitted 5/13/97. Released AS-IS 6/20/97.

SUBJECT CLASS CODE - H

KEYWORDS -
COMPUTER PROGRAM DOCUMENTATION
I CODES
HEAT TRANSFER
FLUID FLOW

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PETROLEUM
COKING
CHEMICAL REACTION KINETICS
MULTIPHASE FLOW
TURBULENCE

EDB SUBJECT CATEGORIES -
990200

SPONSOR - DOE/FE

PACKAGE TYPE - AS - IS