

PACKAGE ID - 001128MLTPL00 PLUG

KWIC TITLE - Plug Flow Reactor Simulator

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LIMITATION CODE -UNL **AUDIENCE CODE** - UNL

COMPLETION DATE - 01/09/1996 **PUBLICATION DATE** - 01/09/1996

DESCRIPTION - PLUG is a computer program that solves the coupled steady state continuity, momentum, energy, and species balance equations for a plug flow reactor. Both homogeneous (gas-phase) and heterogenous (surface) reactions can be accommodated. The reactor may be either isothermal or adiabatic or may have a specified axial temperature or heat flux profile; alternatively, an ambient temperature and an overall heat-transfer coefficient can be specified. The crosssectional area and surface area may vary with axial position, and viscous drag is included. Ideal gas behavior and surface site conservation are assumed.

PACKAGE CONTENTS - Media Directory; software Abstract; SAND96-8211;
Media Includes Source Code;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - PLUG makes use of the CHEMKIN and SURFACE CHEMKIN software packages to handle gas-phase and heterogeneous kinetics as well as thermodynamic properties. The standard implicit code DASSL is then used to solve the set of differential/algebraic equations describing the reactor.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - Any

PROGRAMMING LANGUAGES - FORTRAN

SOFTWARE LIMITATIONS - As currently configured, the code can handle problems involving at most 50 gas-phase species, 46 surface species, 20 bulk species, and 10 phases. However, these limits can easily be increased.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Unlike typical plug flow reactor codes, PLUG is able to handle heterogenous as well as gas-phase chemistry. This requires the solution of a differential/algebraic rather than purely differential system and necessitates a separate calculation for the initial values of the surface species concentrations.

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UNIQUE FEATURES - (CONT)

RELATED SOFTWARE - PLUG must run in conjunction with the CHEMKIN and SURFACE CHEMKIN chemical kinetics packages and the DASSL differential/algebraic system solver.

HARDWARE REQS - The executable produced by PLUG occupies about 0.8 MB of central memory.

TIME REQUIREMENTS - The execution time depends strongly on the size and characteristics of the chemical mechanism and, to a lesser extent, the size of the reactor. However, since a one-dimensional description of the reactor is being used, the computation time tends to be quite modest. For a sample problem involving 17 gas-phase species and 6 surface species, the time required is only a few seconds on a Silicon graphics workstation.

REFERENCES - Richard S. Larson, PLUG: A FORTRAN Program for the Analysis of Plug Flow Reactors with Gas-Phase and Surface Chemistry Version 2.0, SAND96-8211, January 1996.

ABSTRACT STATUS - Submitted 12/04/96. Released AS-IS 12/19/96.

SUBJECT CLASS CODE - OP

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
P CODES
FORTRAN
FLUID FLOW
GASES
ONE-DIMENSIONAL CALCULATIONS
DIFFERENTIAL EQUATIONS
CHEMICAL REACTORS
LOADING RATE
SURFACE PROPERTIES

EDB SUBJECT CATEGORIES -
990200 400100

SPONSOR - DOE/DP

PACKAGE TYPE - AS - IS