PACKAGE ID - 000129DVX1100 DESULF MODEL-FIXS

KWIC TITLE - Desulfurization Model for Fixed-Bed

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

COMPLETION DATE - 03/01/1992 **PUBLICATION DATE -** 03/01/1988

DESCRIPTION - Model was developed to complement the DOE-METC effort to develop a high-temperature process for the desulfurization of coal-derived gases. Computer model capable of describing the sulfidation in fixed-bed reactors have been written and tested. Isothermal conditions have been assumed during the sulfidation phase.

PACKAGE CONTENTS - Media Directory; Software Abstract;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 2 5.25 Diskettes

METHOD OF SOLUTION - The model is based upon the simultaneous solution of the differential equations describing the component material balances and, where necessary, energy balances. The model is heterogeneous in that the solid and fluid phases are considered seperately. Concentration and/or temperature gradients between solid and fluid phases are described in terms of mass and heat transfer coefficients. Plug flow of the gas phase is assumed for the fixed-bed reactor. The single particle kinetic descriptions are based upon a special case of the single particle unreacted core model for the fixed-bed reactor. The resistances associated with mass transfer and product layer diffusion are assumed to dominate while the intrinsic resistance associated with the surface is negligible. The validity of the unreacted core model was established in previous single particle kinetic studies.

COMPUTER - DEC VAX11

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OPERATING SYSTEMS - VMS

PROGRAMMING LANGUAGES - FORTRAN IV

SOFTWARE LIMITATIONS - None.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Only known model for hot gas desulfurization processes.

RELATED SOFTWARE - This is the original software.

OTHER PROG/OPER SYS INFO - File naming convention used is (filename) .DOC. No proprietary or any special sofware is required.

HARDWARE REQS - Standard Features

TIME REQUIREMENTS - Less than 5 minutes

REFERENCES - Final Report on the work performed under Contract No.: DE-AC21-86MC23089, Dynamic Simulation Models for High-Temperature Desulfurization Processes, March 1988, by Louisiana State University, DOE/MC/23089-2601, (DE88010263).

ABSTRACT STATUS - Submitted December 1991.

SUBJECT CLASS CODE - R

KEYWORDS -
COMPUTER PROGRAM DOCUMENTATION
D CODES
DESULFURIZATION
COAL GAS
FLUIDIZED BED REACTORS
ISOTHERMAL PROCESSES
MATHEMATICAL MODELS
COMPUTERIZED SIMULATION
PACKED BEDS

EDB SUBJECT CATEGORIES -
990200 010402

SPONSOR - DOE/FE

PACKAGE TYPE - SCREENED