PACKAGE ID - 000132DVX1100 DESULF MODEL-MOVN

KWIC TITLE - Desulfurization Models for Moving-Bed

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

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DESCRIPTION - Models were developed to complement the DOE-METC effort to develop a high-temperature process for the desulfurization of coal-derived gases. Computer models capable of describing both the sulfidation and regeneration cycles in moving bed reactors have been written and tested. Isothermal conditions have been assumed during the sulfidation phase but the highly exothermic nature of the regeneration reactions make it necessary to consider non isothermal regeneration.

PACKAGE CONTENTS - Media Directory; Software Abstract; User's Manual;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 2 5.25 Diskettes

METHOD OF SOLUTION - All models are based upon the simultaneous solution of the differential equations describing the component material balances and, where necessary, energy balances. The models are heterogeneous in that the solid and fluid phases are considered separately. 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 also assumed. Plug flow of the solid phase is assumed in moving-bed reactor. The single particle kinetic descriptions are based upon a special case of the single particle unreacted core model. The resistances associated with mass transfer and product layer diffusion are assumed to dominate while the intrinsic resistance associated with the surface reaction is negligible. The validity of the unreacted core model was established in previous single particle kinetic

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METHOD OF SOLUTION -(CONT) studies.

COMPUTER - DEC VAX11

OPERATING SYSTEMS - VMS

PROGRAMMING LANGUAGES - FORTRAN IV

SOFTWARE LIMITATIONS - None

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Only known models for hot gas desulfurization/regeneration processes for moving-bed applications.

RELATED SOFTWARE - This is the original software.

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

HARDWARE REQS - Standard Features.

TIME REQUIREMENTS - Less than five 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 -
D CODES
DESULFURIZATION
COMPUTERIZED SIMULATION
COAL GAS
MATHEMATICAL MODELS
ISOTHERMAL PROCESSES
MOVING-BURDEN PROCESS
COMPUTER PROGRAM DOCUMENTATION

EDB SUBJECT CATEGORIES -
990200 010402

SPONSOR - DOE/FE

PACKAGE TYPE - SCREENED