

PACKAGE ID - 000128DVX1100 REGN MODEL FIXR

KWIC TITLE - Regeneration Model for Fixed-Bed

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LIMITATION CODE - UNL

AUDIENCE CODE - UNL

COMPLETION DATE - 03/01/1988

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DESCRIPTION - Model was developed to complement the DOE-METC effort to develop a high-temperature process for the regeneration of sulfided sorbents used to desulfurize the coal-derived gases. Computer model capable of describing the regeneration in fixed-bed reactors have been written and tested. Highly exothermic nature of the regeneration reactions made it necessary to consider non-isothermal regeneration.

PACKAGE CONTENTS - Media Directory; Software Abstract;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 5.25 Diskette

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 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 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 reaction is negligible. The validity of the unreacted core model was established in previous single particle kinetic studies.

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COMPUTER - DEC VAX11

OPERATING SYSTEMS - VMS

PROGRAMMING LANGUAGES - FORTRAN IV

SOFTWARE LIMITATIONS -

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Only known model for high temperature regeneration of sulfided sorbents.

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 is 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 11-26-91.

SUBJECT CLASS CODE - R

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
R CODES
DESULFURIZATION
COAL GAS
PACKED BEDS
FLUIDIZED BED REACTORS
COMPUTERIZED SIMULATION
SORBENT RECOVERY SYSTEMS
MATHEMATICAL MODELS
REGENERATION
SULFIDES

EDB SUBJECT CATEGORIES -
990200 010402

SPONSOR - DOE/FE

PACKAGE TYPE - SCREENED