R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Gasification Technologies

10/2006

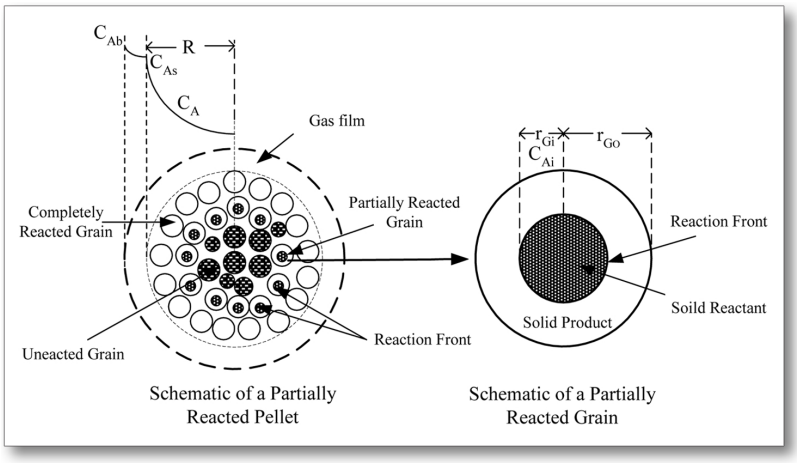
Sulfur Sorption Modeling and Applications

Background

Integrated coal gasification combined cycle (IGCC) power plants represent a highly efficient and environmentally friendly way to generate electricity. The technology is thus a key technology for the 21st century. During the coal gasification process, H_2 and CO are produced in a high temperature gas stream along with other gases such as H_2S. The H_2S must be removed before combustion or it forms sulfur oxides that pollute the air. The objective of this project is to develop an accurate, rapid model to simulate a circulating fluid bed (CFB) and transport reactor that contains a reactant that selectively combines with the H_2S, removing it from the gas stream. In order to reach this objective, NETL is establishing the current knowledge base, identifying operating regimes and transitions and conducting sensitivity analysis of key parameters.

Accomplishments

A mathematical model that simulates hot gas desulfurization (HGD) processes in a transport reactor was developed by integrating hydrodynamic and sulfidation kinetic submodels. This was used to simulate the reactor hydrodynamics as three regions: acceleration, fully developed and deceleration zones. Experimental parameters that went into the simulation were extracted from over 100 cold flow tests based upon scaling laws for CFB reactors. The model was one dimensional, plug flow and included the variable property grain model. The model was validated against experimental data obtained using pilot- and bench-scale transport reactors (GPDU, Transport Reactor). Good agreement between the predicted and experimental data was obtained. Several conference reports and a peer reviewed journal articles that describe the work have been published.



Kinetics Model

CONTACTS

Gary J. Stiegel
Gasification Technology Manager
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236
412-386-4499
gary.stiegel@netl.doe.gov

Lawrence Shadle
Engineering Research Division
National Energy Technology Laboratory
3610 Collins Ferry Road
P. O. Box 880
Morgantown, MV 26507
304-285-4647
lawrence.shadle@netl.doe.gov

PARTNERS

Raghubir Gupta
Research Triangle Institute
3040 Cornwallis Road
Post Office Box 12194
Research Triangle Park, NC 27709-2194
919-541-6000
Gupta@RTI.org

PARTNERS (cont.)

Jerry Schlather
Eastman Chemical
P. O. Box 1974
Kingsport, Tennessee 37662
423-229-2000
gasification@eastman.com

ADDRESS

National Energy Technology Laboratory
1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South
Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

One West Third Street, Suite 1400
Tulsa, OK 74103-3519
918-699-2000

CUSTOMER SERVICE

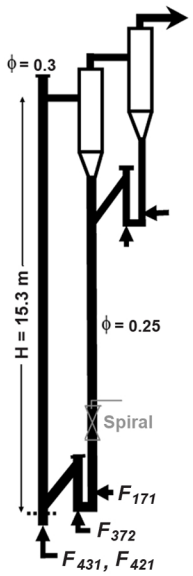
1-800-553-7681

WEBSITE

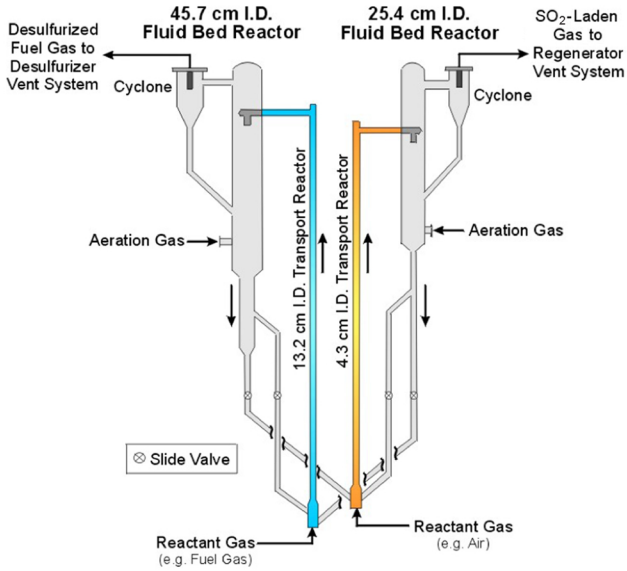
www.netl.doe.gov

Benefits

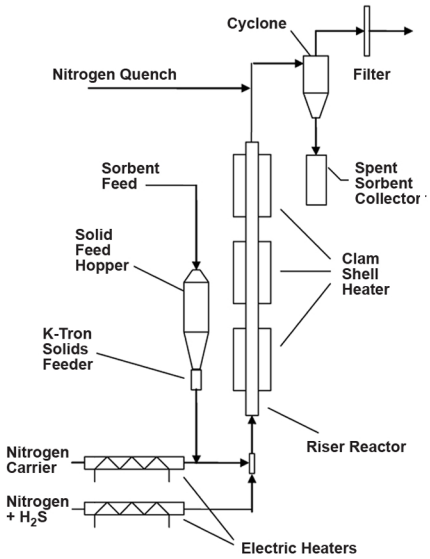
Successful completion of this project will result in a simulator that can be used to support the Eastman-RTI project that is developing warm gas clean-up. This support comes from an improved ability to understand the hydrodynamics and chemistry of both warm and hot gas clean-up. The simulator can also be used to model reactor scale-up issues by predicting the performance of specific process configurations and operational adjustments. It can also be used to predict performance in larger conceptual systems and evaluate the impact of changes in both system configuration and heat integration in the transport absorber and regenerator.



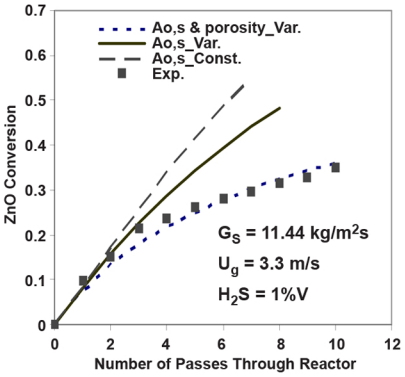
Cold-Flow Circulating Fluid Bed (CFCFB) Test Facility



GPDU in Transport Absorber-Transport Regeneration Configuration



Schematic Diagram of Transport Reactor



Comparison of Experimental Data with Model Predictions Using Variable and Constant BET Surface Area