Simultaneous Production of High-Purity Hydrogen and Sequestration-Ready CO_2 from Syngas: Computer Model Development

Topical Report

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ABSTRACT

Two computer modules are being constructed to model a new process for syngas upgrading and purification. The first module simulates the physical processes occurring in a fluid bed reactor where both gas and solid compositions and flow rates vary significantly along the axis of the reactor. The second module simulates the chemistry and mass transfer between the gas and solid phases. Primitive forms of the two modules have been developed and exercised over a range of performance parameters. These early tests verify that the modules will need to be expanded to model the reactors as series of individual zones in order to attain satisfactory predictive performance.

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1.0 Introduction

GE Energy and Environmental Research Corporation (EER) and Southern Illinois University (SIU) at Carbondale are conducting work on a project titled, "Simultaneous Production of High-Purity Hydrogen and Sequestration-Ready CO_2 from Syngas." This work is sponsored by the U.S. Department of Energy (DOE) under contract number DE-FG26-99FT40682. This project addresses needs to improve methods to efficiently and simultaneously produce streams of high-purity hydrogen (H_2) and sequestration-ready carbon dioxide (CO_2) from the synthesis gas (syngas) that may be produced within a Vision 21 plant.

1.1 Project Objectives

The objectives of this project are to design and build a bench scale dual-bed fluidized reactor/regenerator system for the production of high-purity H_2 (for use in electrochemical fuel cells) and sequestration-ready CO_2. The specific objectives for this project are identified by task as follows:

Task 1: *Laboratory evaluation of the process involved*. Task 1 is being conducted by SIU. The overall objective of this task is to conduct a laboratory scale demonstration of each of the individual subprocesses involved in converting syngas to separate streams of H_2 and CO_2.

Task 2: *Engineering and economic assessments of the process*. Task 2 is being conducted by EER. The objective of this task is to assess the engineering and economic feasibility of the proposed process. These assessments are being accomplished by developing a computer model of the complete process. This topical report covers the computer modeling efforts for the fluidized bed system.

Task 3: *Evaluation of materials*. Task 3 will be conducted by EER and SIU. The overall objective of this task will be to demonstrate the efficacy of the process for CO_2 separation, H_2 production, and isolation of contaminants from the product H_2 stream.

Task 4: *Process design and development*. Task 4 will be conducted by EER and SIU. The overall objectives of this task will be process optimization, cost projections, design of a bench-top sub-scale pilot plant for demonstration of the process under dynamic conditions, and a preliminary system analysis for a full-scale plant.

Task 5: *Bench scale demonstration*. Task 5 will be conducted by EER. The objective of this task will be to collect data on process operation under dynamic conditions. The bench-top sub-scale pilot plant designed from Task 4 will be fabricated and tested.

1.2 Report Purpose

This report is intended to update the reader as to the status of the development of an integrated computer model that numerically simulates the operation and performance of the dual-bed fluidized reactor system. Presently, the model is being developed in two separate modules. One of these calculates the physical behavior of a fluidized bed reactor, while the other module calculates the chemistry and mass transfer between the gas and solid phases. Primitive forms of these modules have been developed and debugged, and are now being exercised against a range of operational parameters including temperature, pressure, and gas-phase compositions.

At their present state of development, these primitive modules treat the dual-bed reactor as two independent batch reactors. However, results of parametric studies using the primitive modules indicate that more detailed model development is required. Presently plans for development of the modules include modeling the dual-bed reactor as a series of independent reactors. This will provide the capability for modeling changes in fluid composition and state properties along the axes of the reactors.

Details of the development of the modules and results of the parametric tests are provided in a confidential attachment to this report.