SECTION IV. TASK 4. APPLICATION OF INTEGRATED CODES

Objective

The objective of this task are to evaluate the integrated comprehensive codes for pulverized coal and fixed-bed reactors and to apply the codes to selected cases of interest to METC.

Task Outline

This task will be accomplished in two subtasks, one for the entrained-bed lasting 45 months and one for the fixed-bed lasting 36 months. Each of these subtasks will consists of three components: 1) Simulation of demonstration cases on BYU computers; 2) Implementation on a work station at AFR; and 3) Simulation of demonstration cases on the workstation.

IV.A. SUBTASK 4.A. - APPLICATION OF GENERALIZED PULVERIZED COAL COMPREHENSIVE CODE

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Objectives

The objectives of this subtask are 1) to implement the comprehensive entrained-bed code developed in Task 3 at AFR and 2) to simulate reactors of interest to METC.

Accomplishments

No work was conducted on this subtask during the past quarter.

Plans

No work is planned for this subtask during the next quarter.

IV.B. SUBTASK 4.3. - APPLICATION OF FIXED-BED CODE

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Objectives

The objective of this subtask is to apply the advanced fixed-bed[1] code developed in Subtask 3.b. to simulate fixed-bed gasifiers of interest to METC. During Phase I, two test cases will be selected, data for validation of these test cases obtained, and initial testing and validation of the code will be performed.

Accomplishments

This subtask was initiated during the past quarter. Fixed-bed technology and data have been reviewed and reported under Subtask 3.b. Based on this review, fixed-bed gasifiers of potential interest for simulation have been identified.

The review was limited to fixed-bed gasification. Stoker boilers were not considered. Several conclusions have been drawn from the review. First, fixed-bed gasification is one of two leading technologies for 1) production of fuel gas from coal, 2) integrated gasification, combined-cycle electric power generation (IGCC), 3) production of synthesis gas from coal, and 4) retrofitting oil-fired power plants and fuel cells. Second, fixed-bed gasification is an important commercial gasification process. Eighty-nine percent of the coal that is gasified is by fixed-bed (Lurgi), ten percent by entrained-bed (Koppers-Totzek, others), and only one percent by fluidized-bed (Winkler). Lurgi's dry-ash gasification process is the only commercial fixed-bed gasification process. Mild gasification has been of increasing interest lately. Fixed-bed gasifiers may be conveniently divided into commercial, demonstration, development, and laboratory units, as shown in Table IV.B-1.

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[1] "Fixed-bed" is in common usage although the bed is actually slowly moving. "Fixed-bed" and "moving-bed" will be used here interchangeably.

TABLE IV B-1. FIXED-BED REACTORS

COMMERCIAL

1. LURGI Dry Ash
   - Sasolburg and Secunda (SASOL), South Africa
   - Westfield, Scotland
   - Beulah (Great Plains), North Dakota

DEMONSTRATION

1. BGC/LURGI Slagging Ash - Westfield, Scotland
2. KILnGAS - Wood River Station, Illinois (Allis-Chalmers and Illinois Power Company)

DEVELOPMENT

1. METC - Morgantown, West Virginia
2. UCC MGU* - Bristol, Virginia
3. WELLMAN-GALUSHA - Minneapolis, Minnesota
4. GEGAS - Schenectady, New York
5. GFETC - Grand Forks, North Dakota
6. RUHR 100 - Dorsten, West Germany
7. KGN - Hueckelhoven, West Germany

LABORATORY

1. Washington University - St. Louis, Missouri
2. Pennsylvania State University - University Park, Pennsylvania
3. METC-SHRODR* - Morgantown, West Virginia
4. UCC* - Bristol, Virginia
5. LLNL* - Livermore, California
6. BNL* - Upton, New York

*Mild gasification

The collection of fixed-bed gasifier design and test data has been initiated. Design test data have been obtained for some of the fixed-bed gasifiers shown in Table IV.B-1. Particular attention has been paid to mild gasification data reported at the recent METC Ninth Annual Gasification and Gas Stream Cleanup Systems Contractors Review Meeting. Detailed profile data of particle temperature, gas temperature, pressure, gas composition, and particle composition in the reactor bed are needed. Unfortunately, only limited detailed data exist, at least in the open literature. There are no published data available for separate gas and solids temperatures and only one set of data for gas composition in the bed. Effluent gas compositions and temperatures, as well as available temperature and pressure profile data, will be used as a basis for model evaluation.

The collection of fixed-bed gasifier design and test data will continue. In order to obtain all the data potentially available for testing and validation of the advanced fixed-bed code, a questionnaire has been prepared. This questionnaire, a copy of which has been included in Appendix C, will be sent to a number of organizations and individuals. The scope and format of the fixed-bed test data have been defined and are presented in Table IV.B-2. A copy of Table IV.B-2 will be included with each questionnaire.

Plans

The collection of fixed-bed gasifier design and test data will continue. The fixed-bed gasification data questionnaire will be mailed. Two fixed-bed gasifiers of interest to METC will be selected for simulation. Data for validation of these two test cases will be obtained, if not already available, and initial testing and validation of the advanced fixed-bed code developed in Subtask 3.b will be performed.

TABLE IV.B-2

SPECIFICATIONS FOR FIXED/MOVING-BED TEST DATA FOR MODEL EVALUATION

Facility and Operational Procedure

- Gasification System
- Reactor Design with Main Dimensions (refractory or water walls, etc.)
- Design and Operation of Inlets and Outlets
- Design and Operation of Coal Distributer, Stirrer and Ash Grate
- Cooling System
- Control System (flow control, pressure control, etc.)
- Fluxing System for Slagging Ash Gasifiers
- Others

Measurement System and Test Procedure

- Instruments
- Sampling Location, Method and Frequency
- Uncertainty in Measurements
- Test Procedure
- Others

Test Results: Inputs

- Coal
  - Feed Rate and Temperature
  - Type (mine, seam, rank)
  - Bulk and Material Density, Size Distribution
  - Proximate and Ultimate Analysis, Heating Value, Free Swelling Index
  - Ash Mineral Analysis, Silica Ratio, Base/Acid Ratio
  - Ash Fusion Temperature
- Oxygen/Air
  - Flow Rate, Pressure, Temperature Composition
- Steam
  - Flow Rate, Pressure, Temperature
- Cooling Water
  - Flow Rate, Pressure, Temperature

Test Results: Outputs

- Gas
  - Flow Rate, Pressure, Temperature, Composition
    Major Species (H_2, CO, CO_2)
    Hydrocarbons (CH_4, C_2H_4, others)
    Nitrogen Species (N_2, NH_3, others)
    Sulphur Species (H_2S, COS, others)
    Others (O_2, others)
    Condensibles (tar, oil, water)
    Particulates
  - Material Density, Molecular Weight, and Heating Value (with and without condensibles and particulates)

TABLE III.B-2 (continued)

- Tar/Oil/Water
  - Flow Rate, Pressure, Temperature, Composition, Heating Value
- Recycle Tar
  - Flow Rate, Pressure, Temperature, Composition, Heating Value
- Particulates
  - Flow Rate, Size Distribution, Composition, Heating Value
- Ash/Slag
  - Flow Rate, Bulk and Material Density, Size Distribution, Temperature, Composition
- Cooling Water
  - Flow Rate, Pressure, Temperature
- Heat Loss

Test Results: Material and Energy Balances

- Material and energy balances by main input and output streams, and material balance by elements. Errors in closures.

Test Results: Axial and Radial Profiles

- Solids/Gas Fractions
- Solids/Gas Bulk and Material Densities, and Composition
- Solids/Gas Velocities
- Solids/Gas Pressures/Stresses
- Solids/Gas Temperatures

Test Results: Transients

- Same as above for steady state tests

Test Results: Others

- Reactor Wall Temperatures
- Coal Bed Height
- Ash Zone Thickness
- Pressure Drops (overall bed, coal bed zone, ash zone)
- Stirrer and Grate Speed and Torque
- Weather Data (temperature, humidity, pressure, precipitation)
- Coal, Char, and Ash/Slag Flow Properties (internal, wall, and effective friction angles, minimum bulk density, compressibility factor, unconfined yield strength, permeability, fragmentation, agglomeration, separation, elutriation, others)
- Coal, Char, and Ash/Slag Bed Zones Heat and Mass Transfer Properties (axial and radial diffusivities, axial and radial conductivities, bed-to-wall heat transfer coefficients, others)
- Coal and Char Reaction Rates (drying, devolatilization, gasification, combustion)
- Others

Comments

1. Please include units with all quantities.
2. Please indicate if specific data are not available.

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