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Biofuels and Biomass

Environmental and Carbon Dioxide Issues

Catalysis and Kinetics

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Accelerating Technology Development through Integrated Computation and Experimentation

This special section of *Energy & Fuels* comprises a selection of papers presented at the topical conference "Accelerating Technology Development through Integrated Computation and Experimentation", sponsored and organized by the United States Department of Energy's National Energy Technology Laboratory (NETL) as part of the 2012 American Institute of Chemical Engineers (AIChE) Annual Meeting held in Pittsburgh, PA, Oct 28–Nov 2, 2012. That topical conference focused on the latest research and development efforts in five main areas related to fossil energy, with each area focusing on the utilization of both experimental and computational approaches: (1) gas separations (membranes, sorbents, and solvents for CO_2, H_2, and O_2 production), (2) CO_2 utilization (enhanced oil recovery, chemical production, mineralization, etc.), (3) carbon sequestration (flow in natural systems), (4) advanced power cycles (oxy-combustion, chemical looping, gasification, etc.), and (5) fuel processing (H_2 production for fuel cells).

More than 100 papers reporting research, along with several plenary and keynote papers, were presented in the topical conference, which provided a forum for researchers in the area of fossil energy to interact, exchange ideas, discuss current developments, and develop collaborations. Because of the high quality of the papers presented and the importance of the topic, it was decided to produce a dedicated section of *Energy & Fuels* to bring together a select set of papers authored by the scientists and engineers who are active in this important area. This special section highlights the latest research and development efforts and draws on the talents and expertise of researchers who are addressing key issues related to energy. In the diverse but related chapters of this dedicated section, readers will find papers covering basic and applied research, systems analysis, modeling and simulation, and studies combining these disciplines. The section should prove informative as well as thought provoking to interested parties wishing to achieve a better understanding of fossil-energy-related research and development aspects.

This section addresses several aspects of carbon capture and storage (CCS), a topic of increasing interest, because CCS holds the potential to mitigate the buildup of greenhouse gases (GHGs), particularly CO_2, in the atmosphere. The papers in this section cover the entire gamut of CCS activities, including carbon capture, transport, and injection into geologic formations for permanent storage. Alternatively, the captured CO_2 can be directed to beneficial uses, such as conversion to polymers. The first step in CCS is capture, and a variety of the papers deal with this aspect. Systems evaluated include membranes, solvents, and sorbents.

An important element in reducing GHG emissions is the deployment of power systems that, because of their advanced designs, produce a concentrated CO_2 stream without extra process costs. Advanced systems being evaluated include integrated gasification combined cycle (IGCC), use of nearly pure oxygen as the oxidizing agent (oxy-fuel combustion), and chemical looping.

Disposal of CO_2 in geologic formations, such as depleted oil and gas reservoirs, unmineable coal seams, and saline formations, holds great promise for reducing GHG emissions to the atmosphere. Much remains to be done to increase our understanding of the behavior of CO_2 in these formations. This will require advanced simulation of fluid flow in porous media, i.e., modeling the behavior of CO_2 injected into geologic formations, including interactions with formation fluids and rocks and migration of the CO_2 plume in porous media.

Fuel cells offer cleaner, efficient, and environmentally friendly energy production compared to combustion-based reciprocating engine processes for a wide range of applications, including transportation and stationary, military, and distributed power. However, the need for a stable and contaminant-free supply of H_2 or H_2-rich synthesis gas is critical for long-term operation of a fuel cell system. Dependent upon the specific application for the fuel cell, a variety of hydrocarbon-based conventional fuels, such as natural gas, liquefied petroleum gas, ethanol, gasoline, jet fuels, kerosene, diesel, and biodiesel, can be converted in a fuel processor to generate H_2 or H_2-rich syngas. High-temperature fuel cells, such as the solid oxide fuel cell, can use CO in the feed along with H_2 and, therefore, are able to use the H_2-rich synthesis gas without any downstream processing (i.e., CO removal). Papers included in the area of fuel processing for hydrogen production provide critical discussion on several aspects of fuel processing: catalyst development, reactor design, system analysis, non-conventional fuel processors such as plasma, membrane, and microchannel, desulfurization for fuel cleanup, chemical looping reformation, and the water–gas shift reaction.

Tying much of this effort together are system analyses that evaluate and compare the economics and feasibility of developing CCS technologies. Various methodologies are used to evaluate the cost and performance of carbon capture, utilization, and storage technologies and to determine how system analyses might be standardized to permit more meaningful comparisons.

The most significant conclusion drawn by the editors from an analysis of the cumulative effort represented by the papers in this section is that meeting the challenge of CCS implementation will require extraordinary information input from many technical disciplines. The editors and authors have enjoyed putting this section together and hope you find it a valuable asset in increasing your knowledge and understanding of CCS technology.

We thank all participants, presenters, and session chairs/co-chairs who contributed to the success of the topical conference.

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