
Theoretical Modeling of Coal and Gas Fired Turbulent Combustion and Gasification Processes This book addresses the science and technology of the gasification process and the production of electricity, synthetic fuels and other useful chemicals. Pursuing a holistic approach, it covers the fundamentals of gasification and its various applications. In addition to discussing recent advances and outlining future directions, it covers advanced topics such as underground coal gasification and chemical looping combustion, and describes the state-of-the-art experimental techniques, modeling and numerical simulations, environmentally friendly approaches, and technological challenges involved. Written in an easy-to-understand format with a comprehensive glossary and bibliography, the book offers an ideal reference guide to coal and biomass gasification for beginners, engineers and researchers involved in designing or operating gasification plants.
Measurement and Modeling of Advanced Coal Conversion Processes Provides a comprehensive review on the brand-new development of several multiphase reactor techniques applied in energy-related processes Explains the fundamentals of multiphase reactors as well as the sophisticated applications Helps the reader to understand the key problems and solutions of clean coal conversion techniques Details the emerging processes for novel refining technology, clean coal conversion techniques, low-cost hydrogen productions and CO2 capture and storage Introduces current energy-related processes and links the basic principles of emerging processes to the features of multiphase reactors providing an overview of energy conversion in combination with multiphase reactor engineering Includes case studies of novel reactors to illustrate the special features of these reactors

Dynamic Modeling and Simulation of a Fluidized Bed Coal Gasification Process The primary objective of this study is to conduct numerical simulation of coal fluidization and gasification in fluidized bed gasifiers. Simulations involve Eulerian-Eulerian multi-phase flow model which is carried out using the Multiphase Flow with Interphase eXchanges (MFiX) computational flow dynamic code. An investigation of coal fluidization is carried out and the influence of numerical diffusion on accuracy of fluidized bed simulations is studied. This is due to the importance of accurate prediction of bubble dynamics and gas-solid mixing in bubbling fluidized beds. The fluidization process is simulated using various numerical schemes, including First Order Upwind (FOU) as well as higher order Total Variation Diminishing (TVD) schemes. Simulations are conducted using wide range of grid resolution and the effect of mesh resolution on the results is studied. It is shown that using higher order discretization schemes is essential to capture correct shape of bubbles, bed height and particle dynamics in the bed. Comparison is also made of computational performance of all numerical schemes considered. The TVD schemes are shown to yield quite different computation times caused by parallelization efficiency on distributed memory platforms. In the gasification simulations, the chemical reaction effects are taken into account using a time-splitting scheme in which the corresponding source terms are directly integrated in a separate step via a stiff ordinary differential equation solver. Simulations are carried out of counterflow and crossflow gasifiers. In the counterflow configuration, bituminous coal is fed into the reactor from the top by gravity and steam serves as the gasifying media which enters from the bottom. Simulation results are compared with the experimental data. Gasification occurs following devolatilization and cracking processes as incoming coal particles heated rapidly to the gasification temperature. Subsequently, gasification process is carried out in an isothermal fashion. As a result, no energy balance is considered in the simulations. Two four-step global mechanisms are used to describe the char gasification and water-gas shift reactions. Comparison is made of the results obtained using these two kinetic models. In the crossflow reactor, sub-bituminous coal enters the gasifier from the side while an upward stream of nitrogen from the bottom is used to fluidize the bed. The devolatilization and gasification processes are described by an eight-step reaction mechanism consisting of three reaction steps to model the devolatilization and cracking processes, as incoming coal particles heated to the gasification temperature; and five reaction steps to represent the char gasification, CO methanation and water-gas shift reactions. In these simulations, energy equation is solved to find the temperature distribution within the reactor. To assess the performance of the time-splitting method, the chemistry effects are also incorporated using the non-splitting method originally implemented in MFiX. It is shown that the splitting scheme, introduced in this study, results in reduction in computation time. In both gasifiers, simulations are shown to reasonably capture the transient behavior of the reactor. The gasification products
predicted by the simulations show favorable agreement with the experimental data.

A Novel Membrane Reactor for Direct Hydrogen Production From Coal

Dynamic Simulation of Coal-based Combined Cycle Plants for Development of Process Control Guidelines Engineering simulations of coal gasifiers are typically performed using computational fluid dynamics (CFD) software, where a 3-D representation of the gasifier equipment is used to model the fluid flow in the gasifier and source terms from the coal gasification process are captured using discrete-phase model source terms. Simulations using this approach can be very time consuming, making it difficult to imbed such models into overall system simulations for plant design and optimization. For such system-level designs, process flowsheet software is typically used, such as Aspen Plus® [1], where each component where each component is modeled using a reduced-order model. For advanced power-generation systems, such as integrated gasifier/gas-turbine combined-cycle systems (IGCC), the critical components determining overall process efficiency and emissions are usually the gasifier and combustor. Providing more accurate and more computationally efficient reduced-order models for these components, then, enables much more effective plant-level design optimization and design for control. Based on the CHEMKIN-PRO and ENERGICO software, we have developed an automated methodology for generating an advanced form of reduced-order model for gasifiers and combustors. The reduced-order model offers representation of key unit operations in flowsheet simulations, while allowing simulation that is fast enough to be used in iterative flowsheet calculations. Using high-fidelity fluid dynamics models as input, Reaction Design's ENERGICO® [2] software can automatically extract equivalent reactor networks (ERNs) from a CFD solution. For the advanced reduced-order concept, we introduce into the ERN a much more detailed kinetics model than can be included practically in the CFD simulation. The state-of-the-art chemistry solver technology within CHEMKIN-PRO allows that to be accomplished while still maintaining a very fast model turn-around time. In this way, the ERN becomes the basis for high-fidelity kinetics simulation, while maintaining the spatial information derived from the geometrically faithful CFD model. The reduced-order models are generated in such a way that they can be easily imported into a process flowsheet simulator, using the CAPE-OPEN architecture for unit operations. The ENERGICO/CHEMKIN-PRO software produces an ERN-definition file that is read by a dynamically linked library (DLL) that can be easily linked to any CAPE-OPEN compliant software. The plug-in unitoperation module has been successfully demonstrated for complex ERNs of coal gasifiers, using both Aspen Plus and COFE process flowsheet simulators through this published CAPE-OPEN interface.

A COMPUTATIONAL WORKBENCH ENVIRONMENT FOR VIRTUAL POWER PLANT SIMULATION The overall objective of this program is the development of predictive capability for the design, scale up, simulation, control and feedstock evaluation in advanced coal conversion devices. This technology is important to reduce the technical and economic risks inherent in utilizing coal, a feedstock whose variable and often unexpected behavior presents a significant challenge. This program will merge significant advances made at Advanced Fuel Research, Inc. (AFR) in measuring and quantitatively describing the mechanisms in coal conversion behavior, with technology being developed at Brigham Young University (BYU) in comprehensive computer codes for mechanistic modeling of entrained-bed gasification. Additional capabilities in predicting pollutant formation will be implemented and the technology will be expanded to fixed-bed reactors. The foundation to describe coal-specified conversion behavior is
ARF's Functional Group (FG) and Devolatilization, Vaporization, and Crosslinking (DVC) models, developed under previous and ongoing METC sponsored programs. These models have demonstrated the capability to describe the time-dependent evolution of individual gas species, and the amount and characteristics of tar and char. The combined FG-DVC model will be integrated with BYU’s comprehensive two-dimensional reactor model, PCGC-2, which is currently the most widely used reactor simulation for combustion or gasification. The program includes: (1) validation of the submodels by comparison with laboratory data obtained in this program, (2) extensive validation of the modified comprehensive code by comparison of predicted results with data from bench-scale and process scale investigations of gasification, mild gasification and combustion of coal or coal-derived products in heat engines, and (3) development of well documented user-friendly software applicable to a workstation environment.

Multiphase Reactor Engineering for Clean and Low-Carbon Energy Applications

This paper presents recent work from an ongoing project at Lawrence Livermore National Laboratory (LLNL) to develop a set of predictive tools for cavity/combustion-zone growth and to gain quantitative understanding of the processes and conditions (natural and engineered) affecting underground coal gasification (UCG). We discuss the application of coupled thermal-hydrologic simulation capabilities required for predicting UCG cavity growth, as well as for predicting potential environmental consequences of UCG operations.

Simulation of UCG cavity evolution involves coupled thermal-hydrological-chemical-mechanical (THCM) processes in the host coal and adjoining rock mass (cap and bedrock). To represent these processes, the NUFT (Nonisothermal Unsaturated-saturated Flow and Transport) code is being customized to address the influence of coal combustion on the heating of the host coal and adjoining rock mass, and the resulting thermal-hydrological response in the host coal/rock. As described in a companion paper (Morris et al. 2009), the ability to model the influence of mechanical processes (spallation and cavity collapse) on UCG cavity evolution is being developed at LLNL with the use of the LDEC (Livermore Distinct Element Code) code. A methodology is also being developed (Morris et al. 2009) to interface the results of the NUFT and LDEC codes to simulate the interaction of mechanical and thermal-hydrological behavior in the host coal/rock, which influences UCG cavity growth. Conditions in the UCG cavity and combustion zone are strongly influenced by water influx, which is controlled by permeability of the host coal/rock and the difference between hydrostatic and cavity pressure. In this paper, we focus on thermal-hydrological processes, examining the relationship between combustion-driven heat generation, convective and conductive heat flow, and water influx, and examine how the thermal and hydrologic properties of the host coal/rock influence those relationships. Specifically, we conducted a parameter sensitivity analysis of the influence of thermal and hydrological properties of the host coal, caprock, and bedrock on cavity temperature and steam production.

Simulation and Economic Evaluation of Coal Gasification with SETS Reforming Process for Power Production

Capture of CO2 from Pre-combustion Gas by Adsorption Processes at High Temperatures

The ongoing discussion about reaching the “peak-oil point” (maximal delivery rate with conventional methods) emphasizes a fundamental change of the frame conditions of oil-based basic products. The alternative with the largest potential is the use of coal. Coal gasification is the production of coal gas (a mixture of mainly hydrogen and carbon monoxide) from coal adding agents like steam/water and oxygen, which can be used in a number of industrial processes (e.g. hydroformulation and Fischer-Tropsch process).
Many different kinds of coal do naturally occur, and due to shrinking natural resources, there has been a substantial gain of interest in poor, ash-rich coal. Beside the quality of coal, there is a number of other parameters influencing the efficiency of coal gasification, such as temperature, pressure, and reactor type. Although several books dealing with the subject of gasification have recently been published, few are strictly focussed on coal as feedstock. This monograph provides the reader with the necessary chemical background on coal gasification. Several types of coal (baseline coal and ash-rich coal) are compared systematically, pointing out the technological efforts achieved so far to overcome this challenge. Using a new, innovative order scheme to evaluate the gasification process at a glance (the ternary diagram), the complex network of chemistry, engineering, and economic needs can be overviewed in a highly efficient way. This book is a must-have for Chemical and Process Engineers, Engineering Students, as well as Scientists in the Chemical Industry.

Characterization of Indiana Coals for Potential Underground Coal Gasification, Including Subsidence Risk and Hydrology

Indirect Coal Gasification Using Aspen-Plus® Model Low Btu gasification/combined cycle power generation (LBG/CCPG) plants and the use of dynamic simulation for developing process control guidelines are described. The formulation of mathematical relationships describing the behavior of various processes within an LBG/CCPG plant (model development) and their solution (simulation) are discussed. A simplified fluidized-bed gasifier model is used as an example. Use of the results of such simulation for developing process control system guidelines is also discussed.

Ett opartiskt ord i jernvägs-frågan Bridging the gap between the well-known technological description of gasification and the underlying theoretical understanding, this book covers the latest numerical and semi-empirical models describing interphase phenomena in high-temperature conversion processes. Consequently, it focuses on the description of gas-particle reaction systems by state-of-the-art computational models in an integrated, unified form. Special attention is paid to understanding and modeling the interaction between individual coal particles and a surrounding hot gas, including heterogeneous and homogeneous chemical reactions inside the particle on the particle interface and near the interface between the solid and gas phases. While serving the needs of engineers involved in industrial research, development and design in the field of gasification technologies, this book’s in-depth coverage makes it equally ideal for young and established researchers in the fields of thermal sciences and chemical engineering with a focus on heterogeneous and homogeneous reactions.

Monthly Catalogue, United States Public Documents

Coal and Biomass Gasification

Mathematical Modeling of Coal Gasification Processes: Countercurrent Reactors and Transient Heating of a Single Briquette This book addresses the science and technology of the gasification process and the production of electricity, synthetic fuels and other useful chemicals. Pursuing a holistic approach, it covers the fundamentals of gasification and its various applications. In addition to discussing recent advances and outlining future directions, it covers advanced topics such as underground coal gasification and chemical looping combustion, and describes the state-of-the-art experimental techniques, modeling and numerical simulations, environmentally friendly approaches, and technological challenges involved. Written in an easy-to-
understand format with a comprehensive glossary and bibliography, the book offers an ideal reference guide to coal and biomass gasification for beginners, engineers and researchers involved in designing or operating gasification plants.

Coal and Biomass Gasification In view of limited liquid fuels, in terms of crude oil reserves and to reduce the use of constantly and rapidly diminishing natural gas reserves, researchers are attracted towards Fisher Tropsch reaction. Aspen Plus(r) has become reliable, acquainted and recognized processes modeling software, extensively in practice for coal and biomass gasification processes. It contains different physical property packages that are useful for solid handling. Aspen Plus(r) model has been proposed to develop a better understanding of the process for geometric analysis of gasifier. This simulation presents an alternate technology for conventional coal gasification to improve the performance of process by varying geometry of gasifier. The Purpose of this study, is entirely focus on the production of synthesis gas from coal, through a process of indirect gasification and using only steam as the gasifying medium. The book serves as reference material for students, engineers and scientists working in the area of syngas production and coal gasification.

Industrial Coal Gasification Technologies Covering Baseline and High-Ash Coal Gasification is a very efficient method of producing clean synthetic gas (syngas) which can be used as fuel for electric generation or chemical building block for petrochemical industries. This study performs detailed simulations of coal gasification process inside a generic two-stage entrained-flow gasifier to produce syngas carbon monoxide and hydrogen. The simulations are conducted using the commercial Computational Fluid Dynamics (CFD) solver FLUENT. The 3-D Navier-Stokes equations and seven species transport equations are solved with eddy-breakup combustion model. Simulations are conducted to investigate the effects of coal mixture (slurry or dry), oxidant (oxygen-blown or air-blown), wall cooling, coal distribution between the two stages, and the feedstock injection angles on the performance of the gasifier in producing CO and H2. The result indicates that coal-slurry feed is preferred over coal-powder feed to produce hydrogen. On the other hand, coal-powder feed is preferred over coal-slurry feed to produce carbon monoxide. The air-blown operation yields poor fuel conversion efficiency and lowest syngas heating value. The two-stage design gives the flexibility to adjust parameters to achieve desired performance. The horizontal injection design gives better performance compared to upward and downward injection designs.

Solid Fuels Combustion and Gasification

Computational Modeling of Underground Coal Gasification

Numerical Simulation of Coal Fluidization and Gasification in Fluidized Beds February issue includes Appendix entitled Directory of United States Government periodicals and subscription publications; September issue includes List of depository libraries; June and December issues include semiannual index.

Thermal-Hydrological Sensitivity Analysis of Underground Coal Gasification Gas Technology Institute has developed a novel concept of a membrane reactor closely coupled with a coal gasifier for direct extraction of hydrogen from coal-derived syngas. The objective of this project is to determine the technical and economic feasibility of this concept by screening, testing and identifying potential candidate membranes under the coal gasification conditions. The best performing membranes were selected for preliminary
reactor design and cost estimate. The overall economics of hydrogen production from this new process was assessed and compared with conventional hydrogen production technologies from coal. Several proton-conducting perovskite membranes based on the formulations of BCN (BaCe{sub 0.8}Nd{sub 0.2}O{sub 3-x}), BCY (BaCe{sub 0.8}Y{sub 0.2}O{sub 3-x}), SCE (Eu-doped SrCeO{sub 3}), and SCTm (SrCe{sub 0.95}Tm{sub 0.05}O{sub 3}) were successfully tested in a new permeation unit at temperatures between 800 and 1040 C and pressures from 1 to 12 bars. The experimental data confirm that the hydrogen flux increases with increasing hydrogen partial pressure at the feed side. The highest hydrogen flux measured was 1.0 cc/min/cm{sup 2} (STP) for the SCTm membrane at 3 bars and 1040 C. The chemical stability of the perovskite membranes with respect to CO{sub 2} and H{sub 2}S can be improved by doping with Zr, as demonstrated from the TGA (Thermal Gravimetric Analysis) tests in this project. A conceptual design, using the measured hydrogen flux data and a modeling approach, for a 1000 tons-per-day (TPD) coal gasifier shows that a membrane module can be configured within a fluidized bed gasifier without a substantial increase of the gasifier dimensions. Flowsheet simulations show that the coal to hydrogen process employing the proposed membrane reactor concept can increase the hydrogen production efficiency by more than 50% compared to the conventional process. Preliminary economic analysis also shows a 30% cost reduction for the proposed membrane reactor process, assuming membrane materials meeting DOE’s flux and cost target. Although this study shows that a membrane module can be configured within a fluidized bed gasifier, placing the membrane module outside the gasifier in a closely coupled way in terms of temperature and pressure can still offer the same performance advantage. This could also avoid the complicated fluid dynamics and heat transfer issues when the membrane module is installed inside the gasifier. Future work should be focused on improving the permeability and stability for the proton-conducting membranes, testing the membranes with real syngas from a gasifier and scaling up the membrane size.

A Hybrid Computer System for the Simulation of a Coal Gasification Process

Coal Combustion and Gasification

Computational Modeling of Underground Coal Gasification

Coupled Geomechanical Simulations of UCG Cavity Evolution

Simulation and Control of the Coal Gasification Combined Cycle Power Plant

This paper presents recent work from an ongoing project to develop predictive tools for cavity/combustion-zone growth and to gain quantitative understanding of the processes and conditions (both natural and engineered) affecting underground coal gasification (UCG). In this paper we will focus upon the development of coupled geomechanical capabilities for simulating the evolution of the UCG cavity using discrete element methodologies. The Discrete Element Method (DEM) has unique advantages for facilitating the prediction of the mechanical response of fractured rock masses, such as cleated coal seams. In contrast with continuum approaches, the interfaces within the coal can be explicitly included and combinations of both elastic and plastic anisotropic response are simulated directly. Additionally, the DEM facilitates estimation of changes in hydraulic properties by providing estimates of changes in cleat aperture. Simulation of cavity evolution involves a range of coupled processes and the mechanical response of the host coal and adjoining rockmass plays a role in every stage of UCG operations. For example, cavity collapse during the burn has significant effect upon the rate of the burn itself. In the vicinity of the cavity, collapse and fracturing may result in enhanced hydraulic conductivity of the rock matrix in the coal and caprock above the burn.
chamber. Even far from the cavity, stresses due to subsidence may be sufficient to induce new fractures linking previously isolated aquifers. These mechanical processes are key in understanding the risk of unacceptable subsidence and the potential for groundwater contamination. These mechanical processes are inherently non-linear, involving significant inelastic response, especially in the region closest to the cavity. In addition, the response of the rock mass involves both continuum and discrete mechanical behavior. We have recently coupled the LDEC (Livermore Distinct Element Code) and NUFT (Non-isothermal Unsaturated Flow and Transport) codes to investigate the interaction between combustion, water influx and mechanical response. The modifications to NUFT are described in detail in a companion paper. This paper considers the extension of the LDEC code and the application of the coupled tool to the simulation of cavity growth and collapse. The distinct element technology incorporated into LDEC is ideally suited to simulation of the progressive failure of the cleated coal mass by permitting the simulation of individual planes of weakness. We will present details of the coupling approach and then demonstrate the capability through simulation of several test cases.

Gasification Studies Task 4 Topical Report As an increasing number of professionals and graduate students enter the field of solid-based power generation, they all require an command of process and equipment, as well as the theory behind it all. However, their informational needs and understanding differ based on their experience and the task at hand. Solid Fuels Combustion and Gasification: Modeling, Simulation, and Equipment Operations, Second Edition explores evolving solid fuel combustion and gasification techniques that are leading to much lower sulfur and nitrogen oxide emissions. It also shows how to increase the efficiency of processes dealing with materials such as coal, biomass, solid residues, etc. Many of the successes of these methods are the result of process optimization resulting from mathematical modeling and simulation. This book introduces and explores these techniques, taking a moderate approach that is neither too narrow nor too basic, making it useful to graduate students, engineers, and professionals. It illustrates the modeling and constructive and operational aspects of equipment used in combustion and gasification of solid fuels. It was written based on the idea that developing models and computer simulators is the optimal method to acquire real and testable understanding of a subject in the area of processing. Model complexity is extended only as far as needed to achieve a reasonable representation of the equipment described in the book, and the author provides specific and carefully selected case studies that: Cover many industrial processes involving combustion or gasification of solid fuels; Provide easy-to-follow examples on how to set simplifying assumptions regarding the operation of real industrial equipment; Enable relatively quick introduction of fundamental equations without the need for unnecessarily complex treatments; The main strategy of the book is to teach by example, and the basic methods illustrated here can be used for modeling a wide range of processes and equipment commonly found in industry. It is a carefully constructed volume which presents essential concepts that minimize the need for other texts, and it can also be used as an introduction to more complex models.

Hydrogen-oriented Underground Coal Gasification for Europe (HUGE) This study is a compilation of the available data on coal properties, hydrology, and lithologic characteristics in nine areas selected as the most promising for underground coal gasification in southwest Indiana. This report includes tables of coal properties important to underground coal gasification and summaries of individual parameters for the Springfield Coal and the Seelyville Coal, as well as maps of the distributions of selected coal properties. This
study indicates that, while much information exists about some of the properties of coal (for example, heating value or ash content), more data are needed on the swelling characteristics of coal, the presence and thickness of clastic partings, and the coal’s geomechanical properties to adequately evaluate the potential for underground coal gasification. Newly obtained analyses of geomechanical properties provide valuable data, but more detailed observations and interpretations of the mechanical behavior of the rock column are necessary to better serve numerical simulations of the gasification process.

Simulation of the CO2 - A cceptor Process for Coal Gasification The book deals with development of comprehensive computational models for simulating underground coal gasification (UCG). It starts with an introduction to the UCG process and process modelling inputs in the form of reaction kinetics, flow patterns, spalling rate, and transport coefficient that are elaborated with methods to generate the same are described with illustrations. All the known process models are reviewed, and relative merits and limitations of the modeling approaches are highlighted and compared. The book describes all the necessary steps required to determine the techno-economic feasibility of UCG process for a given coal reserve, through modeling and simulation.

Computer-lösung gewöhnlicher Differentialgleichungen

Process analysis and simulation of underground coal gasification

Modeling Underground Coal Gasification Using the Tough2 Reservoir Simulator The capture and storage of CO2 from coal have received considerable attention due to a growing demand for green use of carbon-based resources concerning its global warming effect. There are usually two ways of capturing CO2 from coal-related gases according to locations of capture blocks, post-combustion and pre-combustion. The conventional approach for pre-combustion CO2 capture is liquid absorption. However, one potential limitation of this process is that the liquid scrubbing must occur at relatively low temperatures (near ambient). By contrast, adsorbent based processes offer the potential of higher temperature capture eliminating the intermediate cooling and reheating steps. Therefore there is a motivation to develop high temperature adsorption processes. This project investigates the capture of CO2 by solid adsorbents from pre-combustion coal gasification syngas in an Integrated Gasification Combined Cycle (IGCC) process at high temperatures. The project covers materials development and process testing on both a real gasifier and a synthetic pre-combustion gas stream provided in our laboratory. Adsorbents screening was performed with real coal gasification syngas from a pilot coal gasifier. Breakthrough and regeneration experiments with hydrotalcite Mg 70, calcium chabazite, and zeolite 13X were performed on the custom-made gas separation apparatus at 120 °C and 200 °C. Zeolite 13X was found to be a potentially good adsorbent for CO2 separation provided T200 °C. Thereafter, different VPSA processes using zeolite 13X were designed to pursue a CO2 purity of 95% with synthetic syngas. The designed processes were then validated with real coal gasification gas. However, simulation results for the separation from full scale syngas showed that using zeolite 13X to reach a purity of > 95% would be very costly. High temperature adsorbents composed of MgO and K2CO3 were prepared and characterized by various means. These prepared adsorbents possessed high CO2 sorption capacity and cycling stability both under dry and wet conditions. An adsorption model was proposed for the prepared adsorbent and provided an adequate description of the adsorption and desorption experiments performed on a thermogravimetric analyser. The derived isotherm from the proposed model was also able to represent the experimental isothermal adsorption data well. Although the CO2 adsorption kinetics of these
adsorbents were higher than other reported high temperature adsorbents, they were still much slower than widely used physical adsorbents, which makes it currently not very efficient for pressure swing adsorption processes. In future work, efforts will be focused on increasing the adsorption and desorption kinetics by, for example making these adsorbents to nanoscale, possibly supported on porous substrates.

Simulation of Coal Gasification Process Inside a Two-stage Gasifier An analysis of various options of coal gasification technologies with different gasification media, process parameters and coal types, as well as mathematical and thermodynamic modelling of the planned trials, have been conducted. Moreover, a pseudo-homogeneous mathematical model for the adsorption of CO₂ on the CaO-rich minerals was developed. For the purpose of the experiments an ex situ reactor was constructed. The reactor was used for the simulation of real underground conditions in respect to both the coal seams and the surrounding rock layers. Large blocks of coal were prepared for the reactor by the industrial partner of the project. In total, six experiments were performed. The experiments demonstrated the possibility of coal gasification in hard coal block and lignite, and tested the methodology of the experiment. Tests with smaller coal blocks in a pressurised reactor were also performed. Moreover, tests on the migration of heavy metals to water during the gasification process, as well as tests of the behaviour of the strata, have been conducted. The concept of the underground georeactor at a process development unit scale was elaborated. The location of the georeactor was chosen and an analysis of the surrounding space was carried out. The process design, together with the technical design of the generator and the monitoring system, has been carried out. After all the necessary infrastructure had been built, an underground trial in the in situ reactor in the experimental mine was conducted. The trial lasted 16 days. The underground experiment enabled the identification of potential problems related to the operation of the UCG process. After the in situ trial, the impact of the UCG process on the natural environment was analysed, as well as the impact of the UCG process on life standards, and the implementation criteria for the selected UCG technological option were elaborated. The results of the project were presented during 17 international conferences, in 15 publications in journals and one patent application.

Gasification Processes The book deals with development of comprehensive computational models for simulating underground coal gasification (UCG). It starts with an introduction to the UCG process and process modelling inputs in the form of reaction kinetics, flow patterns, spalling rate, and transport coefficient that are elaborated with methods to generate the same are described with illustrations. All the known process models are reviewed, and relative merits and limitations of the modeling approaches are highlighted and compared. The book describes all the necessary steps required to determine the techno-economic feasibility of UCG process for a given coal reserve, through modeling and simulation.

Computer modeling of coal gasification reactors

Computer Simulation, Second-law Analysis and Economics of Coal Gasification Processes In this report is described the work effort to develop and demonstrate a software framework to support advanced process simulations to evaluate the performance of advanced power systems. Integrated into the framework are a broad range of models, analysis tools, and visualization methods that can be used for the plant evaluation. The framework provides a tightly integrated problem-solving environment, with plug-and-play.
functionality, and includes a hierarchy of models, ranging from fast running process models to detailed reacting CFD models. The framework places no inherent limitations on the type of physics that can be modeled, numerical techniques, or programming languages used to implement the equipment models, or the type or amount of data that can be exchanged between models. Tools are provided to analyze simulation results at multiple levels of detail, ranging from simple tabular outputs to advanced solution visualization methods. All models and tools communicate in a seamless manner. The framework can be coupled to other software frameworks that provide different modeling capabilities. Three software frameworks were developed during the course of the project. The first framework focused on simulating the performance of the DOE Low Emissions Boiler System Proof of Concept facility, an advanced pulverized-coal combustion-based power plant. The second framework targeted simulating the performance of an Integrated coal Gasification Combined Cycle - Fuel Cell Turbine (IGCC-FCT) plant configuration. The coal gasifier models included both CFD and process models for the commercially dominant systems. Interfacing models to the framework was performed using VES-Open, and tests were performed to demonstrate interfacing CAPE-Open compliant models to the framework. The IGCC-FCT framework was subsequently extended to support Virtual Engineering concepts in which plant configurations can be constructed and interrogated in a three-dimensional, user-centered, interactive, immersive environment. The Virtual Engineering Framework (VEF), in effect a prototype framework, was developed through close collaboration with NETL supported research teams from Iowa State University Virtual Reality Applications Center (ISU-VRAC) and Carnegie Mellon University (CMU). The VEF is open source, compatible across systems ranging from inexpensive desktop PCs to large-scale, immersive facilities and provides support for heterogeneous distributed computing of plant simulations. The ability to compute plant economics through an interface that coupled the CMU IECM tool to the VEF was demonstrated, and the ability to couple the VEF to Aspen Plus, a commercial flowsheet modeling tool, was demonstrated. Models were interfaced to the framework using VES-Open. Tests were performed for interfacing CAPE-Open-compliant models to the framework. Where available, the developed models and plant simulations have been benchmarked against data from the open literature. The VEF has been installed at NETL. The VEF provides simulation capabilities not available in commercial simulation tools. It provides DOE engineers, scientists, and decision makers with a flexible and extensible simulation system that can be used to reduce the time, technical risk, and cost to develop the next generation of advanced, coal-fired power systems that will have low emissions and high efficiency. Furthermore, the VEF provides a common simulation system that NETL can use to help manage Advanced Power Systems Research projects, including both combustion- and gasification-based technologies.

Package Equivalent Reactor Networks as Reduced Order Models for Use with CAPE-OPEN Compliant Simulation

Computer modeling of coal gasification reactors The use of coal is required to help satisfy the world's energy needs. Yet coal is a difficult fossil fuel to consume efficiently and cleanly. We believe that its clean and efficient use can be increased through improved technology based on a thorough understanding of fundamental physical and chemical processes that occur during consumption. The principal objective of this book is to provide a current summary of this technology. The past technology for describing and analyzing coal furnaces and combustors has relied largely on empirical inputs for the complex flow and chemical reactions that occur while more formally treating the heat-transfer effects. Growing concern over control of combustion-generated air pollutants revealed a lack of understanding of the relevant fundamental physical and chemical mechanisms. Recent technical advances in computer speed and storage
capacity, and in numerical prediction of recirculating turbulent flows, two-phase flows, and flows with chemical reaction have opened new opportunities for describing and modeling such complex combustion systems in greater detail. We believe that most of the requisite component models to permit a more fundamental description of coal combustion processes are available. At the same time there is worldwide interest in the use of coal, and progress in modeling of coal reaction processes has been steady.