

# Simulation Of Coal Gasification Process Using Aspen Plus

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In contrast to traditional combustion, gasification technologies offer the potential for converting coal and low or negative-value feedstocks, such as petroleum coke and various waste materials into usable energy sources or chemicals. With a growing number of companies operating and marketing systems based on gasification concepts worldwide, this b

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 Bridging the gap between theory and application, this reference demonstrates the operational mechanisms, modeling, and simulation of equipment for the combustion and gasification of solid fuels. Solid Fuels Combustion and Gasification: Modeling, Simulation, and Equipment Operation clearly illustrates procedures to improve and optimize the de

Underground Coal Gasification (UCG) is carried out in unmined coal seams, using wells drilled from the surface and converting coal into synthesis gas. The gas can be used for power generation and synthesis of automotive fuels, fertilizers and other products. UCG offers financial, social, and environmental benefits over conventional coal extraction and utilization methods and may play a critical role in ensuring energy security in the future. Underground Coal Gasification and Combustion provides an overview of underground coal gasification technology, its current status and future directions. Comprehensive in approach, the book covers history, science, technology, hydrogeology, rock mechanics, environmental performance, economics, regulatory and commercial aspects of UCG projects. The first book on the subject in forty years, it is unique in analysing more than a century of global UCG developments by experts from

Australia, Canada, Poland, Russia, Ukraine, United Kingdom, the USA and Uzbekistan. Provides researchers, engineers, industry, educators and regulators with an authoritative overview of science and practical applications of underground coal gasification technologies Offers insight into efficiency, environmental performance, costs, permitting issues and commercial aspects of UCG projects Written by scientists and practitioners of UCG technology sharing hands-on experience of step-by-step UCG implementation

Integrated Gasification Combined Cycle (IGCC) Technologies discusses this innovative power generation technology that combines modern coal gasification technology with both gas turbine and steam turbine power generation, an important emerging technology which has the potential to significantly improve the efficiencies and emissions of coal power plants. The advantages of this technology over conventional pulverized coal power plants include fuel flexibility, greater efficiencies, and very low pollutant emissions. The book reviews the current status and future developments of key technologies involved in IGCC plants and how they can be integrated to maximize efficiency and reduce the cost of electricity generation in a carbon-constrained world. The first part of this book introduces the principles of IGCC systems and the fuel types for use in IGCC systems. The second part covers syngas production within IGCC systems. The third part looks at syngas cleaning, the separation of CO<sub>2</sub> and hydrogen enrichment, with final sections describing the gas turbine combined cycle and

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presenting several case studies of existing IGCC plants. Provides an in-depth, multi-contributor overview of integrated gasification combined cycle technologies Reviews the current status and future developments of key technologies involved in IGCC plants Provides several case studies of existing IGCC plants around the world 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 CO<sub>2</sub> 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

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 CO<sub>2</sub> 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.

Biomass can be converted to energy, biofuels, and bioproducts via thermochemical

conversion processes, such as combustion, pyrolysis, and gasification. Combustion technology is most widely applied on an industrial scale. However, biomass gasification and pyrolysis processes are still in the research and development stage. The major products from these processes are syngas, bio-oil, and char (called also biochar for agronomic application). Among these products, biomass chars have received increasing attention for different applications, such as gasification, co-combustion, catalysts or adsorbents precursors, soil amendment, carbon fuel cells, and supercapacitors. This Special Issue provides an overview of biomass char production methods (pyrolysis, hydrothermal carbonization, etc.), characterization techniques (e.g., scanning electronic microscopy, X-ray fluorescence, nitrogen adsorption, Raman spectroscopy, nuclear magnetic resonance spectroscopy, X-ray photoelectron spectroscopy, and temperature programmed desorption and mass spectrometry), their properties, and their suitable recovery processes.

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.

The primary objective of this study is to conduct numerical simulation of coal fluidization and gasification in fluidized bed gasifiers. Simulations involve Eulerian-Eulerian multiphase 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.

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

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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.

Skyrocketing energy costs have spurred renewed interest in coal gasification. Currently available information on this subject needs to be updated, however, and focused on specific coals and end products. For example, carbon capture and sequestration, previously given little attention, now has a prominent role in coal conversion processes. This book approaches coal gasification and related technologies from a process engineering point of view, with topics chosen to aid the process engineer who is interested in a complete, coal-to-products system. It provides a perspective for engineers and scientists who analyze and improve components of coal conversion processes. The first topic describes the nature and availability of coal. Next, the fundamentals of gasification are described, followed by a description of gasification technologies and gas cleaning processes. The conversion of syngas to electricity, fuels and chemicals is then discussed. Finally, process economics are covered. Emphasis is given to the selection of gasification technology based on the type of coal fed to the gasifier and desired end product: E.g., lower temperature gasifiers produce substantial quantities of methane, which is undesirable in an ammonia synthesis feed. This book also reviews gasification kinetics which is informed by recent papers and process design studies by the US Department of Energy and other groups, and also largely

ignored by other gasification books. • Approaches coal gasification and related technologies from a process engineering point of view, providing a perspective for engineers and scientists who analyze and improve components of coal conversion processes • Describes the fundamentals of gasification, gasification technologies, and gas cleaning processes • Emphasizes the importance of the coal types fed to the gasifier and desired end products • Covers gasification kinetics, which was largely ignored by other gasification books Provides a perspective for engineers and scientists who analyze and improve components of the coal conversion processes Describes the fundamentals of gasification, gasification technologies, and gas cleaning processes Covers gasification kinetics, which was largely ignored by other gasification books Combining the knowledge involved in process engineering and process modeling, this is the first book to cover all modeling methods applicable to process intensification. Both the editors and authors are renowned experts from industry and academia in the various fields of process modeling and integrated chemical processes. Following an introduction to the topic, the book goes on to look at equipment and operational methods, monolithic catalysis, HEX, micro- and reverse flow reactors, catalytic and reactive distillation, the simulated-moving bed and vibration bubble column as well as ultrasound and ultrasonic reactors. A final chapter is devoted to processes under supercritical conditions. In its treatment of hot topics of multidisciplinary interest, this book is of great value to researchers and engineers alike.

### Simulation of Coal Gasification Process Inside a Two-stage Gasifier

This book is the outcome of contributions by many experts in the field from different disciplines, various backgrounds, and diverse expertise. This book provides information on biomass volume calculation methods and biomass valorization for energy production. The chapters presented in this book include original research and review articles. I hope the research presented in this book will help to advance the use of biomass for bioenergy production and valorization. The key features of the book are: Providing information on biomass volume estimation using direct, nondestructive and remote sensing methods Biomass valorization for energy using thermochemical (gasification and pyrolysis) and biochemical (fermentation) conversion processes.

Besides being one of the best Clean Coal Technologies, fluidized beds are also proving to be the most practical option for biomass conversion. Although the technology is well established, the field lacks a comprehensive guide to the design and operating principles of fluidized bed boilers and gasifiers. With more than 30 years of research and industrial experience, Prabir Basu answers this pressing need with *Combustion and Gasification in Fluidized Beds*. This book is a versatile resource that explains how fluidized bed equipment works and how to use the basic principles of thermodynamics and fluid mechanics in design while providing insight into planning new projects, troubleshooting existing equipment, and appreciating the capabilities and limitations of the process. From hydrodynamics to construction and maintenance, the author covers all of the essential information needed to understand, design, operate, and maintain a complete fluidized bed system. It is a must for clean coal technology as well as for biomass power generation. Beginning with a general introduction to fossil or

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biofuel conversion choices, the book surveys hydrodynamics, fundamentals of gasification, combustion of solid fuels, pollution aspects including climate change mitigation, heat transfer in fluidized beds, the design and operation of bubbling and circulating fluidized bed boilers, and various supporting components such as distributor grates, feeding systems, and gas-solid separators.

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

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

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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.

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.

A comprehensive and example oriented text for the study of chemical process design and simulation *Chemical Process Design and Simulation* is an accessible guide that offers information on the most important principles of chemical engineering design and includes illustrative examples of their application that uses simulation software. A comprehensive and practical resource, the text uses both Aspen Plus and Aspen Hysys simulation software. The author describes the basic methodologies for computer aided design and offers a description of the

basic steps of process simulation in Aspen Plus and Aspen Hysys. The text reviews the design and simulation of individual simple unit operations that includes a mathematical model of each unit operation such as reactors, separators, and heat exchangers. The author also explores the design of new plants and simulation of existing plants where conventional chemicals and material mixtures with measurable compositions are used. In addition, to aid in comprehension, solutions to examples of real problems are included. The final section covers plant design and simulation of processes using nonconventional components. This important resource: Includes information on the application of both the Aspen Plus and Aspen Hysys software that enables a comparison of the two software systems Combines the basic theoretical principles of chemical process and design with real-world examples Covers both processes with conventional organic chemicals and processes with more complex materials such as solids, oil blends, polymers and electrolytes Presents examples that are solved using a new version of Aspen software, ASPEN One 9 Written for students and academics in the field of process design, Chemical Process Design and Simulation is a practical and accessible guide to the chemical process design and simulation using proven software.

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 H<sub>2</sub>. 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.

Underground coal gasification (UCG) is an important technique for future coal utilization. It has the potential to be a clean technology and to tap un-mineable,

deep coal deposits across the world. Commercialization of UCG has been riddled with a variety of issues, including public perception and a lack of clear comprehension about underlying physicochemical phenomena. This book will bridge the gap in knowledge and highlight the modern findings related to the complex interactions in UCG. With a focus on the chemical reactions in UCG and treating the underground coal cavity as “nature’s own chemical reactor”, various mathematical modeling studies that serve to unravel some of the mysteries of this decades-old technique will be revealed.

Harness State-of-the-Art Computational Modeling Tools Computational Modeling of Pulverized Coal Fired Boilers successfully establishes the use of computational modeling as an effective means to simulate and enhance boiler performance. This text factors in how computational flow models can provide a framework for developing a greater understanding of the underlying processes in PC boilers. It also provides a detailed account of the methodology of computational modeling of pulverized coal boilers, as well as an apt approach to modeling complex processes occurring in PC boilers in a manageable way. Connects Modeling with Real-Life Applications Restricted to the combustion side of the boiler (the authors assume some prior background of reaction engineering and numerical techniques), the book describes the individual aspects of

combustion and heat recovery sections of PC boilers that can be used to further improve the design methodologies, optimize boiler performance, and solve practical boiler-related problems. The book provides guidelines on implementing the material in commercial CFD solvers, summarizes key points, and presents relevant case studies. It can also be used to model larger boilers based on conventional, super-critical, or ultra-super critical technologies as well as based on oxy-fuel technologies. Consisting of six chapters, this functional text: Provides a general introduction Explains the overall approach and methodology Explores kinetics of coal pyrolysis (devolatilization) and combustion and methods of its evaluation Presents computational flow modeling approach to simulate pulverized coal fired boiler Covers modeling aspects from formulation of model equations to simulation methodology Determines typical results obtained with computational flow models Discusses the phenomenological models or reactor network models Includes practical applications of computational modeling

Computational Modeling of Pulverized Coal Fired Boilers explores the potential of computational models for better engineering of pulverized coal boilers, providing an ideal resource for practicing engineers working in utility industries. It also benefits boiler design companies, industrial consultants, R & D laboratories, and engineering scientists/research students.

This book presents the current carbonaceous fuel conversion technologies based on chemical looping concepts in the context of traditional or conventional technologies. The key features of the chemical looping processes, their ability to generate a sequestration-ready CO<sub>2</sub> stream, are thoroughly discussed. Chapter 2 is devoted entirely to the performance of particles in chemical looping technology and covers the subjects of solid particle design, synthesis, properties, and reactive characteristics. The looping processes can be applied for combustion and/or gasification of carbon-based material such as coal, natural gas, petroleum coke, and biomass directly or indirectly for steam, syngas, hydrogen, chemicals, electricity, and liquid fuels production. Details of the energy conversion efficiency and the economics of these looping processes for combustion and gasification applications in contrast to those of the conventional processes are given in Chapters 3, 4, and 5. Finally, Chapter 6 presents additional chemical looping applications that are potentially beneficial, including those for H<sub>2</sub> storage and onboard H<sub>2</sub> production, CO<sub>2</sub> capture in combustion flue gas, power generation using fuel cell, steam-methane reforming, tar sand digestion, and chemicals and liquid fuel production. A CD is appended to this book that contains the chemical looping simulation files and the simulation results based on the ASPEN Plus software for such reactors as gasifier, reducer,

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oxidizer and combustor, and for such processes as conventional gasification processes, Syngas Chemical Looping Process, Calcium Looping Process, and Carbonation-Calcination Reaction (CCR) Process. Note: CD-ROM/DVD and other supplementary materials are not included as part of eBook file.

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