Simulation Of Methanol Production From Synthesis Gas

This monograph focuses on methanol and its utilization in transportation sector, namely in spark ignition (SI) engines. The contents focus on methanol production and presents a variety of production technologies from different feedstocks. The potential of methanol utilization in transportation in SI engines is discussed, its challenges, limitations, aspects related to its utilization and current global use of methanol are also presented. The book also contains chapters related to pollutant formation and exhaust emissions from methanol fuelled SI engines, one chapter is focused specifically on formaldehyde emissions, which possesses one of the greatest challenges of methanol use in IC engines. Readers will learn about the production aspects of methanol, its potential as a sustainable fuel, its utilization in SI engine and the effect of methanol and its utilization techniques on engine performance, combustion, exhaust emissions, efficiency and other important parameters. This volume will be a useful guide for professionals, post-graduate students involved in alternative fuels, spark ignition engines, and environmental research.

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.

Provides a holistic approach to multiphase catalytic reactors from their modeling and design to their applications in industrial manufacturing of chemicals Covers theoretical aspects and examples of fixed-bed, fluidized-bed, trickle-bed, slurry, monolith and microchannel reactors Includes chapters covering experimental techniques and practical guidelines for lab-scale testing of multiphase reactors Includes mathematical content focused on design equations and empirical relationships characterizing different multiphase reactor types together with an assortment of computational tools Involves detailed coverage of multiphase reactor applications such as Fischer-Tropsch synthesis, fuel processing for fuel cells, hydrotreating of oil fractions and biofuels processing

My work was the fist of its kind in our University.I studied the kinetics & thermodynamics of the RD process to produce the MTBE simultaneously.Methyl tertiary butyl ether (MTBE) is primarily used in gasoline blending as an octane enhancer to improve hydrocarbon combustion efficiency. Of all the oxygenates, MTBE is attractive for a variety of technical reasons. It has a low vapor pressure. It can be blended with other fuels without phase separation. It has the

desirable octane characteristics.MTBE is produced via direct addition of methanol to isobutylene using sulphonated ion exchange resin as catalysts. There are two ways to produce MTBE, one is the conventional process which is mainly a reactor and separate distillation column with conversion range 87-92%. Another method for the production of MTBE is newly established and date back to the way in 1980 as the scientist Smith recorded the first patent for the production of MTBE through this method, this method called Reactive Distillation Process, and there are a lot of features that makes this process attractive and practical with a conversion reached 99.2%.

Chemical modelling covers a wide range of disciplines and this book is the first stop for any materials scientist, biochemist, chemist or molecular physicist wishing to acquaint themselves with major developments in the applications and theory of chemical modelling. Containing both comprehensive and critical reviews, it is a convenient reference to the current literature. Coverage includes, but is not limited to, boron clusters, molecular modeling of inclusion complexes, modelling of circular dichroism for DNA and proteins, and the interface effect of nanocomposites as electrode materials for Li/Na ion batteries.

Sustainability has become an important factor in the chemical process and energy industries with a strong drive for process improvements towards more environmentally conscious solutions. However, there are many ways of defining sustainability and even more ways of trying to determine how sustainable a process is. This work looks into applying a conjunction of tools including; process simulation, multi-criteria decision matrices and life-cycle assessment to more quantitatively determine sustainability metrics. We have applied these tools for the production of electricity, methanol and dimethyl ether. A novel method of electricity production, in chemical looping combustion (CLC), was used that inherently involves carbon dioxide capture. Experimental work was conducted for two different oxygen carriers, CaSO4 and CuO, using thermogravimetric analysis (TGA). Process simulations were developed for both coal and natural gas (NG) feedstocks to produce power and heat. Sustainability metrics were developed based on simulated data showing electricity prices of 23.7 ¢/kWhr (NG) and 7.8 ¢/kWhr (coal) while reducing CO2 emissions 0.38 (NG) and 3.38 (coal) metric ton/MWhr electricity. Renewable methanol production was also simulated in Aspen Plus. This process used wind based electrolytic hydrogen and captured CO2 as feedstocks. This work presents a multi-criteria decision matrix for the inclusion of sustainability metrics alongside economic indicators in feasibility analysis. A comparison of renewable methanol to NG based methanol using this matrix shows that the renewable process is feasible. We continued this work to conduct a full (cradle-to-grave) life-cycle assessment of alternative fuels based on this renewable methanol and its conversion to dimethyl ether. Using renewable methanol as a fuel reduces greenhouse gas emissions 86% and fossil fuel use by 91% compared to conventional gasoline. Using dimethyl ether reduces greenhouse gas emissions 80% and fossil fuel use 81% when compared to ultra-low sulfur diesel. This whole work focuses on developing sustainability metrics helps identify a quantified measure of sustainability that can be used along economic indicators in a multi-criteria decision matrix for a better and comprehensive feasibility evaluation of energy systems and chemical 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

Methanol: Science and Engineering provides a comprehensive review of the chemistry, properties, and current and potential uses and applications of methanol. Divided into four parts, the book begins with a detailed account of current production methods and their economics. The second part deals with the applications of methanol, providing useful insights into future applications. Modeling of the various reactor systems is covered in the next section, with final discussions in the book focusing on the economic and environmental impact of this chemical. Users will find this to be a must-have resource for all researchers and engineers studying alternative energy sources. Provides the latest developments on methanol research Reviews methanol production methods and their economics Outlines the use of methanol as an alternative green transportation fuel Includes new technologies and many new applications of methanol

The Hynol Process for conversion of coal and natural gas to methanol as a liquid fuel consists of three consecutive unit operations (1) hydrogasification of coal, (2) steam reforming of the methane formed and added natural gas feedstock, and (3) catalytic methanol synthesis. The Hynol Process is a total recycle process. Using a process simulation computer program, mass and energy balances and yields and efficiency data have been obtained for a range of natural gas to coal feedstock ratios. Although the methanol yield increases with natural gas to coal feed ratio, the cost of feedstock per unit methanol is insensitive over a wide range of feedstock ratios. The Hynol Process produces a 13% increase in methanol yield compared to the equivalent of two separate conventional coal gasification and natural gas reforming plants. The CO2 emissions are reduced by 22% for the Hynol plant compared to the conventional processes with greater CO2 reductions at lower gas to coal feedstock ratios. A preliminary cost estimate for a 10,000 Tons/Day Hynol methanol plant indicates a lower production cost than the current cost of methanol by the conventional natural gas reforming plant. The lower unit energy cost for coal is beneficial in reducing the methanol cost in the Hynol Process.

Carbon Dioxide Recovery and Utilization is a complete and informative resource on the carbon dioxide sources and market at the European Union level, with reference to the world situation. The book covers the following themes: - Sources of carbon dioxide and their purity, - Market of carbon dioxide and its uses, - Separation techniques of carbon dioxide from flue gases, - Analysis of the potential of each technique and application, - Basic science and technology of supercritical CO2, - Reactions in supercritical CO2 and its use as reactive solvent, - Utilization of CO2 in the synthesis of chemicals with low energy input, - Conversion of CO2 into fuels: existing techniques, - Dry reforming of methane, - Assessment of the use of carbon dioxide for the synthesis of methanol. This book is unique in providing integrated information and a perspective on innovative technologies for the use of carbon dioxide. The book is suitable for use as a textbook for courses in chemical engineering and chemistry. It is also of great interest as a general reference for those involved with technologies for avoiding carbon dioxide production and for economists. This is an invaluable reference for specialists on synthetic chemistry, gas separation, supercritical fluids, carbon

dioxide marketing, renewable energy and sustainable development. In addition, it will be useful for those working in the chemical industry and for policy makers for carbon dioxide mitigation, innovative technologies, carbon recycling, and power generation.

Operating Training Simulator (OTS) is a computer-based training system. The OTS applies a simulation of an industrial process to generate the appropriate data of the plant''s process operation. In addition, the OTS is widely accepted in the industry as an enabling technology for employee competency and proficiency training and enhancement. This system is deemed as the effective application in order to develop the highest skill levels and proficiency of the operator. This project presents the first-hand experience of developing a process simulator system using Aspen Simulation Workbook (ASW). The production of acetic acid from methanol carbonylation is used as a case study. Aspen Plus is used for the modelling of the methanol carbonylation process and will be linked with Excel using Aspen Simulation Workbook. The simulation can be operated in Aspen Simulation Workbook by manipulating the value of the variables. This case study is about to determine the changes of output variable by manipulates the input variables. This would contribute towards the solution of training issues related to control and operate a process and act as a tool to educate and train the engineering students for supporting training in control and operate certain processes respectively. The operator training tool is developed successfully in Aspen Simulation Workbook.

Beyond its identification with the second law of thermodynamics, entropy is a formidable tool for describing systems in their relationship with their environment. This book proposes to go through some of these situations where the formulation of entropy, and more precisely, the production of entropy in out-of-equilibrium processes, makes it possible to forge an approach to the behavior of very different systems. Whether for dimensioning structures; influencing parameter variability; or optimizing power, efficiency, or waste heat reduction, simulations based on entropy production offer a tool that is both compact and reliable. In the case of systems marked by complexity, it appears to be the only way. In that sense, realistic optimization can be carried out, integrating within the same framework both the system and all the constraints and boundary conditions that define it. Simulations based on entropy give the researcher a powerful analytical framework that crosses the disciplines of physics and links them together.

Biodiesel is a clean burning alternative fuel, produced from domestic, renewable resources such as plant oils, animal fats, used cooking oil and even new sources such as algae. Biodiesel is also defined as fuel which has the same characteristics with commercial diesel in terms of its molecular formula. The transesterification reaction can be carried out using both homogeneous (acid or base) and heterogeneous (acid, base, or enzymatic) catalyst. Homogeneous catalysts provide much faster reaction rates than heterogeneous catalysts, but it is considerably more costly to separate homogenous catalysts from the reaction

mixture (Liu et al., 2008). Therefore, heterogeneously base catalysts are studied in this research. The objective of this study is to find the feasibility of new type of heterogeneous catalyst in determining the best operating parameters and design factors which affecting the performance of biodiesel production. Aspen Plus 12.1 is used to performed the simulation study for feasibility of the biodiesel production using heterogeneous catalyst through a plug flow reactor (PFR). The simulation was done by incorporating the reaction kinetics and thermodynamics model into the reactor model. The NRTL of thermodynamics model is used in this research in order to perform the separation process for two liquid phases in the transesterification of vegetable oil process. The simulation was run after all the important property data had been incorporated into Aspen Plus simulator. After running all the operating parameters, it shows that the best temperature is 65 0C, the best molar ratio of methanol to oil is 6:1, the best mass ratio of catalyst to oil is 3% and the best space velocity is 0.25 hr-1 on oil conversion and biodiesel yield percentage. The PFR reactor schemes which are in single PFR, two PFR in series and PFR to CSTR were proposed as a suitable scheme for the production of biodiesel. Hence that, at the optimum operating condition, the conversion is 91.5%.

The objective of the Biomass to Methanol Systems Analysis Project is the determination of the most economically optimum combination of unit operations which will make the production of methanol from biomass competitive with or more economic than traditional processes with conventional fossil fuel feedstocks. This report summarizes the development of simulation models for methanol production based upon the Institute of Gas Technology (IGT) "Renugas" gasifier and the Battelle Columbus Laboratory (BCL) gasifier. This report discusses methanol production technology, the IGT and BCL gasifiers, analysis of gasifier data for gasification of wood, methanol production material and energy balance simulations, and one case study based upon each of the gasifiers.

Hydrogen is the fuel of future. It has found its uses as an alternate energy source either by direct combustion or by electricity generation through fuel-cell. Hydrogen being the lightest gas has storage problems and risk hazards. In order to overcome these challenges idea of on-board production of hydrogen is popular among researchers. For on-board production of hydrogen process of partial oxidation of methanol is proposed and discussed in this work. For partial oxidation of methanol a fixed bed catalytic reactor is designed. In order to explain the method in detail, computer aided modeling and simulation of process is carried out using Aspen-HYSYS V7.1 tool. Simulation studies are focused to optimize the process for best possible conversion of methanol to desired product hydrogen. By simulation various parameters and response of fixed bed reactor is studied in detail. Reaction kinetics is explained on the basis of Langmuir Hinshelwood model in this work. In order to make the whole process reliable experimental rig is also designed for physical production of hydrogen by partial

oxidation of methanol. Results from both simulation and experimental work are analyzed and compared.

Methanol synthesis has been the subject of many improvements over the last decades since it became more cost effective and scalable than earlier high pressure technology. The synthesis of methanol from syngas has conventionally been carried out in adiabatic quench-type reactor in the gas phase where the only way to moderate the temperature is to inject shots of syngas at various position of the rector. However, because of the highly exothermic behavior of methanol synthesis reactions, the dissipation of heat has been a bottle-neck in the reactor design, and reactor configurations have a tendency to be complicated. This dissertation is divided into three parts presents a mathematical model of double-tube methanol reactor which was developed through cooperation between Mitsubishi Heavy Industries (MHI) and Mitsubishi Gas Company (MGC), methanol synthesis process flowsheet was developed and fully integrated with the Genetic Algorithms that generated a set of optimal operating conditions with respect to upper and lower limits and several constraints, and a dynamic optimization approaches to derive the ideal operating conditions for a Lurgi type reactor in the presence of catalyst deactivation. This study proposes a new approach based on a hybrid algorithm combining genetic algorithm (GA) and generalized pattern search (GPS) derivative-free methodologies to provide a sufficiently good solution to this dynamic optimization problem. The hybrid GA-GPS algorithm has the advantage of sequentially combining GA and GPS logics; while GA, as the most popular evolutionary algorithm, effectively explore the landscape of the fitness function and identify promising areas of the search space, GPS efficiently search existing basins in order to find an approximately optimal solution. The simulation results showed that implementing the shell temperature trajectory derived by the proposed approach with 5% recycle ratio of CO2 increased the production of methanol by approximately 2.5% compared to the existing operating conditions.

Any mention of the "greenhouse effect" tends to ignite controversy. While the rising atmospheric concentrations of greenhouse gases-especially carbon dioxide- are certainly among the most pressing issues today, theoretical and perceived consequences have been subject to conjecture and misinformation. That raging debate has obscured an important fact: scientists and engineers are hard at work on methods to reduce CO2 emissions, and devise practical methods for their remediation. Greenhouse Gas Carbon Dioxide Mitigation: Science and Technology sheds light on the most recent advancements, documented by two of the world's leading researchers on CO2. Aware of the complexity and still-unknown factors behind climatic change, the authors consider the need to make CO2 mitigation viable for both environmental and economic gain. To that end, Professor Halmann offers new insights into interesting chemical pathways for the conversion of CO2 to useful products. Steinberg adds real-life engineering solutions, applicable to heavy CO2-producing industrial processes, and improving efficiency of energy conversion. Exciting theories and pilot projects are also testing the potential for CO2 utilization, conversion, reduction, and disposal. Greenhouse Gas Carbon Dioxide Mitigation: Science and Technology reports on the use of biomass, such as ocean fertilization and "energy farms," to put CO2 to practical and safe use. Professional and

academic readers involved with CO2 research will find Greenhouse Gas Carbon Dioxide Mitigation: Science and Technology an invaluable roadmap for information and inspiration-a way to move beyond argument, and into action.

To evaluate the risks and potential pay-offs of a new technology, a systematic approach for assessment must be developed. Characterization of the performance and emissions of the technology must be made comparable to conventional and other advanced alternatives. This study deals with the design and implementation of a performance and emission model for a gasification based power system fueled with municipal solid waste (MSW) and coal in ASPEN PLUS --C a chemical process simulation software package. The power system modeled is an integrated gasification combined cycle (IGCC) and has several advantages over conventional combustion plants including lower pollutant emissions; higher thermal efficiencies; and the ability to co-produce several products aside from electricity. The model was developed to analyze and quantify the expected benefits associated with MSW gasification. This research models a British Gas/Lurgi (BGL) Slagging gasifer-based IGCC power and methanol production facility firing coal and MSW. The ASPEN PLUS IGCC model consists of 153 unit operation blocks, 24 FORTRAN blocks and 32 design specifications. The performance model calculates mass and energy balances for the entire IGCC system. For validation, the model was calibrated to a design study by the Electric Power Research Institute (EPRI) of a BGL gasifier based IGCC system (Pechtl et al., 1992). First developed and calibrated for a coal fueled IGCC system, the model was then converted to process MSW. Three fuels are used in this study: a Pittsburgh No. 8 bituminous coal; a German waste blend; and an American 75/25 percent mixture of Refuse Derived Fuel (RDF) and Pittsburgh No. 8 Bituminous coal. Methanol plant sizes of 10,000, 20,000 and 40,000 lb methanol/hr, each with and without recycling the methanol plant purge gas to the gas turbine, were modeled for each fuel. Regardless of the type of fuel fired, all systems were more efficient when the purge gas from the methanol plant was recycled for.

ASPEN computer simulation cases involving methanol, ethanol and propanol recycle have been completed. The results indicate that the yield of higher alcohols increased slightly until the quantity of recycled lower alcohol equaled the amount of that alcohol produced (i.e. when there is no net formation of the recycled alcohol). Above this point, no change in higher alcohol yield was observed. All cases were based on a 2/1 H2/CO feed ratio at 70 atm and 275°C. ASPEN PLUS simulations of the thermodynamics of higher alcohol synthesis were carried out based on non-ideal, equation-of-state models. The models used were the Peng-Robinson and the Redlich-Kwong-Aspen equations of state. The results of these simulations indicate very little difference between the results obtained with the ideal fluid model and the non-ideal models. No significant changes were found in reactant conversion, product distribution or product yield. All laboratory renovations are now complete.

Methanol is a valuable commodity with many uses. It is used to manufacture other chemicals such as olefins, formaldehyde, and methyl-tert-butyl ether (MTBE). Methanol is also being researched as an alternative fuel for vehicles. Global methanol demand is increasing, making it a valuable chemical to manufacture. Methanol production requires three main steps: syngas production, methanol production, and methanol purification. Syngas is a mix of carbon monoxide and hydrogen that can be made through the reforming of natural gas. The production of syngas is done through many methods. Three primary methods are steam methane reforming (SMR), partial oxidation (POX), and autothermal reforming (ATR). Once syngas is produced, it is sent to a methanol reactor where three main reactions occur: the hydrogenation of CO, the hydrogenation of CO2, and the water-gas shift reaction. A product stream with methanol is then purified in using distillation. The company Technology Convergence Inc. (TCI) made a process for manufacturing methanol in 2004 called the Green Methanol Process. This process involved the use of a POX reformer and an electrolyser to

provide the required hydrogen and oxygen. TCI is now known as Advanced Chemical Technologies (AChT), and they have since updated their Green Methanol Process. The new process still uses an electrolyser to generate hydrogen and oxygen, but now uses an ATR for syngas production. Aspen Plus was used in this work to simulate the updated AChT process. Heat integration was successfully implemented into the simulation. Additionally, the syngas production method was changed over from POX to ATR. An initial analysis of the amine reboiler of a CO2 capture unit was done. Finally, it was discovered that the waste stream contained a large amount of hydrogen. To remedy this, a method of hydrogen purification was studied called pressure swing adsorption (PSA). A version of the methanol process simulation was done with the PSA hydrogen recycle system added. An economic analysis looked into the OPEX and CAPEX of the process with and without PSA hydrogen recycling. Without hydrogen recycling, the CAPEX and OPEX were found to be $248 CAD/metric tonne (MT) methanol and $300 CAD/MT methanol, respectively, while producing 217 MTPD (metric tonne per day) of methanol. This resulted in a combined overall cost of $548 CAD/MT methanol produced. With hydrogen recycling, the CAPEX and OPEX were found to be $223 CAD/MT methanol and $280 CAD/MT methanol respectively, while producing 249 MTPD of methanol. This resulted in a combined cost of $503 CAD/MT methanol. Overall, it was found that the implementation of a PSA hydrogen recycle system was a good investment. Additionally, hourly Ontario electricity price (HOEP) data from 2018 were used to determine on average the most expensive consecutive 11-day period. Since the plant was planned to be shut down for 11 days for maintenance, this would inform when the best time to shut down would be to save the most on electricity. The best day to start the maintenance was found to be January 5th. The next most expensive periods started on December 4th and April 9th.

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The development of innovative drugs is becoming more difficult while relying on empirical approaches. This inspired all major pharmaceutical companies to pursue alternative model-based paradigms. The key question is: How to find innovative compounds and, subsequently, appropriate dosage regimens? Written from the industry perspective and based on many years of experience, this book offers: - Concepts for creation of drug-disease models, introduced and supplemented with extensive MATLAB programs - Guidance for exploration and modification of these programs to enhance the understanding of key principles - Usage of differential equations to pharmacokinetic, pharmacodynamic and (patho-) physiologic problems thereby acknowledging their dynamic nature - A range of topics from single exponential decay to adaptive dosing, from single subject exploration to clinical trial simulation, and from empirical to mechanistic disease modeling. Students with an undergraduate mathematical background or equivalent education, interest in life sciences and skills in a high-level programming language such as MATLAB, are encouraged to engage in model-based pharmaceutical research and development.

Reactive distillation column (RD column) is a hybrid equipment that combines two of major equipment, i.e. reactor and distillation column. RD column brings many advantages to the chemical industries especially in reducing the cost of building plant, and energy consumption. Biodiesel is an excellent substitute for conventional diesel fuel because of being renewable, nontoxic and biodegradable. In the biodiesel industry, mainly for the biodiesel production from Jatropha Curcas seed oil (JCO oil); the reactive distillation is still being a new technology. The JCO oil contains high percentage of triolein and oleic acid which are really useful for engine performance. This study is mainly based on simulation method by using Aspen Plus 12.1 software. The biodiesel routes process used is triglyceride hydrolysis and fatty acid esterification process. This study will focus on oleic acid esterification with methanol in the reactive distillation column to produce methyl oleate. The simulation was done in equilibrium

stage model incorporate with kinetic of reaction model using RADFRAC unit as the RD column model. The purpose of the simulation carried out is to determine the effect of important parameters, i.e. reflux ratio, column pressure, feed temperature, etc, that affect the RD column performance and design the optimized RD column condition to achieve highest product conversion. In the nutshell, the optimum parameters for simulated RD column are; reflux ratio 0.01, feed temperature at 363.15K @ 900C, column pressure at 100 kPa, 14 stages with 6 reactive stages, and oleic acid and methanol feed locations, accordingly, at 3nd stage and 8th stage, to achieve 99.65% of oleic acid conversion to biodiesel.

Cyclic Separating Reactors is a critical examination of the literature covering periodically operated separating reactors incorporating an adsorbent as well as a catalyst, aiming to establish the magnitude of performance improvement available with this type of reactor compared to systems in which the reactor and separator are separate units. The adequacy of present models is considered by comparison of simulation and experimental studies, and gaps in understanding or experimental verification of model predictions are identified. Separating reactors, including chromatographic reactors and pressure swing reactors, are an expeditious means of process intensification, reducing both capital and operating costs, particularly where reactions are equilibrium limited. For this reason, cyclically operating separating reactors are attracting considerable interest across the range of chemical manufacturing industries, so this book is a timely and valuable summary of the literature available to the engineer. Following an introduction to multifunctional reactors and to periodic reactor operation, Cyclic Separating Reactors covers both chromatographic and pressure swing adsorption reactors, and is written for chemical engineers in both industry and academe. First book to critically examine the literature surrounding Cyclically Operating Separating Reactors providing a straightforward entry to, and detailed appraisal of, the literature, so the reader does not have to engage in an expensive and time consuming literature review Evaluates current models and understanding to give the engineer clear information on what performance can be expected of these reactors and where current information needs to be augmented when designing systems for commercial operation.

The Hynol process is proposed to meet the demand for an economical process for methanol production with reduced CO2 emission. This new process consists of three reaction steps: (a) hydrogasification of biomass, (b) steam reforming of the produced gas with additional natural gas feedstock, and (c) methanol synthesis of the hydrogen and carbon monoxide produced during the previous two steps. The H2-rich gas remaining after methanol synthesis is recycled to gasify the biomass in an energy neutral reactor so that there is no need for an expensive oxygen plant as required by commercial steam gasifiers. Recycling gas allows the methanol synthesis reactor to perform at a relatively lower pressure than conventional while the plant still maintains high methanol yield. Energy recovery designed into the process minimizes heat loss and increases the process thermal efficiency. If the Hynol methanol is used as an alternative and more efficient automotive fuel, an overall 41% reduction in CO2 emission can be achieved compared to the use of conventional gasoline fuel. A preliminary economic estimate shows that the total capital investment for a Hynol plant is 40% lower than that for a conventional biomass gasification plant. The methanol production cost is $0.43/gal for a 1085 million gal/yr Hynol plant which is competitive with current U.S. methanol and equivalent gasoline prices. Process flowsheet and simulation data using biomass and natural gas as cofeedstocks are presented. The Hynol process can convert any condensed carbonaceous material, especially municipal solid waste (MSW), to produce methanol.

This book closes the gap between Chemical Reaction Engineering and Fluid Mechanics. It provides the basic theory for momentum, heat and mass transfer in reactive systems. Numerical methods for solving the resulting equations as well as the interplay between physical and numerical modes are discussed. The book is written using the standard

terminology of this community. It is intended for researchers and engineers who want to develop their own codes, or who are interested in a deeper insight into commercial CFD codes in order to derive consistent extensions and to overcome "black box" practice. It can also serve as a textbook and reference book.

The following study entails process simulations and techno-economic analysis based investigations of novel chemical looping partial oxidation processes. The moving bed reactor system analyzed in this dissertation provides chemical looping technologies several intrinsic advantages over conventional energy processing schemes. Chapter 2 focusses on optimizing the counter-current moving bed chemical looping system for H2 production from natural gas. The chemical looping process for H2 production from natural gas is optimized based on isothermal thermodynamic limits of an iron-based counter-current moving bed reactor system. The iso-thermal analysis is followed by a parametric sensitivity for energy balance for satisfying the auto-thermal heat balance. This is completed by computing temperature swings based on a net heat duty calculation for individual chemical looping reactors. Overall the chemical looping process is shown to have a cold gas efficiency of 77.6% (HHV basis) and an effective thermal efficiency of 75.1% (HHV basis), both of which are significantly higher than the baseline case. Chapter 3 discusses the Shale gas to Syngas process for integration into a Gas to Liquid fuel (GTL) plant. Following the methodology for an isothermal and an adiabatic analysis from Chapter 2, Chapter 3 identifies a suitable auto-thermal operating condition for the chemical looping reactors. The process simulation model is used to derive cost estimates based on standard engineering assumptions and completes a sensitivity analysis for several important economic parameters. The STS process is shown to require significantly lower natural gas feedstock than the conventional process baseline for producing the same amount of liquid fuels. The STS process lowers the capital cost investment for the syngas production section of a GTL plant by over 50% and if commercialized can be disruptive to liquid fuel production markets. Chapter 4 discusses the Coal to syngas (CTS) process for its technical and economic performance when integrated into a 10,000 tpd methanol plant. This chapter details the equipment sizing philosophy and cost methodology used in this dissertation for calculating economic performance of the novel processes developed. Further, sensitivity studies which analyze effect of economic parameters like the capital charge factor, natural gas price are considered to identify the critical technology parameters necessary to be de-risked for pilot scale and commercial scale operation of the CTS technology. The CTS process reduced the coal consumption by 14% for the same amount of methanol production. The CTS process also reduced the methanol required selling price by 21% over the corresponding baseline case with greater than 90% carbon capture. Chapter 5 discusses the two reducer chemical looping configurations and the fixed bed chemical looping configurations. The two reducer chemical looping configurations provide the flexibility for designing two different reducer reactors, each optimized to a specific fuel feedstock. The two reducer chemical looping configurations can improve over thermodynamic performance of a single reducer chemical looping configuration by providing the flexibility to get high solids conversion with high fuel conversions. The fixed bed operating strategy opens up ways to operate iron-based chemical looping system without solids circulation for high-efficiency production of syngas.

Dimethyl ether (DME) as a clean fuel seems to be a superior candidate for high-quality diesel fuel in near future. In this study, a comprehensive three-dimensional dynamic heterogeneous model developed to simulate the flow behavior and catalytic coupling reactions for synthesis of the DME from hydrogenation of the CO and CO2, dehydration of methanol to dimethyl ether and water gas shift reaction in a fixed bed reactor. For this purpose, a CFD simulation was articulated where the standard k-? model with 10% turbulence tolerations implemented. Then the concentration and temperature profiles along the reactor were determined. It was revealed that under conditions considered, a single phase physiochemical system under equilibrium

existed for which simulations were performed. Ultimately, generated results of the model under appropriate industrial boundary conditions compared with those of others available in the open literature to verify the developed model. Then, the effects of various operating parameters including the pressure, temperature and flow rate of the feed to the reactor upon the DME production as well as; selectivity were examined. The CFD modeling results generated from the present work revealed reasonable agreement with obtained data of these authors and other experimental available in the open literature which considering the complexity of the task performed was rather satisfying.

Gasification is a thermo-chemical process which transforms biomass into valuable synthesis gas. Integrated with a biorefinery it can address the facility's residue handling challenges and input demands. A number of feedstock, technology, oxidizer and product options are available for gasification along with combinations thereof. The objective of this work is to create a systematic method for optimizing the design of a residual biomass gasification unit. In detail, this work involves development of an optimization superstructure, creation of a biorefining scenario, process simulation, equipment sizing & costing, economic evaluation and optimization. The superstructure accommodates different feedstocks, reactor technologies, syngas cleaning options and final processing options. The criterion for optimization is annual worth. A biorefining scenario for the production of renewable diesel fuel from seed oil is developed; gasification receives the residues from this biorefinery. Availability of Soybeans, Jatropha, Chinese Tallow and woody biomass material is set by land use within a 50-mile radius. Four reactor technologies are considered, based on oxidizer type and operating pressure, along with three syngas cleaning methods and five processing options. Results show that residual gasification is profitable for large-scale biorefineries with the proper configuration. Low-pressure air gasification with filters, water-gas shift and hydrogen separation is the most advantageous combination of technology and product with an annual worth of $9.1 MM and a return on investment of 10.7%. Low-pressure air gasification with filters and methanol synthesis is the second most advantageous combination with an annual worth of $9.0 MM. Gasification is more economic for residue processing than combustion or disposal, and it competes well with natural gas-based methanol synthesis. However, it is less economic than steam-methane reforming of natural gas to hydrogen. Carbon dioxide credits contribute to profitability, affecting some configurations more than others. A carbon dioxide credit of $33/t makes the process competitive with conventional oil and gas development. Sensitivity analysis demonstrates a 10% change in hydrogen or electricity price results in a change to the optimal configuration of the unit. Accurate assessment of future commodity prices is critical to maximizing profitability.

This book is designed to apprise the students of chemical engineering with a variety of different processes of chemical technologies. The book is richly illustrated and covers the essential information with the help of flow diagrams, enabling the students to gain a full understanding of both the fundamental concepts and chemical reactions involved in process technologies. Newer technologies have been dealt with and some technologies which have lost their relevance have been omitted. Computer simulation methods have been described for many important technologies. In short, the book considers computer design tools and design software, in a manner that integrates this knowledge smoothly into the main subject. The book is expected to become useful not only to the students for courses in Chemical Technology but also to practising engineers and process designers for innovative process development. There are topics on natural products and fermentation process chemicals, organic chemicals, inorganic chemicals, refinery operations, oil and gas operations and nanotechnology products. In some of these topics, computer simulation and costing examples are included. An illustration of modelling and simulation using C++, is also given as an example of user-written programs for simulation. Another method that can be used for simulation is the use of spreadsheets,

which is also described with the help of an example. A new important topic of today being ‘polysilicon’ used in the manufacture of computer chips and solar panels, is also covered in detail.

The 2012 International Conference on Applied Biotechnology (ICAB 2012) was held in Tianjin, China on October 18-19, 2012. It provides not only a platform for domestic and foreign researchers to exchange their ideas and experiences with the application-oriented research of biotechnology, but also an opportunity to promote the development and prosperity of the biotechnology industry. The proceedings of ICAB 2012 mainly focus on the world's latest scientific research and techniques in applied biotechnology, including Industrial Microbial Technology, Food Biotechnology, Pharmaceutical Biotechnology, Environmental Biotechnology, Marine Biotechnology, Agricultural Biotechnology, Biological Materials and Bio-energy Technology, Advances in Biotechnology, and Future Trends in Biotechnology. These proceedings are intended for scientists and researchers engaging in applied biotechnology. Professor Pingkai Ouyang is the President of the Nanjing University of Technology, China. Professor Tongcun Zhang is the Director of the Key Laboratory of Industrial Fermentation Microbiology of the Ministry of Education at the College of Bioengineering, Tianjin University of Science and Technology, China. Dr. Samuel Kaplan is a Professor at the Department of Microbiology & Molecular Genetics at the University of Texas at Houston Medical School, Houston, Texas, USA. Dr. Bill Skarnes is a Professor at Wellcome Trust Sanger Institute, United Kingdom.

While the PSE community continues its focus on understanding, synthesizing, modeling, designing, simulating, analyzing, diagnosing, operating, controlling, managing, and optimizing a host of chemical and related industries using the systems approach, the boundaries of PSE research have expanded considerably over the years. While early PSE research was largely concerned with individual units and plants, the current research spans wide ranges of scales in size (molecules to processing units to plants to global multinational enterprises to global supply chain networks; biological cells to ecological webs) and time (instantaneous molecular interactions to months of plant operation to years of strategic planning). The changes and challenges brought about by increasing globalization and the the common global issues of energy, sustainability, and environment provide the motivation for the theme of PSE2012: Process Systems Engineering and Decision Support for the Flat World. Each theme includes an invited chapter based on the plenary presentation by an eminent academic or industrial researcher Reports on the state-of-the-art advances in the various fields of process systems engineering Addresses common global problems and the research being done to solve them

Increasing awareness of the environmental issues forces a strong drive towards the development of new, sustainable processes for renewable energy production. Likewise, the economic issues related to the increasing prices of crude oil, and its derivatives lead to the recognition of advantages of alternative fuels, thus a significant interest in biomass-derived, synthetic fuels is observed. Among various thermo-chemical conversion processes, biomass gasification is one of the most effective, efficient and sustainable solutions to the production of renewable energy. It provides a gaseous fuel, composed mainly of carbon monoxide and hydrogen, suitable to produce chemicals, heat, and energy. In particular, syngas can be used to obtain methanol (MeOH) and dimethyl ether (DME), both energy carriers of great interest for many advanced energy applications. The herein presented work provides the reader with a comparison of the technicalities as well as economics of methanol and DME production from biomass-derived syngas, by different pathways. For that purpose a process simulation by means of the ChemCAD® commercial code was used. The developed simulation strategies include both, optimization of the kinetic models and unique solution of fuel refinement.

Computer-aided process engineering (CAPE) plays a key design and operations role in the process industries, from the molecular scale through managing complex manufacturing sites. The research interests cover a wide range of interdisciplinary problems related to the current needs of society and industry. ESCAPE 23 brings together researchers and practitioners of computer-aided process engineering interested in modeling, simulation and optimization, synthesis and design, automation and control, and education. The proceedings present and evaluate emerging as well as established research methods and concepts, as well as industrial case studies. Contributions from the international community using computer-based methods in process engineering Reviews the latest developments in process systems engineering Emphasis on industrial and societal challenges

Facilitates the process of learning and later mastering Aspen Plus® with step by step examples and succinct explanations Step-by-step textbook for identifying solutions to various process engineering problems via screenshots of the Aspen Plus® platforms in parallel with the related text Includes end-of-chapter problems and term project problems Includes online exam and quiz problems for instructors that are parametrized (i.e., adjustable) so that each student will have a standalone version Includes extra online material for students such as Aspen Plus®-related files that are used in the working tutorials throughout the entire textbook

This book is part of a two-volume work that offers a unique blend of information on realistic evaluations of catalyst-based synthesis processes using green chemistry principles and the environmental sustainability applications of such processes for biomass conversion, refining, and petrochemical production. The volumes provide a comprehensive resource of state-of-the-art technologies and green chemistry methodologies from researchers, academics, and chemical and manufacturing industrial scientists. The work will be of interest to professors, researchers, and practitioners in clean energy catalysis, green chemistry, chemical engineering and manufacturing, and environmental sustainability. This volume focuses on catalyst synthesis and green chemistry applications for petrochemical and refining processes. While most books on the subject focus on catalyst use for conventional crude, fuel-oriented refineries, this book emphasizes recent transitions to petrochemical refineries with the goal of evaluating how green chemistry applications can produce clean energy through petrochemical industrial means. The majority of the chapters are contributed by industrial researchers and technicians and address various petrochemical processes, including hydrotreating, hydrocracking, flue gas treatment and isomerization catalysts.

23 European Symposium on Computer Aided Process EngineeringProduction of Methanol and Dimethyl ether from biomass derived syngas – a comparison of the different synthesis pathways by means of flowsheet simulationElsevier Inc. Chapters

Energy Systems Engineering is one of the most exciting and fastest growing fields in engineering. Modeling and simulation plays a key role in Energy Systems Engineering because it is the primary basis on which energy system design, control, optimization, and analysis are based. This book contains a specially curated collection of recent research articles on the modeling and simulation of energy systems written by top experts around the world from universities and research labs, such as Massachusetts Institute of Technology, Yale University, Norwegian University of Science and Technology, National Energy Technology Laboratory of the US Department of Energy,

University of Technology Sydney, McMaster University, Queens University, Purdue University, the University of Connecticut, Technical University of Denmark, the University of Toronto, Technische Universität Berlin, Texas A&M, the University of Pennsylvania, and many more. The key research themes covered include energy systems design, control systems, flexible operations, operational strategies, and systems analysis. The addressed areas of application include electric power generation, refrigeration cycles, natural gas liquefaction, shale gas treatment, concentrated solar power, waste-to-energy systems, micro-gas turbines, carbon dioxide capture systems, energy storage, petroleum refinery unit operations, Brayton cycles, to name but a few.