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Editorial

Special Issue on "Dynamic Modeling and Control in Chemical and Energy Processes"

Dimitris Ipsakis

Industrial, Energy and Environmental Systems Lab (IEESL), School of Production Engineering and Management, Technical University of Crete, 73100 Chania, Greece; dipsakis@pem.tuc.gr; Tel.: +30-28210-37362

Recent energy policies have enforced the need to minimize GHG emissions. As a consequence, significant improvements have been made in novel process systems, as well as in the upgrading of the existing facilities that deal with fossil fuels. This Special Issue, entitled "Dynamic Modeling and Control in Chemical and Energy Processes", collects a set of high-quality research studies that address issues pertinent to the broad areas of modeling (e.g., process-related, kinetics and diffusion models), simulation and control. There are three subsections within this Special Issue, entitled "Modeling and Control in Energy Systems", "Reactive and Separation Technologies" (e.g., membrane reactors, carbon capture and storage) and "Diffusion and Kinetic Modeling in Fossil-Fuel-Based Feedstocks". All these aspects are considered crucial in forming the basis of concrete dynamic and control modeling studies. The latter are necessary as we move from bench-scale applications to industrial unit implementations. Overall, eleven research studies have been submitted, and are available online at: https://www.mdpi.com/journal/processes/special_issues/Modeling_Chemical_Energy (accessed on 26 November 2021).

1. Modeling and Control in Energy Systems

The modeling and control of energy systems that involve steam turbines, H_2 production units and novel power management in buildings are essential tools in unraveling complex dynamics and predicting a system's performance. Efforts towards tackling such issues have been well identified in the following research studies. In one of these, the well-known challenges in pressurized marine steam power plants (e.g., shipping navigation) were addressed effectively. As stated in [1], marine steam turbine rotational speed control systems must be constructed on the basis of Newton's second law, and an inherent disadvantage of the model is its non-linearity and complex structure. Considering this problem, S. Liu et al. [1] converted the non-linear model into a linear one and developed a novel Model Predictive Controller that addressed the rotational speed control problem of the marine steam turbine. As presented, the control system managed to maintain minimal overshoot and excellent set-point tracking. The simulation scenarios revealed that such an approach is feasible and significantly improves the dynamic characteristics of the system. Another research study focused on smart city organization through efficient energy control in buildings. As described in [2], building electricity consumption needs to be controlled by considering local environmental factors such as the working day, temperature and humidity (or a combination of these). Moreover, the implementation of an optimal electricity consumption strategy is challenging from a microgrid electricity management viewpoint. For this purpose, S. Lee et al. [2] employed neural network modeling with training data generation in order to predict a building's energy consumption (actual electricity consumption data from a shopping mall in Dalian, China were used). Based on the testing of their training data, the authors developed a robust building energy management strategy and were able to improve the energy efficiency, performance and reliability. Advancing towards the evaluation of novel thermal/energy systems, B. Tashtoush et al. [3] provided a comprehensive energy and exergoeconomic analysis of a transcritical refrigeration cycle with a suitable working fluid. As shown, the design and evaluation of the transcritical

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refrigeration cycle resulted in better performance compared with a traditional ejector refrigeration cycle. A set of advantages included lower exergy destruction, longer lifetime and improved safety (among others). Clearly, the proposed transcritical refrigeration cycle is highly recommended for enhancing the cycle performance and reducing the optimum pressure in heat/energy-related systems based on CO_2 working fluids. Following the progress surrounding H_2-based technologies, D. Ipsakis et al. [4] provided insights into controlling the operation of a coupled reformer/combustion system for H_2 production. In this study, a distributed control scheme based on PID controllers (each one tuned via the Ziegler–Nichols methodology) was applied and assessed under a set of realistic simulation scenarios featuring set-point tracking (e.g., temperature) despite the emergence of sudden disturbances (e.g., catalyst deactivation). It was revealed that accurately tuned controllers led to a quick start-up operation, minimum overshoot regarding reactor/burner temperature and quick settling during the disturbance's effect. Such a simplified yet compact study can be considered to form a basis for advanced process control schemes that can be implemented in similar reforming pilot plants. Unrelated to process systems but still within the area of system dynamics, J. Sun et al. [5] studied issues related to safety investment and the need to overcome the different types of hazards that a port operation might be exposed to. In this study, the authors analyzed several influencing factors and explored the interactions between the safety investment and system risk level. By analyzing the key factors affecting the port operation and their mutual relationships within a man–machine–environment management system, a decision-making model for safety investment in a port enterprise was established through system dynamics.

2. Reactive and Separation Technologies

A significant research area that has attracted the interest of industrial stakeholders is the implementation of separation technologies, either utilizing solvents (e.g., CO_2 capture) or by preferentially removing one or more components (e.g., membranes). Solvent-based post-combustion carbon capture can mitigate climate change but, at the same time, the increased energy requirements (due to solvent regeneration) require the development of effective control systems. Y. H. Chen et al. [6] proposed an optimal control approach and compared their results with a conventional control scheme, proving that the advanced process control scheme ensures faster responses during a disturbance (changes in flue gas conditions). Moreover, the proposed control structure ensured: (a) the maintenance of pre-defined set points (CO_2 capture efficiency), (b) a lower reboiler heat duty and (c) savings in solvent utilization, which are crucial for the economics of power plants integrated with carbon capture and storage technologies. As a connected outcome of [4,6], it was concluded that hydrogen purification and CO_2 capture are of great importance in refineries and power plants. Hence, dual-membrane separators could offer an alternative approach for improving H_2/CO_2 separation efficiency in downstream processes. Along these lines, W. Xiao et al. [7] developed a hollow-fiber dual separator with an integrated polyimide (PI) membrane and polydimethylsiloxane/polyetherimide composite membrane. The effects of process parameters including stage cut, operating temperature, operating pressure and membrane area ratio on the separation performance were investigated. At high stage cut, the dual-membrane separator has significant advantages over a single-membrane separator, and the operating temperature has a significant impact on gas permeation rates. Specifically, the proposed dual-membrane separator can obtain the highest purity H_2 and CO_2 at room temperature and increased pressures. Such concepts are expected to play a key industrial role in the recovery of H_2 and in the reduction of greenhouse gas emissions.

3. Diffusion and Kinetic Modeling in Fossil-Fuel-Based Feedstocks

Diffusion and kinetic modeling can provide insights into larger-scale control studies. Such theoretical concepts can form the basis that is needed for identifying the driving forces (e.g., reaction rates and diffusion rates) that favor the production or separation of added-value components. Coalbed methane recovery and CO_2-enhanced coalbed methane production are upstream processes that require detailed and reliable information on gas sorption and flow. More specifically, gas sorption determines methane reserves, whereas CO_2 sorption determines the capacity in coal. J. Zang et al. [8] presented experimental measurements of three fractional adsorption curves at different equilibrium pressures. In particular, these curves were modeled and screened with single, double and triple (mainly) fitting parameters that could predict the non-monotonous dependences of diffusivity on gas and coal properties. Within a similar topic, J. Zang et al. [9] shed light on the effects of particle size on gas diffusivity and related kinetics. In this study, a set of ethane desorption experimental data from two anthracites (a hard and a brittle coal type) were fitted through the unipore and bidisperse diffusion kinetic models. It was revealed that the relationship between diffusivity and particle size was different for the two coals: (a) the brittle coal had more abundant macropores than the hard coal and (b) the diffusivity in the hard coal decreased with increasing particle size. Overall, it was concluded that the effects of particle size on diffusivity may be coal-dependent, and the effects of particle size can be influenced by other factors, including coal structure. As an important issue regarding coalbed methane recovery, it was identified that coals with fine particles can complete desorption more quickly and desorb more methane in the same period, compared with coals with coarse particles. In a related research area, the progress made on analytical techniques applied to heavy petroleum fractions was presented. Initially, a study on the catalytic oxidation of heavy residual oil was carried out by A.V. Vakhin et al. [10]. The thermodynamic parameters of heavy residual oil oxidation products were studied using pulsed nuclear magnetic resonance, and the relationship between nuclear magnetic resonance parameters, the viscosity of heavy residual oil and its oxidation products was established. Specifically, the authors proved the possibility of using pulsed nuclear magnetic resonance as a flow-line method for the rapid analysis of intermediate and final products related to heavy residual oil oxidation (a process applied in refineries). Next, the work by A. I. Lakhova et al. [11] was devoted to obtaining data on the structure and the quantitative and qualitative compositions of structural formations of a petroleum dispersed system. According to the component composition data, the proportion of a complex structural unit was estimated in relation to the dispersion medium (petroleum dispersed system). Based on the IR spectroscopy data, the authors showed that the proportion of paraffinic structures relative to aromatic ones (aliphaticity) can be calculated by using the ratio of optical absorption densities. Using this parameter, the structural affinity coefficients of neighboring structural formations of the petroleum dispersed system could be quantified.

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