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Editorial

Special Issue: Modeling and Simulation of Energy Systems

Thomas A. Adams II

Department of Chemical Engineering, McMaster University, 1280 Main St W, Hamilton, ON L8S4L7, Canada; tadams@mcmaster.ca; Tel.: +1-905-525-9140

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Abstract: This editorial provides a brief overview of the Special Issue "Modeling and Simulation of Energy Systems." This Special Issue contains 21 research articles describing some of the latest advances in energy systems engineering that use modeling and simulation as a key part of the problem-solving methodology. Although the specific computer tools and software chosen for the job are quite variable, the overall objectives are the same—mathematical models of energy systems are used to describe real phenomena and answer important questions that, due to the hugeness or complexity of the systems of interest, cannot be answered experimentally on the lab bench. The topics explored relate to the conceptual process design of new energy systems and energy networks, the design and operation of controllers for improved energy systems performance or safety, and finding optimal operating strategies for complex systems given highly variable and dynamic environments. Application areas include electric power generation, natural gas liquefaction or transportation, energy conversion and management, energy storage, refinery applications, heat and refrigeration cycles, carbon dioxide capture, and many others. The case studies discussed within this issue mostly range from the large industrial (chemical plant) scale to the regional/global supply chain scale.

Keywords: modeling; simulation; energy; energy systems; process systems engineering; optimization; process design; operations

1. Introduction

Energy systems are currently a subject of rapidly growing interest within the engineering research community. Energy conversion and consumption impacts nearly all aspects of our lives, including the food we eat, the water we drink, the products we buy, how we battle the elements, how we communicate, how we move people and goods from place to place, how we work, and even how we are entertained. Although this has always been true throughout human history, the scale at which energy is consumed today is larger and expanding more quickly than ever before. The associated impacts of our energy consumption on our planet are now becoming so significant that the makeup of the atmosphere itself, particularly with regard to atmospheric CO_2 concentration, is being impacted.

Since the possible consequences are so alarming, energy systems engineering has become an extremely important area of research since one key aspect of solving this problem relates to the development of energy systems with far lower environmental impacts. Although energy is used in very diverse ways at scales from large to very small, large-scale systems, such as electric power plants, chemical plants, refineries, and oil and gas supply chains, are the easiest targets for improvement and the likeliest places where meaningful environmental impact reductions can be achieved. This is why almost all of the systems discussed in this Special Issue are in these application areas and, at large scales, range from 100 MW to 1000 MW class plants to massive international supply chains. Moreover, about half of the studies in this issue concern electric power generation, in a large part because fossil-based combustion systems tend to be the largest single-point sources of CO_2 emissions in the world. To address these concerns, the articles in this Special Issue took a variety of approaches, including the design of new energy systems and networks, improved control strategies for existing systems, and improved daily or hourly operational strategies for very complex systems. As a consequence of the large scales involved, even relatively small percentage improvements to efficiency or emissions can result in meaningful large-scale impacts.

2. Modeling Types

This issue focuses on the modeling and simulation of energy systems, or more precisely, research which relies heavily on mathematical models in order to address critical issues within energy systems. The issue begins with an extensive review of how modeling and simulation is used in energy systems research by Subramanian et al. [1], which examined and categorized over 300 papers on the subject. They proposed the modeling taxonomy shown in Figure 1 and noted that the "Process Systems Engineering Approach" to modeling energy systems focuses on mathematical modeling using the bottom-up approach. This means that mathematical models of individual process units, pieces of equipment, or process sections are written in the form of equations that describe the thermo-physical phenomena associated with it.

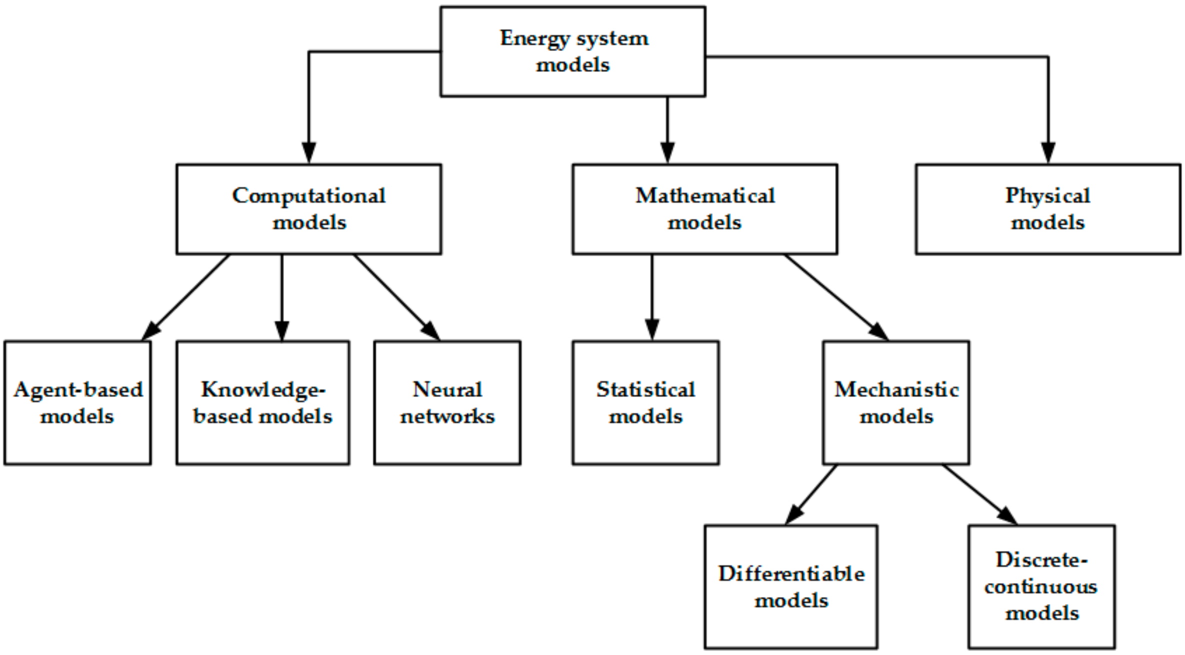

Figure 1. Taxonomy of energy systems modeling proposed by Subramanian et al. [1]. Reproduced with permission from MDPI.

Most of the articles in this issue use mechanistic models via a "first principles" approach, in which the equations and constraints derive from fundamental theory related to the first and second laws of thermodynamics, such as mass, energy, and momentum balances. These are usually coupled with equations that represent the physical properties of various chemicals or mixtures under different conditions, as well as equations describing physical or mechanical behaviour of the process equipment. The model parameters for physical property and equipment models are usually empirically determined in prior studies and are readily available through physical property databases or other sources.

As noted in the review by Subramanian et al. [1], statistical models are becoming increasingly more important in energy systems due to the increasing availability of data and computational capabilities in data analytics. Statistical models attempt to capture important characteristics of processes or process units without the use of fundamental first principles models. The benefits are usually improved computational speed at the risk of losing model rigor, extrapolative power, or certain nuances. For example, in this issue, Riboldi and Nord [2] use Kriging-type statistical models to create a surrogate of a much larger and more complex first principles model. The surrogate model is used for optimization purposes in place of the more rigorous one to help significantly reduce the computation time of optimization, which would be mostly intractable when using the fully-rigorous model. Similarly, Zimmerman et al. [3] create a statistical model from a more rigorous one, which is used for model predictive control (MPC). MPC requires very fast model solution times since it must re-solve the model frequently and repeatedly in order to determine ongoing control actions.

3. Implementation and Solution Frameworks

Interestingly, the software and implementation frameworks on which the models were built and simulated in this Special Issue varied widely from article to article. The list of software and packages includes, but is not limited to, the following: Aspen Custom Modeler, Aspen Exchanger and Design Rating, Aspen HYSYS, Aspen Plus, Aspen Plus Dynamics, Aspen Properties, casADi, Dymola, EcoInvent, GAMS, JuliaPro, JuMP, LINGO, MATLAB, Minitab, Modellica, Plant Engineering And Construction Estimator, PVWatts, Thermoflex, and other software developed in-house specifically for the articles in this issue, such as SoLCAT and EVA. There were generally two approaches for construction of the models. Most rigorous models of chemical processes were constructed with flowsheeting software (most commonly with the Aspen suite), in which the software builds the overall flowsheet model from a convenient model library containing models of the individual unit operations and connections. Models with a lower resolution (often because the boundaries of the model are at a much larger scale, such as a supply chain), models not based on mass and energy balances, and models with less rigour intended for use in optimization, tended to be implemented in general equation solving software such as GAMS or MATLAB, in which all of the equations needed to be strictly written out by the user. However, the diversity of software packages and implementation methods indicates the wide variety of problem types that were considered throughout this Special Issue.

4. Issue Summary

A summary of the articles in this Special Issue is provided in Table 1. It is an interesting snapshot of important research in energy systems and demonstrates both the breadth of problems considered and the depth of detail and understanding involved. Almost all articles use mathematical optimization to some degree, whether to find optimal designs, optimal controllers, or optimal operational strategies.

Table 1. Summary of articles in this Special Issue, categorized by problem type.

Authors/Ref	Application	Models and Software	Comments
		Reviews	
Subramanian, Gundersen, and Adams [1]	Field-wide survey of models in energy systems.	Modelling taxonomy proposed	Proposed connecting the PSE-style bottom-up approach with top-down approach used in energy economics.
		Energy System Design	
Riboldi and Nord [2]	Offshore power plants, integrated with renewables.	1st Principles + Kriging. Thermoflex, Plant Engineering, and Construction Estimator, MATLAB.	Dynamic considerations with regard to wind and electricity demand. Surrogate models used for optimization purposes.
Surindra, Caesarendra, Prasetyo, Mahlia, and Taufik [4]	Organic Rankine cycles in geothermal energy systems.	1st Principles of thermodynamic cycles.	Blends physical models (experimental apparatus) with mathematical ones.
Mussati, Mansouri, Gernaey, Morosuk, and Mussati [5]	Adsorption refrigeration cycles.	1st Principles. GAMS.	Optimal design with a superstructure approach.

Table 1. *Cont.*

Authors/Ref	Application	Models and Software	Comments
Yadav, Fabiano, Soh, Zimmerman, Sen, and Seider [6]	Transesterification of triolein to methyl-oleate (biofuels).	1st Principles. Aspen Plus with custom models.	Experimental validation of models in some conditions. Models used to predict performance in other conditions.
Vikse, Watson, Gundersen, and Barton [7]	Multi-stream heat exchanger (MHEX) design for natural gas liquefaction.	1st Principles. Julia. Aspen Plus for comparison.	Presents nonsmooth framework and algorithm for designing optimal MHEXs when standard methods fail.
Ridha, Li, Gençer, Siirola, Miller, Ribeiro, and Agrawal [8]	Shale gas condensate to oligomers and alkanes at the wellhead.	1st Principles. Aspen Plus, Aspen Economic Analyzer.	Techno-economic analysis. Premise: Cheaper to transport oligomers than Natural Gas Liquids.
Stuber [9]	Concentrated solar power with thermal energy storage.	1st Principles with empirical elements. JuliaPro/JuMP.	Equation oriented, differentiable model for determination of optimal design params.
Al-Aboosi and El-Halwagi [10]	Integrated water and energy between systems.	Mostly empirical models. LINGO.	Optimal design of integrated multi-product, multi-source systems considering time-varying solar.
Li, Demirel, and Hasan [11]	Automatically generate work-heat exchanger networks (WHEN).	1st Principles. GAMS. Phenomena level models.	Algorithm to create optimal WHENs from sources and sinks using building block superstructures.
Control Systems			
Sarda, Hedrick, Reynolds, Bhattacharyya, Zitney, and Omell [12]	Load-following Supercritical pulverized coal (SCPC).	1st Principles with reduced models. Aspen Plus Dynamics, Aspen Custom Modeler, Aspen Exchanger, and Design Rating.	Plant-wide dynamic model for designing and simulating plant-wide control system.
Zimmerman, Kyprianidis, and Lindberg [3]	Combustion of fuel derived from waste (refuse).	1st Principles. Modellica.	MPC with feedforward system developed. Soft sensors. Experimental validation.
Rahman, Zaccaria, Zhao, and Kyprianidis [13]	Micro gas turbine systems.	1st Principles with data-driven model tuning. EVA (in-house).	Dynamic models. Fault detection and diagnostics.
Pravin, Guidi, and Bhartiya [14]	Integrated reformer-membrane fuel cell systems.	1st Principles ODEs with some empirical characteristics. MATLAB.	Controllability analysis. Certain design considerations must be made for controllability purposes.
Decardi-Nelson, Liu, and Liu [15]	Flexible post-combustion CO_2 capture systems.	1st Principles. casADI, Python, Aspen Properties.	Economic MPC for disturbances. Look-up table made from Aspen Properties for fast use.
Flexible Operations and Operational Strategies			
Chen and Bollas [16]	Flexible, load-following subcritical coal power plant.	1st Principles. Dymola. Modelon Thermal-Power Library, MATLAB.	Dynamic optimization of transitions during load changes.
Corengia and Torres [17]	Optimal operating schedule of grid-scale battery energy storage.	1st Principles. GAMS.	Considers degradation of the batteries, demand cycles, and local tariff policies.
Kazda and Li [18]	Optimal operations of natural gas transport networks.	1st Principles. GAMS.	Created piecewise linear models to capture nonlinearities with optimization problem tractability.
Du and Cluett [19]	Operational improvements to existing Naphtha recovery units.	1st Principles and statistical models (Principle Component Analysis). Aspen Plus, Minitab.	Aspen Models released. Statistical models suggest unintuitive options, explained by Aspen model.

Table 1. *Cont.*

Authors/Ref	Application	Models and Software	Comments
		Systems Analysis	
Miller, Gençer, and O'Sullivan [20]	Life cycle analysis (LCA) of integrated solar PV, wind, and batteries.	Empirical/data driven models. SoLCAT (in-house). Ecoinvent. PVWatts.	LCA focused on emissions from use/manufacture of various power sources in several case studies.
Siddiqui, Taimoor, and Almitan. [21]	Supercritical CO_2 Brayton cycles coupled with bottoming cycles.	1st Principles. Aspen HYSYS.	Energy and exergy cycle analysis for working fluid screening.

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