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Editorial: special issue contributed from CHEMECA 2008 - mathematical modeling

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Editorial: special issue contributed from CHEMECA 2008 - mathematical modeling

Abstract

The papers in this issue of Chemical Product and Process Modeling are substantially those that arose from special sessions on "mathematical modeling" at the 36th Australasian Chemical Engineering Conference (held between 28th September to 1st October 2008, in Newcastle, Australia).

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Editorial: Special Issue Contributed from CHEMECA 2008-Mathematical Modeling

Mark I. Nelson, Brent Young, and Harvinder S. Sidhu

Abstract

The papers in this issue of Chemical Product and Process Modeling are substantially those that arose from special sessions on "mathematical modeling" at the 36th Australasian Chemical Engineering Conference (held between 28th September to 1st October 2008, in Newcastle, Australia). The papers in this special issue are available at: www.bepress.com/cppm/vol4/iss3.

KEYWORDS: CHEMECA

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The papers featured in this issue have been revised and extended from CHEMECA and re-reviewed before publication. All the papers in this issue revolve around mathematical modeling. However, this special issue only features a small number of the presentations at CHEMECA that use mathematical modeling. Modeling finds many practical applications within chemical engineering and consequently presentations involving mathematics were featured in many special sessions throughout CHEMECA. Some of these presentations will appear in special issues elsewhere.

The papers in this special issue cover a variety of topics. Gomes et al (<http://www.bepress.com/cppm/vol4/iss3/2>) develop experimental protocols and mathematical models for understanding and characterizing semi-batch emulsion polymerization in the presence of a xanthate-based transfer agent. The development of validated mathematical models in this area will lead to better control of product properties.

The generation of emulsions using micro-scale devices is based upon the breakup of laminar liquid jets. Phan & Evans (<http://www.bepress.com/cppm/vol4/iss3/3>) investigate the breakup of liquid/liquid jets experimentally at Reynolds number as low as 0.4. Three existing mathematical models are applied to predict droplet size. None of these is found to adequately describe jet breakup.

There is a growing demand for steel having a carbon content in the ultra low range (<30 ppm). Mondal et al (<http://www.bepress.com/cppm/vol4/iss3/4>) use computational fluid dynamics to study the Revolutionary Degassing Activator (REDA) method. It has been claimed that the REDA process can achieve carbon content below 10ppm. They find that the design of the snorkel significantly affects the melt circulation of the bath.

Methyl methacrylate is a precursor to several commercially important polymers. The standard process to manufacture it produces large quantities of toxic byproducts which have promoted new research into alternative methods of synthesis via methacrolein and methacrylic acid intermediates. Kendell et al (<http://www.bepress.com/cppm/vol4/iss3/5>) report upon a kinetic simulation of methacrolein and lactone production from the catalytic oxidation of iso-butane over lanthanide phosphomolybdates.

The choice of the control system remains a critical issue in many industrial processes. But process operability does not depend entirely upon the control system as it also depends upon the inherent properties of the process itself. Santoso et al. (<http://www.bepress.com/cppm/vol4/iss3/6>) investigate these issues

by presenting a dynamic operability analysis of a Methyl Tertiary Butyl Ether (MTBE) reactive distillation column. The effects of two design parameters, the reboiler duty and the reflux ratio, on the operability of the reactive distillation system are studied. The method developed to investigate these problems has the advantage that it can be used in the early design stages when knowledge of the process is limited.

A long standing problem in the process industry is stiction in a control valve. This can lead to oscillations in process variables which lead to lower product quality and productivity. It also accelerates equipment wear and tear. Zabiri & Samyudia (<http://www.bepress.com/cppm/vol4/iss3/7>) apply the Mixed-Integer Quadratic Programming (MIQP)-based Model Predictive Controller (MPC) to a system with the control valve stiction. Simulation studies show that MIQP-based MPC can improve the closed-loop performance of a fluid catalytic cracking unit subject to stiction by reducing oscillations in the process variables.

Heat stress and skin burns are occupational hazards for firefighters. Mercer & Sidhu (<http://www.bepress.com/cppm/vol4/iss3/8>) show how by combining classic heat-transfer principles with knowledge of the heat-transfer characteristics of the skin the performance of novel protective clothing that has an embedded phase change layer can be investigated. The mathematical model is used to predict the duration of fire exposure during which the garment is able to protect the firefighter from getting first and second degree burns. It is shown that substantial improvements in the thermal performance of the clothing can be achieved if clothing can be designed to have a minimum air gap between the clothing and the wearer.

The use of simple one-step irreversible reaction models has provided many insights into the phenomena of combustion. However, they do not qualitatively describe all processes occurring in flames. Thus there is a growing interest in the use of two-step mechanisms to predict the generic behavior of flames. Sidhu et al (<http://www.bepress.com/cppm/vol4/iss3/9>) provide a numerical investigation into traveling nonadiabatic combustion waves for the case of a two-step chain branching reaction mechanism. The extinction behavior for nonadiabatic systems is shown to be quite different for that of their adiabatic counterparts.

Counter-flow burners have long provided a standard geometry for studying combustion and extinction processes in diffusion and premixed flames. Luo et al (<http://www.bepress.com/cppm/vol4/iss3/10>) report on the first systematic investigation into the structure of a three-dimensional methane-air counter-flow

non-premixed flame. After validating the model it was used to carefully examine the self-similarity assumptions normally invoked in simulating counter-flow non-premixed flames.

Tham et al (<http://www.bepress.com/cppm/vol4/iss3/11>) report on a two-dimensional computational fluid dynamics simulation for the ohmic heating of whole milk solutions in an annular geometry. The authors investigate how the applied voltage and flow rate affect the temperature field and the concentration profile of the protein types in the solution. The implications of the concentration and temperature distributions for fouling on the electrode surfaces are discussed.

The molecule CF_3I has been identified, in both experimental and modeling studies, as one of the effective and efficient fire suppressants. Luo et al (<http://www.bepress.com/cppm/vol4/iss3/12>) extend earlier investigations by systematically studying the inhibition of premixed flames in the presence of CF_3I . The reaction mechanism comprised 100 species and 880 reverse reaction steps. Reaction pathway analysis identified four major inhibition cycles. A linear expression is developed linking the normalized rate of heat release with the ratio of laminar burning velocities of mitigated and non-mitigated flames.

A key process unit of a strip mill in a steel plant is the reheating furnace, in which slabs are heated to uniform target temperatures. Considerable energy savings can be achieved by ensuring that the discharged slabs are heated as closely as possible to the target temperature. Waelen et al

(<http://www.bepress.com/cppm/vol4/iss3/13>) developed a novel supervisory control system for a boutique, walking beam-type, natural gas-fired industrial reheating furnace run by New Zealand Steel. Compared to other reheating furnaces the control problem considered here is complicated because a temporary steady state solution is not attainable. A control system is developed to provide furnace temperature set points for the operators by solving a two-dimensional slab conduction and radiation model in real time. The heat-transfer models are steel grade specific. The estimated control performance is at least as good as that currently achieved manually.

In the final paper of the special issue, Nelson et al

(<http://www.bepress.com/cppm/vol4/iss3/14>) investigate the behavior of a reaction described by Michaelis-Menten kinetics in an immobilized enzyme reactor in which the catalyst must be activated before the reaction can proceed. It is shown that the concentration of product is maximized at low residence times whereas the productivity of the reactor is maximized at high residence times.