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Editorial: Special Issue Contributed by the 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008

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Abstract

The 10th International Chemical and Biological Engineering Conference - CHEMPOR 2008, was held in Braga, Portugal, from the 4th to the 6th of September, 2008. The conference was jointly organized by the University of Minho, the "Ordem dos Engenheiros," and the Institute for Biotechnology and Bioengineeing, with the support of "Sociedade Portuguesa de Química" and "Sociedade Portuguesa de Biotecnologia".

The CHEMPOR series traditionally brings together both young and established researchers and end users to discuss recent developments in different areas of Chemical Engineering. The scope of this edition was extended to Biological Engineering research. One of the major core areas of the conference program was life quality, due to the importance that Chemical and Biological Engineering plays in this area. "Integration of Life Sciences & Engineering" and "Sustainable Process-Product Development through Green Chemistry" were two of the leading themes with papers addressing such important issues. This was complemented with additional leading themes including "Advancing the Chemical and Biological Engineering Fundamentals," "Multi-Scale and/or Multi-Disciplinary Approach to Process-Product Innovation", "Systematic Methods and Tools for Managing the Complexity", and "Educating Chemical and Biological Engineers for Coming Challenges." Papers contributed for this special issue represent a good sample of the important themes that were addressed.

This special issue presents a set of fifteen selected research papers, which have undergone the peer-review process of Chemical Product and Process Modeling journal. We wish to thank the authors who have contributed to yield a high scientific standard to this special issue. We also extend our gratefulness to all reviewers, through their dedicated efforts, having assisted us in this task.

KEYWORDS: Process-Product Innovation, Systematic Methods and Tools for Managing the Complexity, Sustainable Process-Product Development

Summary of Papers

In the first paper Filipe *et al*. analyzed the use of performance indicators for the design of reactive distillation columns, in particular a cost indicator previously used in the classification and screening of several thousands of preliminary designs. A further refinement of this indicator was proposed, with the incorporation of an additional term, which accounts for the cost of catalyst. This ensures a more stringent choice of candidate configurations at the early stages of design.

In the second paper Chernykh *et al.* presents ChemPAK, a software package for kinetics scheme evaluation. ChemPAK works with the systems of chemical reactions stored in the network database or obtained via the package interface. The program automatically generates a numerical model of the chemical reaction system, allowing the user to adjust the chemical kinetic scheme, and to promptly evaluate the resulting scheme.

In the third paper Brito *et al*. address the modification of the Maxwell-Stefan model, by considering both the concentration polarization and the transport through the membrane. The modified model was tested for the simulation of Dextran T70 aqueous solutions filtration. Numerical simulations by solving the model equations with an adaptive resolution algorithm, based on the Adaptive Method of Lines, determined the concentration profiles in the polarization layer and inside the membrane pore. The authors have shown that the formation of significant solute accumulation at the membrane/polarization interface leads to high levels of apparent rejection.

In the fourth paper Springer *et al*. have studied the repartition of the wall shear stress on cylindrical, square, triangular and hybrid channels by numerical simulation. The authors aimed at establishing predictions for different commercial ceramic membranes and predict the geometry that tends to enhance mass transport characteristics by enhancing hydrodynamics conditions. Numerical simulations were performed over a typical range of Reynolds numbers inside different channel geometry under laminar and turbulent conditions. This work intended to enhance the performances of these processes by maximizing the average wall shear stress on the membrane surface by numerical simulation. A comparison with experimental results has been realized and a good agreement was obtained. A new membrane was designed according to the whole CFD results consistent with experimental results.

The next tree papers (Cuel *et al.*; Furlan *et al.*; Silva *et al.*) are concerned with adsorption processes. Cuel *et al*. applied a new transient simulation method, called the sequencing method, to solve a model representing a fixed bed adsorption column. In each time step, convection and mass transfer were applied successively on the column's mesh. Numerical simulations were given for linear adsorption isotherms. These results were compared with the traditional finite difference method. The results have shown that the sequencing method yields excellent fluid and solid concentration profiles along the column's length and a more accurate prediction of breakthrough time than the finite difference method. The removal of reactive dyes from the textile industry through a combined coagulation/adsorption in fixed bed columns was studied by Furlan *et al.* Adsorption results for the reactive dyes were analyzed by Langmuir and Freundlich isotherm models and showed good correlation. The presence of sodium chloride in the mixture resulted in significant adsorption improvement. The influence of increased temperature plus sodium chloride on the dye removal from aqueous solution showed the feasibility of adsorption and its endothermic nature. In the paper by Silva *et al.* a mathematical model was proposed to simulate a supercritical fluid extraction unit. The model was solved using the method of lines and finite differences with flow correction. Experimental data was fitted fairly well by both models with equivalent accuracy. Two operating regimes were detected in the selected experimental conditions: equilibrium and mass transfer controlled. The last one was more difficult to simulate, requiring specific mass transfer parameters for series and parallel alternatives, for its accurate representation.

The paper by Esquivel *et al.* addresses the effects of temperature and antioxidant extracts concentration on the induction time of vegetable oils using a sequence of simple factorial designs. The antioxidant extracts were obtained from aromatic plants by hydrodistillation followed by liquid-liquid extraction using diisopropyl ether as a solvent. Vegetable oils and lard were spiked with those extracts and then subjected to oxidation in a Rancimat apparatus. A simple equation was derived trying to relate the induction time with the extract concentration. The model was validated with data obtained from rosemary, peppermint, lemon balm and marjoram in virgin olive oil and sunflower oil.

The fluidization behaviour of three geometrical shaped food particulates - cylindrical (beans), parallelepiped (potato) and spherical (green peas) - with change in moisture content in a fluidized bed dryer is addressed in the paper by

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Senadeera. An empirical relationship was developed for change of minimum fluidization velocity with moisture content during drying for cylindrical particulates for the L:D ratio 1:1, and spherical behaviour was best fitted to the linear model. The experimentally determined minimum fluidisation velocities were compared with predicted minimum fluidization velocities using a generalised equation.

The paper by Nucci et al. is concerned with the application of fuzzy logic to a Penicillin G acylase (PGA) production process in a bench-scale bioreactor. Several variables were tested to identify the best fuzzy inputs. The results have shown that batch time, carbon dioxide concentration and its derivate were the best choice. The fuzzy algorithm could accurately infer the time for bioreactor harvesting and the output linguistic variable "stop cultivation" was defined between 0 and 100% certainty. The best experimental result was obtained when the dissolved oxygen concentration was maintained close to 0.5% of saturation.

The paper by Curvelo-Santana et al. aimed at finding optimal conditions to use the amylases from *A. niger* in starch hydrolysis and alcohol production from manioc root starch. New models for starch hydrolysis kinetics were compared for substratum dependence. Results have shown that exponential models fitted better than Michaelis-Menten model.

Redundant measurements in the air quality monitoring network of Lisbon and Tagus Valley were evaluated by Pires *et al.*. The minimum number of monitoring sites that should operate was determined using principal component analysis (PCA). The air pollution data (CO, NO_2, PM_{10} and O_3) was collected in twenty monitoring sites. The principal components were selected representing at least 95% of the original data variance. The PCA results showed that, from twenty studied monitoring sites, only ten for CO, eleven for NO_2, five for O_3 and nine for PM_{10} were needed to characterize the region. The air pollutant analysers corresponding to the redundant measurements can be installed in non-monitored regions, allowing the enlargement of the air quality monitoring network.

In Koçak's paper a SIMULINK® application is presented to solve a benchmark feedback control problem. The controller's task is to raise the temperature of a heterogeneous batch reactor to a certain level as rapidly as possible, with minimum overshoot, and maintain it for the remainder of the reaction. A non-linear S-function block is introduced for housing both the reactor and the temperature control loop.

In a paper by Eslamloueyan & Hosseinzadeh a predictive control system based on neural network model of process is presented for handling and suppressing riser-slugging flow regime that can occur in multiphase pipeline-riser systems. An ANN model of the plant is used to predict future response of the nonlinear process. The authors argued that the proposed neural model predictive controller improved significantly the set-point tracking especially for higher step change in the set-point value.

We hope you enjoy reading this special issue of the CPPM journal dedicated to CHEMPOR2008 as much as we have enjoyed compiling it!

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