Special Issue on Feature Papers for Celebrating the Fifth Anniversary of the Founding of Processes

Authors:

Michael A. Henson

Abstract:

The Special Issue "Feature Papers for Celebrating the Fifth Anniversary of the Founding of Processes„ represents a landmark for this open access journal covering chemical, biological, materials, pharmaceutical, and environmental systems as well as general computational methods for process and systems engineering. [...]

Special Issue on Feature Papers for Celebrating the Fifth Anniversary of the Founding of *Processes*

Michael A. Henson

Department of Chemical Engineering and the Institute for Applied Life Sciences, University of Massachusetts Amherst, N527 Life Sciences Laboratories, 240 Thatcher Way, Amherst, MA 01003, USA; mhenson@umass.edu; Tel.: +01-413-545-3481

The Special Issue "Feature Papers for Celebrating the Fifth Anniversary of the Founding of *Processes*" represents a landmark for this open access journal covering chemical, biological, materials, pharmaceutical, and environmental systems as well as general computational methods for process and systems engineering. The Special Issue is available online at: https://www.mdpi.com/journal/processes/special_issues/Feature_Papers.

Chemical Processes

A major focus of *Processes* is chemical process engineering with applications to both traditional industries and emerging industries for renewable chemicals and energy production. The Special Issue contains four papers in this area. The first paper describes the development and simulation of a model prediction controller for achieving the desired viscosity curve in the continuous production of a non-Newtonian fluid [1]. The second paper addresses the problem of minimizing fuel consumption in fuel gas networks through a superstructure-based method and mixed-integer nonlinear programming [2]. The interesting possibility of extending the favorable characteristics of cuboid packed-bed devices originally designed for chromatographic separations to packed-bed chemical reactors is explored in the third paper [3]. The fourth paper addresses the optimal design of ammonia production plants based on adsorption for unreacted nitrogen and hydrogen recovery and wind energy for electricity generation [4].

Biological Systems

The development of system models and process technology for biological applications is a major focus area of *Processes*. The Special Issue contains five papers in this area. The first paper shows the development of a systems model for investigating patient outcomes from liver surgery and determining the processes responsible for liver failure [5]. The extension of the cybernetic modeling approach to lipid metabolism in mouse bone marrow-derived macrophage cells is the focus of the second paper [6]. The third paper addresses the metabolic modeling of cell-free protein expression through adaptation of a genome-scale metabolic model and direct incorporation of metabolite measurements [7]. The engineering of cuboid packed-bed devices is revisited in the fourth paper by investigating the effect of the length-to-width aspect ratio on chromatographic separation efficiency [8]. The fifth paper reports on the computational development of a novel method for constraint-based metabolic modeling of intracellular glycosylation reactions [9].

Materials Processes

Processes covers a wide range of materials related topics including fundamental modeling, process technology, and applications. This diversity is reflected in the Special Issue through six contributions. The first paper provides a literature-based comparison of rotor-stator mixing devices operated in batch

and continuous modes [10]. Two contributions focus on challenges in pharmaceutical manufacturing. The first paper describes the development of a database of multiphase reactions for synthesizing small-molecule pharmaceutical to facilitate investigation of reaction-separation schemes [11], while the second paper provides a complementary study on developing an ontological information infrastructure for integrating data from pharmaceutical manufacturing plants and analytical laboratories [12]. The Special Issue also contains two contributions focusing on polymerization processes. One paper investigates the experimental validation of a kinetic model for thermal spontaneous polymerization of n-butyl acrylate) [13], while the other paper presents a MATLAB-based tool for copolymerization reactivity ratio estimation based on error-in-variables models [14]. The sixth paper in this area addresses the problem of materials processing through the development of a classification method for identifying a promising experimental design region from a literature database [15].

Computational Methods

The development of novel computational methods with applications to systems modeling and engineering is an important area of *Processes*. The Special Issue has two papers in this area. The first paper addresses the problem of model-based experimental design based on global parameter sensitivity measures and demonstrates the application of the methods through a case study on the synthesis of a precursor for protein kinase inhibitors [16]. The second contribution describes the development of a maximum entropy-based simulation method for analysis of metabolic pathways with application to the central metabolism of the mold *Neurospora crassa* [17].

Other Topics

Processes contains an "Other Topics" section to compile papers that do not fit well in the other four sections. The Special Issue contains two papers in this section, both focused on water systems. The first contribution presents a combined feedforward/feedback model predictive control strategy for minimizing disturbance effects in military water networks [18]. The second contribution investigates the problem of optimal capacity planning in seawater desalination systems from a multiscale perspective [19].

The Future of *Processes*

The Special Issue covers a broad range of topics consistent with the mission of *Processes* to become a highly visible outlet for publishing novel studies in systems modeling, process engineering, and associated applications. The journal will continue to solicit high-quality contributions in these domains.

Michael A. Henson
Founding Editor-in-Chief of Processes.

Conflicts of Interest: The author declares no conflicts of interest.

References

1. Mei, R.; Grosso, M.; Corominas, F.; Baratti, R.; Tronci, S. Multivariable Real-Time Control of Viscosity Curve for a Continuous Production Process of a Non-Newtonian Fluid. *Processes* **2018**, *6*, 12. [CrossRef]
2. Li, J.; Demirel, S.; Hasan, M. Fuel Gas Network Synthesis Using Block Superstructure. *Processes* **2018**, *6*, 23. [CrossRef]
3. Ghosh, R. Cuboid Packed-Beds as Chemical Reactors? *Processes* **2018**, *6*, 44. [CrossRef]
4. Palys, M.; McCormick, A.; Cussler, E.; Daoutidis, P. Modeling and Optimal Design of Absorbent Enhanced Ammonia Synthesis. *Processes* **2018**, *6*, 91. [CrossRef]
5. Verma, B.; Subramaniam, P.; Vadigepalli, R. Modeling the Dynamics of Human Liver Failure Post Liver Resection. *Processes* **2018**, *6*, 115. [CrossRef]

6. Aboulmouna, L.; Gupta, S.; Maurya, M.; DeVilbiss, F.; Subramaniam, S.; Ramkrishna, D. A Cybernetic Approach to Modeling Lipid Metabolism in Mammalian Cells. *Processes* **2018**, *6*, 126. [CrossRef]

7. Dai, D.; Horvath, N.; Varner, J. Dynamic Sequence Specific Constraint-Based Modeling of Cell-Free Protein Synthesis. *Processes* **2018**, *6*, 132. [CrossRef]

8. Chen, G.; Ghosh, R. Effect of the Length-to-Width Aspect Ratio of a Cuboid Packed-Bed Device on Efficiency of Chromatographic Separation. *Processes* **2018**, *6*, 160. [CrossRef]

9. Hutter, S.; Wolf, M.; Papili Gao, N.; Lepori, D.; Schweigler, T.; Morbidelli, M.; Gunawan, R. Glycosylation Flux Analysis of Immunoglobulin G in Chinese Hamster Ovary Perfusion Cell Culture. *Processes* **2018**, *6*, 176. [CrossRef]

10. Håkansson, A. Rotor-Stator Mixers: From Batch to Continuous Mode of Operation—A Review. *Processes* **2018**, *6*, 32. [CrossRef]

11. Papadakis, E.; Anantpinijwatna, A.; Woodley, J.; Gani, R. A Reaction Database for Small Molecule Pharmaceutical Processes Integrated with Process Information. *Processes* **2017**, *5*, 58. [CrossRef]

12. Cao, H.; Mushnoori, S.; Higgins, B.; Kollipara, C.; Fermier, A.; Hausner, D.; Jha, S.; Singh, R.; Ierapetritou, M.; Ramachandran, R. A Systematic Framework for Data Management and Integration in a Continuous Pharmaceutical Manufacturing Processing Line. *Processes* **2018**, *6*, 53. [CrossRef]

13. Riazi, H.; Shamsabadi, A.; Corcoran, P.; Grady, M.; Rappe, A.; Soroush, M. On the Thermal Self-Initiation Reaction of n-Butyl Acrylate in Free-Radical Polymerization. *Processes* **2018**, *6*, 3. [CrossRef]

14. Scott, A.; Penlidis, A. Computational Package for Copolymerization Reactivity Ratio Estimation: Improved Access to the Error-in-Variables-Model. *Processes* **2018**, *6*, 8. [CrossRef]

15. McBride, M.; Persson, N.; Reichmanis, E.; Grover, M. Solving Materials' Small Data Problem with Dynamic Experimental Databases. *Processes* **2018**, *6*, 79. [CrossRef]

16. Schenkendorf, R.; Xie, X.; Rehbein, M.; Scholl, S.; Krewer, U. The Impact of Global Sensitivities and Design Measures in Model-Based Optimal Experimental Design. *Processes* **2018**, *6*, 27. [CrossRef]

17. Cannon, W.; Zucker, J.; Baxter, D.; Kumar, N.; Baker, S.; Hurley, J.; Dunlap, J. Prediction of Metabolite Concentrations, Rate Constants and Post-Translational Regulation Using Maximum Entropy-Based Simulations with Application to Central Metabolism of *Neurospora crassa*. *Processes* **2018**, *6*, 63. [CrossRef]

18. James, C.; Webber, M.; Edgar, T. Minimizing the Effect of Substantial Perturbations in Military Water Systems for Increased Resilience and Efficiency. *Processes* **2017**, *5*, 60. [CrossRef]

19. Baaqeel, H.; El-Halwagi, M.M. Optimal Multiscale Capacity Planning in Seawater Desalination Systems. *Processes* **2018**, *6*, 68. [CrossRef]