

CHEMICAL PRODUCT AND PROCESS MODELING

EDITORS-IN-CHIEF

Rahmat Sotudeh-Gharebagh, University of Tehran, Iran

Navid Mostoufi, University of Tehran, Iran

Jamal Chaouki, Ecole Polytechnique de Montreal, Canada

ASSOCIATE EDITORS

Ricardo Aguilar-López, CINVESTAV-IPN, México

Sameer Al-Asheh, Jordan University of Science and Technology, Jordan

Adel Al-Taweel, Dalhousie University, Canada

Costin Sorin Bildea, University Politehnica of Bucharest, Romania

Miryan Cassanello, Universidad de Buenos Aires, Argentina

Alkis Constantinides, Rutgers, State University of New Jersey, USA

Marc-Olivier Coppens, University College London, UK

Mario R. Eden, Auburn University, USA

Eugénio C. Ferreira, Universidade do Minho, Portugal

Iftekhar Karimi, National University of Singapore, Singapore

Eugeny Kenig, University of Paderborn, Germany

Jiri Klemes, University of Pannonia, Hungary

Andrzej Kraslawski, University of Lappeenranta, Finland

Surendra Kumar, Indian Institute of Technology Roorkee, India

Jae W. Lee, The City College of New York, USA

Patrick Linke, Texas A&M University at Qatar, Qatar

Norman W. Loney, New Jersey Institute of Technology, USA

Davide Manca, Politecnico di Milano, Italy

Mark Nelson, University of Wollongong, Australia

Heinz A. Preisig, Norwegian University of Science and Technology, Norway

Fernando Preto, CANMET Energy Technology Centre, Canada

Todd Pugsley, University of Saskatchewan, Canada

Luis Puigjaner, Universitat Politecnica de Catalunya, Spain

Jean-Michel Reneaume, Ecole Nationale Supérieure en Génie des Technologies Industrielles, ENSGTI, France

Sohrab Rohani, University of Western Ontario, Canada

Panos Seferlis, Aristotle University of Thessaloniki and Centre for Research and Technology, Greece

Paul Stuart, Ecole Polytechnique de Montreal, Canada

Bill Svrcek, University of Calgary, Canada

Jan Verstraete, IFP Energies nouvelles, France

Johan Warna, Abo Akademi University, Finland

Joachim Werther, Technical University Hamburg, Germany

Brent Young, University of Auckland, New Zealand

Yifang Zhu, UCLA School of Public Health, USA

ABSTRACTED/INDEXED IN Celdes; CNKI Scholar (China National Knowledge Infrastructure); CNPIEC; EBSCO Discovery Service; Elsevier: Compendex, Engineering Village, SCOPUS; Google Scholar; Inspec; J-Gate; Naviga (Softweco); Polymer Library; Primo Central (ExLibris); ProQuest: Advanced Technologies Database with Aerospace, Aerospace Database, Aluminium Industry Abstracts, ANTE: Abstracts in New Technologies and Engineering, Ceramic Abstracts/World Ceramics Abstracts, Civil Engineering Abstracts, Computer and Information Systems Abstracts, Copper Technical Reference Library, Corrosion Abstracts, Earthquake Engineering Abstracts, Electronics and Communications Abstracts, Engineered Materials Abstracts, Engineering Research Database, Materials Business File, Materials Research Database, Mechanical & Transportation Engineering Abstracts, METADEX (Metals Abstracts), Solid State and Superconductivity Abstracts, Technology Research Database; SCImago (SJR); Summon (Serials Solutions/ProQuest); TDOne (TDNet); WorldCat (OCLC)

Chemical Product and Process Modeling (CPPM) is the premier forum for theoretical and applied research on product and process modeling, simulation and optimization. Thanks to its international editorial board, the journal assembles the best papers from around the world on modern modeling, simulation and optimization techniques and it also covers the gap between product and process. The range of topics includes equation-oriented modeling and simulation, sequential and modular simulation, performance of industrial process simulators, computational fluid dynamics, environmental, food, pharmaceutical and fine chemical process modeling. The journal brings together chemical engineering researchers, practitioners, and software developers in a new forum for the international modeling and simulation community. Editors represent top engineering institutions across the globe, such as the University of Tehran, the Ecole Polytechnique de Montreal, Rutgers, Indian Institute of Technology, the Technical University Hamburg, and the University of Buenos Aires.

The publisher, together with the authors and editors, has taken great pains to ensure that all information presented in this work (programs, applications, amounts, dosages, etc.) reflects the standard of knowledge at the time of publication. Despite careful manuscript preparation and proof correction, errors can nevertheless occur. Authors, editors and publisher disclaim all responsibility for any errors or omissions or liability for the results obtained from use of the information, or parts thereof, contained in this work.

The citation of registered names, trade names, trademarks, etc. in this work does not imply, even in the absence of a specific statement, that such names are exempt from laws and regulations protecting trademarks etc. and therefore free for general use.

ISSN 2194-6159 · e-ISSN 1934-2659

All information regarding notes for contributors, subscriptions, Open Access, back volumes and orders is available online at www.degruyter.com/cppm.

RESPONSIBLE EDITOR Rahmat Sotudeh-Gharebagh, Department of Chemical Engineering, College of Engineering, University of Tehran, P.O. Box 11155-4563, Tehran, IRAN, Email: sotudeh@ut.ac.ir

JOURNAL MANAGER Theresa Haney, De Gruyter, Genthiner Straße 13, 10785 Berlin, Germany, Tel.: +49 (0)30 260 05 – 375, Fax: +49 (0)30 260 05 – 325, Email: theresa.haney@degruyter.com

RESPONSIBLE FOR ADVERTISEMENTS Panagiota Herbrand, De Gruyter, Mies-van-der-Rohe-Straße 1, 80807 Munich, Germany, Tel.: +49 (0)89 769 02 – 394, Fax: +49 (0)89 769 02 – 350, Email: panagiota.herbrand@degruyter.com

TYPESETTING Integra Software Services Pvt. Ltd., Pondicherry, India

PRINTING Franz X. Stickle Druck und Verlag e.K., Ettenheim

© 2013 Walter de Gruyter GmbH, Berlin/Boston

Printed in Germany



Offenlegung der Inhaber und Beteiligungsverhältnisse gem. § 7a Abs. 1 Ziff. 1, Abs. 2 Ziff. 3 des Berliner Pressegesetzes: Gisela Cram, Rentnerin, Berlin; Dr. Annette Lubasch, Ärztin, Berlin; Elsbeth Cram, Pensionärin, Rosengarten-Alvesen; Margret Cram, Studienrätin i. R., Berlin; Brigitta Duvenbeck, Oberstudienrätin i. R., Bad Homburg; Dr. Georg-Martin Cram, Unternehmens-Systemberater, Stadtbergen; Maike Cram, Berlin; Jens Cram, Mannheim; Renate Tran, Zürich; Gudula Gädeke M.A., Atemtherapeutin/Lehrerin, Tübingen; Martin Gädeke, Einzelunternehmer, Würzburg; John-Walter Siebert, Pfarrer, Oberstenfeld; Dr. Christa Schütz, Ärztin, Mannheim; Sonja Schütz, Berlin; Dorothee Seils, Apothekerin, Stuttgart; Gabriele Seils, Journalistin, Berlin; Ingrid Cram, Betriebsleiterin, Tuxpan / Michoacan (Mexiko); Sabina Cram, Mexico DF (Mexiko); Dr. Clara-Eugenie Seils, Oberstudienrätin i.R., Reppenstedt; Christoph Seils, Journalist, Berlin; Susanne Cram-Gomez, Mexico DF (Mexiko); Silke Cram, Wissenschaftlerin, Mexico DF (Mexiko); Björn Cram, Aachen; Ella Anita Cram, Rentnerin, Berlin; Dr. Sven Fund, geschäftsführender Gesellschafter, Berlin; Walter de Gruyter Stiftung, Berlin; Berit Cram, Greifswald; Walter Cram-Heydrich, Mexico DF (Mexico), Juliane Schütz, Berlin; Antje Schütz, Berlin; Valentin Schütz, Berlin.

Contents

Santhi Raju Pilli, Tamal Banerjee, and
Kaustubha Mohanty

**Ionic Liquids as Green Solvents for the Extraction of
Endosulfan from Aqueous Solution: A Quantum
Chemical Approach — 1**

R. Karthikeyan, K. Manickavasagam, Shikha Tripathi,
and K.V.V. Murthy

**Neuro-Fuzzy-Based Control for Parallel Cascade
Control — 15**

Arun Gupta, Patrick Jordan and Shusheng Pang
**Modelling the Heat and Mass Transfer during Hot
Pressing of Medium Density Fibreboard — 27**

Seyed Hashem Samadi, Barat Ghobadian, GholamHassan
Najafi, Ali Motevali, and Saeid Faal

**Drying of Apple Slices in Combined Heat and Power
(CHP) Dryer: Comparison of Mathematical Models and
Neural Networks — 41**

Amit Kumar Singh, Barjeev Tyagi, and Vishal Kumar

**First Principle Modeling and Neural Network–Based
Empirical Modeling with Experimental Validation of
Binary Distillation Column — 53**

Ali Akbar Amooey

**The Correlation of Activity Coefficients of Ionic Species
of Aqueous Electrolytes Using a New Model — 71**

