Reaction Chemistry & Engineering

Bridging the gap between chemistry and chemical engineering rsc.li/reaction-engineering

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2058-9883 CODEN RCEEBW 8(9) 2099-2376 (2023)



Cover See Richard J. Whitby *et al.*, pp. 2134–2140. Image reproduced by permission of Dawid Drelinkiewicz from *React. Chem. Eng.*, 2023, **8**, 2134.



Inside cover See Roland Wohlgemuth, pp. 2109–2118. Image reproduced by permission of Roland Wohlgemuth from *React. Chem. Eng.*, 2023, **8**, 2109.

REVIEWS

C ROYAL SOCIETY PAPER OF CHEMISTRY The select-off met

2109

Route selection and reaction engineering for sustainable metabolite synthesis

Roland Wohlgemuth*



2119

Combining computational fluid dynamics, photon fate simulation and machine learning to optimize continuous-flow photocatalytic systems

Gabriela X. de Oliveira, Simon Kuhn, Humberto G. Riella, Cíntia Soares* and Natan Padoin*



Editorial Staff

Executive Editor Maria Southall

Deputy Editor

Bianca Provost

Editorial Production Manager Cara Sutton

Assistant Editors

Sean Browner, Molly Colgate, Paul Scott, Alison Winder

Editorial Assistant Basita Javeed

Publishing Assistant Allison Holloway

Publisher

Sam Keltie

For queries about submitted papers, please contact Cara Sutton, Editorial Production Manager in the first instance. E-mail: reactionchemeng@rsc.org

For pre-submission queries please contact Maria Southall, Executive Editor. E-mail: reactionchemeng-rsc@rsc.org

Reaction Chemistry & Engineering (electronic: ISSN 2058-9883) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park,

Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry Thomas Graham House, Science Park, Milton Road, Cambridge,

CB4 OWF, UK

Tel +44 (0)1223 432398; E-mail: orders@rsc.org

2023 Annual (electronic) subscription price: £2584; \$4262. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office Burlington House, Piccadilly, London W1J 0BA, UK,

Telephone: +44 (0) 207 4378 6556. Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail: advertising@rsc.org

For marketing opportunities relating to this journal. contact marketing@rsc.org

Reaction Chemistry & Engineering

rsc.li/reaction-engineering

Bridging the gap between chemistry and chemical engineering

Editorial Board

Editor-in-Chief Klavs F Jensen, Massachusetts Institute of Technology, USA Associate Editors Ian R Baxendale, Durham University, UK Richard Bourne, University of Leeds, UK

Saif A Khan, National University of Singapore, Singapore Francesca Paradisi, University of Bern, Switzerland Laura Torrente, University of Cambridge, UK Haihui Wang, Tsinghua University, China

Oliver Kappe, University of Graz, Austria

Beata Kilos-Réaume, Dow, USA

Laboratory, India

Thessaloniki, Greece

Netherlands

Slovenia

Australia

USA

Alexander Katz, University of California, Berkeley,

Francesca Kerton, Memorial University, Canada

Dong Pyo Kim, POSTECH, Republic of Korea

Shu Kobayashi, University of Tokyo, Japan

Amol Kulkarni, National Chemical Research

Alexei Lapkin, University of Cambridge, UK

Hélène Lebel, University of Montreal, Canada

Angeliki Lemonidou, Aristotle University of

Guangsheng Luo, Tsinghua University, China

Haresh Manyar, Queen's University Belfast, UK

Rebecca Meadows, AstraZeneca, UK

Shane Grosser Merck USA Petra de Jongh Utrecht University Netherlands

Members

NJ, USA

Germany

USA

Belgium

Heather Kulik, Massachusetts Institute of Technology, USA Anita Maguire, University College Cork, Ireland Megan Smyth, Almac Sciences

Rebecca Ruck, Merck & Co. Inc., Kenilworth.

Andrew Rutter, GlaxoSmithKline, UK

Susannah Scott, UC Santa Barbara, USA

Doris Segets, University of Duisburg-Essen,

Annette Taylor, University of Sheffield, UK

Enrico Tronconi, University of Milan, Italy

Veronique Van Speybroeck, Ghent University,

Dionisios G Vlachos, University of Delaware, USA

Ning Sun, Lawrence Berkeley National Laboratory,

Basu Saha, Lancaster Univeristy, UK

Jay Siegel, Tianjin University, China

Manish Sharma, BASF, USA

Advisory Board

Malcolm Berry, MB Chemistry Consulting Ltd., UK Claude de Bellefon, University of Lyon, France Donna G Blackmond, Scripps Research Institute, USA

Wayne Blaylock, Dow Chemical Company, USA Cara Brocklehurst, Novartis AG, Switzerland Jian-Feng Chen, Beijing University of Chemical Technology, China

Ya-Huei Chin, University of Toronto, Canada Evelina Colacino, University of Montpellier, France Avelino Corma, Polytechnical University of Valencia. Spain

Anna Croft, University of Nottingham, UK Paul Dauenhauer, University of Minnesota, USA Stevan Djuric, Abbvie, USA

Raj Gounder, Purdue University, USA Raju Kumar Gupta, Indian Institute of Technology Kanpur, India

Dorota Gryko, Polish Academy of Sciences, Poland Ryan Hartman, New York University, USA

Joel M Hawkins, Pfizer Worldwide R&D, USA Ive Hermans, University of Wisconsin- Madison,

Volker Hessel, University of Adelaide, Australia Lin Huang, Trunk & Petal Pte Ltd., Singapore Marty Johnson, Eli Lillv. USA

Information for Authors

Full details on how to submit material for publication in Reaction Chemistry & Engineering are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made via the journal's homepage: rsc.li/reaction-engineering. Submissions: The journal welcomes submissions of manuscripts for publication as Review Articles and Minireviews, Full Papers and Communications should describe original work of high quality and impact.

Additional details are available from the Editorial Office or http://www.rsc.org/authors

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)-Reproduced by permission of the Royal Society of Chemistry

Massimo Morbidelli, Milano Politecnico, Italy Siegfried Waldvogel, Johannes Gutenberg Timothy Noël, University of Amsterdam, Universität Mainz, Germany Robin White, Luxembourg Institute for Science & Matthew O'Brian, Keele University, UK Technology, Luxembourg Tatsuya Okubo, University of Tokyo, Japan Karen Wilson, RMIT University, Australia Polona Žnidaršič Plazl, University of Ljubljana, Sheryl L. Wiskur, University of South Carolina, USA Wen-De Xiao, Shanghai Jiao Tong University, Anastasios Polyzos, University of Melbourne, China Zhen Yao, Zhejiang University, China Jeffrey Rimer, University of Houston, USA This journal is © The Royal Society of Chemistry 2023. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the

Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

ROYAL SOCIETY OF CHEMISTRY



2134

The switch-off method: rapid investigation of flow photochemical reactions

Dawid Drelinkiewicz, Stephen T. Alston, Thomas Durand and Richard J. Whitby*





2141

Tuning the catalytic performance of a Cu supported silica modified $\gamma\text{-Al}_2\text{O}_3$ nanocatalyst via cobalt-doping for A^3-coupling

Manpreet Kaur, Shally Sharma, Anu Choudhary and Satya Paul*



2156

You get what you screen for: a benchmark analysis of leaf branch compost cutinase variants for polyethylene terephthalate (PET) degradation

Stefanie Fritzsche, Florentin Tischer, Wolfgang Peukert and Kathrin Castiglione*



2170

Process intensification of continuous-flow seATRP by a sonicated multi-reactor setup

Suqi Zhang, Tanja Junkers and Simon Kuhn*



2177



Aromatic hydroxylation of substituted benzenes by an unspecific peroxygenase from *Aspergillus brasiliensis*

Fabian Schmitz, Katja Koschorreck, Frank Hollmann and Vlada B. Urlacher*



An efficient and green procedure for transformation of thiols to disulfides and thioamides in AGA8 aqueous micelles

Hao Jin, Penghao Liu, Yuxiang Wang, Shuai Zhang, Qi Meng* and Qiaoqiao Teng*

219



Efficient removal of organic dyestuff in water contamination over a MOF-derived Co-based adsorbent

Yuxi Yang, Yaqi Xue, Jing Li, Haihong Xia and Minghao Zhou*





Making photochemistry scalable – an operationally simple falling film looping photoreactor

Shibu Naskar, Daniel Kowalczyk, Susital Mal, Subrata Das,* Debabrata Mandal, Prakash Kumar and Dirk Ziegenbalg*

2223

Effect of temperature on the CO_2 splitting rate in a DBD microreactor

Deema Khunda, Sirui Li, Nikolay Cherkasov, Mohamed Z. M. Rishard, Alan L. Chaffee and Evgeny V. Rebrov*



2234

Mechanistic modeling, parametric study, and optimization of immobilization of enzymatic cascades in porous particles

Leandros Paschalidis, Sara Arana-Peña, Volker Sieber and Jakob Burger*



2245

Relationship between feeding strategies and nitrogen sources in platform chemical bio-based 2,3-butanediol production in fed-batch fermentation

Daniel Tinôco,* Rui de Paula Vieira de Castro, Douglas Teixeira, Francisco de Assis Beltrão Junior, Eduardo de Oliveira Júnior, Paulo Luiz de Andrade Coutinho and Denise Maria Guimarães Freire



2258

Rare-earth doped hexagonal NaYbF₄ nanoprobes with size-controlled and NIR-II emission for multifunctional applications

Yu Min, Xin Ding, Bing Yu,* Hailin Cong* and Youqing Shen





From at-line to online NMR: coupling probe-based autosampler with benchtop NMR

Yining Ji,* Zhihao Lin,* Latevi Lawson,* François Lévesque, David A. Foley, Robert Espina and Hector Robert

Multi-platform synthesis of ondansetron featuring process intensification in flow

Yoshio Hato and Timothy F. Jamison*

2284

2275



[Flow]

Single-task ML Optimizer

SeMOpt

Step 2 [ref. 12]

Dt

Equipping data-driven experiment planning for Selfdriving Laboratories with semantic memory: case studies of transfer learning in chemical reaction optimization

Riley J. Hickman, Jurģis Ruža, Hermann Tribukait,* Loïc M. Roch* and Alberto García-Durán



Optimizing dissolved gas composition in a doublebath-type sonoreactor for efficient production of ultrasonic-activated water with stable oxygen and nitrogen reactive species

Bao-Ngoc T. Le, Nguyen-Phuong Nguyen, Thanh-Linh H. Duong, Tri Nguyen, Tien-Cuong Hoang, Hong-Ha T. Nguyen, Dai-Viet N. Vo,* Hoang-Duy P. Nguyen and Thuy-Phuong T. Pham*

2309

Demonstration and experimental model validation of the DME synthesis by reactive distillation in a pilot-scale pressure column

Malte Semmel, Innokentij Bogatykh, Benedikt Steinbach, Jörg Sauer, Jens-Uwe Repke and Ouda Salem*



2323

Magnetic separation of immobilized biocatalyst enables continuous manufacturing with a solidsforming reaction

Colton E. Lagerman, Grant D. Marshall, Matthew A. McDonald, Patrick R. Harris, Martha A. Grover, Ronald W. Rousseau and Andreas S. Bommarius*



2332

Efficient recovery of indium from waste indium tin oxide (ITO) targets by pressure leaching with sulfuric acid

Qianyou Pu, Ba Zhang, Shiwei Zhou,* Yonggang Wei, Bo Li and Hua Wang



2342

Laccase-mediator co-immobilized doped-HKUST-1 cellulose composite beads and their application for the biodegradation of carbazole

Jia Juan, Xue Ping,* Liu Xueping, Xu Chongrui, Gu Yaohua and Li Peng







Dioxygen-triggered oxidation of benzylic C-H bonds: insight on the synergistic effect of Cu-Fe bimetallic oxide

Aniruddha Singha, Anil Chandra Kothari, Rajaram Bal and Biswajit Chowdhury*



Metal-organic framework-supported ionic liquids for lipase immobilization: design, characterization, and investigation of catalytic performance

Hongbo Suo, Qi Qi, Xusheng Dai, Xinyue Geng, Qi Li, Jie Yang, Guoyun Liu,* Renmin Liu* and Lili Xu*