



7th International Conference
on Population Balance Modelling



2022

May 9-11

Lyon - France

Monday, May 9, 2022

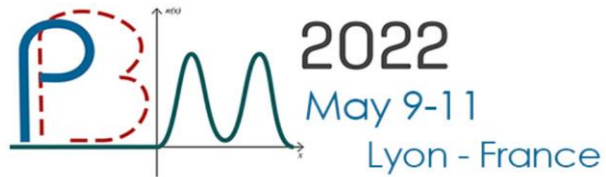
- 08:00-08:30 Registration
08:30-08:45 Welcome and opening
Chair: Heiko Briesen, Technische Universität München / Germany
08:45-09:30 Keynote lecture
Simplifying population balances to promote broader use in industry
R. Bertrum Diemer
University of Delaware / USA

Session 1: PBM for crystallization and precipitation

- 09:30-09:55 *Simulation of continuous Ni-Mn-co hydroxide co-precipitation by compartmental population balance modelling*
Mohsen Shiea, Andrea Querio, Antonio Buffo, Gianluca Boccardo, Daniele Marchisio
Politecnico di Torino / Italy
- 09:55-10:20 *A population balance model for aluminum oxide precipitation in a laminar flow around a burning aluminum particle*
Jannis Finke, Fabian Sewerin
Otto-von-Guericke-Universität Magdeburg / Germany.
- 10:20-10:50 Coffee Break and poster session**
- Chair: Christine Frances, LGC Toulouse / France*
- 10:50-11:15 *Derivation and validation of a novel secondary nucleation rate model for modeling crystallization processes*
Byeongho Ahn, Luca Bosetti, Michele Chen, Marco Mazzotti
ETH Zurich / Switzerland
- 11:15-11:40 *Population balance based modeling of diastereomeric salt crystallization process of pregabalin tartrate*
Álmos Botond Orosz, Miklós Hunor Bosits, Hajnalka Pataki, Szalay Zsófia, Ádám Demeter, Botond Szilágyi
Budapest University of Technology and Economics; Gedeon Richter Plc / Hungary
- 11:40-12:05 *Digital design of an agrochemical crystallization process using a two-dimensional population balance modeling approach*
Wei-Lee Wu, Chris Chappelow, Paul Larsen, Jasson Patton, Aaron Shinkle, Zoltan Nagy
Purdue University; Corteva Agriscience / USA
- 12:05-12:30 *Population balance model-based investigation of polymorphic steady-states in continuous crystallization*
Brigitta Bodák, Andraž Košir, Luca Bosetti, Ramona Achermann, Marco Mazzotti
ETH Zurich / Switzerland
- 12:30-13:30 Lunch break and poster session**



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Session 2: PBM for liquid / liquid systems

Chair: Frederic Augier, IFP Energies Nouvelles / France

- 13:30-13:55 *A modelling perspective of the breakage phenomena from single oil droplet breakage experiments in turbulent flow*
Nicolas La Forgia, Hugo Atle Jakobsen
Norwegian University of Science and Technology / Norway.
- 13:55-14:20 *PBM modelling of single and double emulsions preparation using static mixers*
Noureddine Lebaz, Nida Othman
University of Lyon / France.
- 14:20-14:45 *PBM modelling of Pickering emulsions for Janus particles synthesis*
Graziano Frungieri, Heiko Briesen
Technische Universität München / Germany
- 14:45-15:10 *Modeling of surfactant and drop size dynamics in counter-current extraction columns*
Ville Alopaeus
Aalto University / Finland
- 15:10-15:50 Coffee Break and poster session**

Session 3: PBM for polymerization and granulation

Chair: Nicodemo Di Pasquale, University of Nottingham / UK

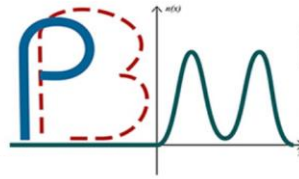
- 15:50-16:15 *Phase inversion prediction during the bulk synthesis of high-impact polystyrene: a population balance approach*
Juan M. Maffi, Diana A. Estenoz
Instituto Tecnológico de Buenos Aires; Instituto de Desarrollo Tecnológico para la Industria Química / Argentina
- 16:15-16:40 *Modelling the molecular weight distribution in a step-growth polymerization process: an inverse problem approach*
Balazs Bordas, Kutup Kurt, Andreas Bamberg, Sebastian Engell
Merck KGaA; TU Dortmund / Germany
- 16:40-17:05 *Granulation of alumina powder in a ploughshare mixer: experimental studies and population balance modeling*
Swati Sahu, Aswin Muthachikavil, Vishnu Masampally, Venkata Sudheendra Buddhiraju, Venkatarmana Runkana
Tata Research Development and Design Centre / India
- 17:05-17:30 *Towards a generic population balance model for twin-screw wet granulation: from material properties to particle size distribution*
Ana Alejandra Barrera Jiménez, Daan Van Hauwermeiren, Kensaku Matsunami, Michiel Peeters, Thomas De Beer, Ingmar Nopens
Ghent University / Belgium

19:00-20:00 - Social activity

Visiting Lyon by boat: Croisières Promenades - Les Bateaux Lyonnais, 2 Quai des Célestins



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Tuesday, May 10, 2022

Chair: Alain Liné, INSA Toulouse / France

08:30-09:15

Keynote lecture

Twenty years of quadrature-based moment methods: What have we learned?

Rodney O. Fox

Iowa State University / USA

Session 1: PBM Modelling and numerical methods

09:15-09:40

Prediction of PSD and grain morphology in SPVC industrial reactors by a combination of multi-scale population balances and Monte Carlo computational methods

Costas Kiparissides, Prokopis Pladis

CERTH, Aristotle University of Thessaloniki / Greece

09:40-10:05

Modelling the collision kernel for non-spherical nanoparticle agglomerates

Maximilian Karsch, Andreas Kronenburg

University of Stuttgart / Germany

10:05-10:30

Identification of Mg(OH)₂ precipitation kinetics with population balances and CFD

Antonello Raponi, Giuseppe Battaglia, Salvatore Romano, Andrea Cipollina, Antonio Buffo, Gianluca Boccardo, Marco Vanni, Daniele Marchisio

Politecnico di Torino; And Università di Palermo / Italy

10:30-11:00

Coffee Break and poster session

Chair: Ville Alopaeus, Aalto University / Finland

11:00-11:25

Parametrization and PBM modelling of the interaction of crystal growth and abrasion

Simon A. Schiele, Rolf Meinhardt, Heiko Briesen

University of Munich / Germany

11:25-11:50

State and parameter estimation for continuous fluidized bed spray agglomeration

Jessica Behrens, Eric Otto, Robert Dürr, Achim Kienle

Max-Planck-Institute for Dynamics of Complex Technical Systems, Otto von Guericke University Magdeburg, and Magdeburg-Stendal University of Applied Sciences / Germany

11:50-12:15

Experimental analysis of aggregate size and population balance modelling using extended Kalman filter

Carole Coufort, Saudejaud, Léa Cot, Christine Frances

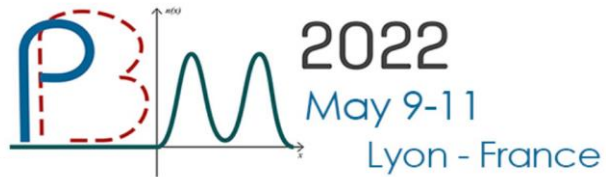
Université de Toulouse / France

12:15-13:30

Lunch break and poster session



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Session 2: Multiscale coupling

Chair: Alfredo Soldati, Vienna University of Technology / Austria; University Udine / Italy

- 13:30-13:55 *Direct numerical simulation of continuous (nano-) particle synthesis for various chemical systems: similarities and differences*
Tobias Schikarski, Marc Avila, Wolfgang Peukert
Friedrich-Alexander-University Erlangen-Nuremberg; University of Bremen / Germany
- 13:55-14:20 *A CFD-DEM coupling approach for the prediction of the coalescence and the breakage kernels in the wet granulation process*
Mohamed HAMOU, Safae EL MISAOU, Achraf NAJIHI, Lhachmi KHAMAR
University of Mohamed VI Polytechnique / Morocco
- 14:20-14:45 *Challenges of the coupling between CFD and PBE in aerated stirred tanks with phase segregation*
Francesco Maluta, Alessandro Paglianti, Giuseppina Montante
University of Bologna / Italy
- 14:45-15:10 *CFD-PBM simulation of the aggregation of yeast particles with air bubbles and coalescence of foam bubbles in a flotation system*
Felix Ulmer, Ali Khajehesamedini
Technical University of Munich / Germany
- 15:10-15:50 Coffee Break and poster session**

Session 3: Analytical and numerical solutions of PB

Chair: Daniele Marchisio, Politecnico di Torino / Italy

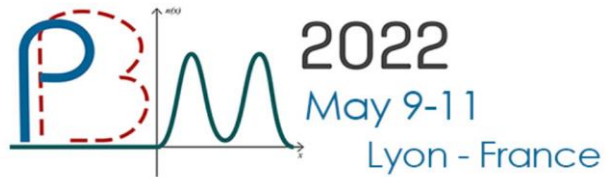
- 15:50-16:15 *Analytical approximate solutions of aggregation and fragmentation population balance equation*
Gurmeet Kaur, Heiko Briesen
Technical University of Munich / Germany
- 16:15-16:40 *A conservative finite volume approach to joint aggregation breakage problems on arbitrary grids*
Daniel O'Sullivan, Stelios Rigopoulos
Imperial College London / UK
- 16:40-17:05 *A Eulerian characteristics-based model reduction approach for the spatially inhomogeneous population balance equation*
Fabian Sewerin
Otto-von-Guericke-Universität Magdeburg / Germany
- 17:05-17:30 *Solution of the bivariate population balance equation using an open-source finite element framework*
Deepak K. Singh, Pablo R. Brito-Parada, Gaurav Bhutani
Indian Institute of Technology Mandi / India; Imperial College London / UK

19:30 – Conference dinner

Restaurant Vatel Lyon, 8 rue Duhamel, Lyon.



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Wednesday, May 11, 2022

Chair: Ingmar Nopens, Ghent University / Belgium

08:30-09:15

Keynote lecture

Control of particle formation in fluidized beds

Achim Kienle

Max Planck Institute and Otto von Guericke; University of Magdeburg / Germany

Session 1: New applications of PBM

09:15-09:40

Influence of density and viscosity on deformation, breakage and coalescence of bubbles in turbulence

Francesca Mangani, Giovanni Soligo, Alessio Roccon, Alfredo Soldati

Institute of Fluid Mechanics and Heat Transfer / Austria; Complex Fluids and Flows Unit / Japan; University of Udine / Italy

09:40-10:05

Population balance model for gravitational separation; axial dispersion and densely packed volume fraction restriction

Moein Assar, Sebastien Charles Simon, Brian Arthur Grimes

Norwegian University of Science and Technology / Norway

10:05-10:30

Population balance equation for porous media: Upscaled dynamics and evolution

Nicodemo Di Pasquale, Matteo Icardi

University of Nottingham / UK

10:30-11:00

Coffee Break and poster session

Chair: Giuseppina Montante, University of Bologna / Italy

11:00-11:25

Modeling the viscosity of boehmite gel structured under shear

Iana Sudreau, Mathilde Auxois, Marion Servel, Sébastien Manneville, Thibault Divoux

IFP Énergies Nouvelles; Université de Lyon / France.

11:25-11:50

Mass based population balance model as a cornerstone for integral modelling of drinking water treatment plants

Beñat Elduayen-Echave, Paloma Grau, Eduardo Ayesa

CEIT-Basque Research and Technology Alliance; Universidad de Nava / Spain

11:50-12:15

Integrating molecular dynamics with population balances to model fresh cement rheology

Juan Pablo Gallo-Molina, Karel Lesage, Ingmar Nopens

Ghent University / Belgium

12:15-12:45

Closing remarks / Poster Award Ceremony