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Editorial

Special Issue on "Recent Advances in Population Balance Modeling"

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Population Balance Modeling (PBM) is a powerful modeling framework that allows the prediction of the dynamics of distributed properties of a population of individuals at the mesoscale. This is of particular interest when such a property is a critical quality attribute of a production system (e.g., particle size distribution and particle composition). The framework found its roots in the chemical engineering field in the 1960s and boomed in the late 1990s with increasing computational power. It is now gaining ground in other application fields, such as pharmaceutical engineering and biotechnology.

Population balance models come in different forms. They can be formulated taking into account different continuous and discrete mechanisms such as nucleation, growth, aggregation and breakage. For these mechanisms, process rates or kernels need to be defined. Calibration and validation of these kernels based on experimental data is of particular interest to secure the model's predictive power and, hence, successful use in scenario analysis for process operational and design optimization.

Moreover, PBM can include one or more distributed properties and either be embedded in a Computational Fluid Dynamics framework or spatial compartments to include the effect of spatial heterogeneities. Recently, it has been integrated with stochastic and machine learning-based approaches as well. Specific numerical and computational burden challenges arise when doing so.

The latest research in this intriguing field of research was discussed at the 6th International Conference on Population Balance Modeling (PBM2018) held in Ghent, Belgium on 7–9 May 2018 organized by Ghent University in collaboration with the Technical University of Denmark and supported by the European Federation of Chemical Engineering (EFCE). The past five International Conferences on Population Balance Modeling, held in Kona (Hawaii, 2000), Valencia (Spain, 2004), Quebec (Canada, 2007), Berlin (Germany, 2010) and Bangalore (India, 2013) have stimulated the increasing interest in the development and application of the PBM framework.

The issue is a reflection of high-quality and invited papers presented at PBM2018, a conference with international participants and several keynote speakers. This Special Issue on "Population Balance Modeling" aims to show the most recent advances in applications, parameter estimation/model calibration, numerical methods and stochastic methods of population balance modeling. As summarized below, this Special Issue provides a collection of twelve papers on original advances in population balance modeling.

1. Applications

This Special Issue contains five contributions covering applications of PBM in a wide range of applications ranging from crystallization, granulation and flotation to social aspects. Majumder [1] discussed the preferential crystallization as a promising separation technology for conglomerate-forming enantiomers, which is a challenge in pharmaceutical

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Citation: Mansouri, S.S.; Briesen, H.; Gernaey, K.V.; Nopens, I. Special Issue on "Recent Advances in Population Balance Modeling". *Processes* **2021**, *9*, 122. https://doi.org/10.3390/pr9010122

Received: 6 January 2021
Accepted: 6 January 2021
Published: 8 January 2021

manufacturing to develop different therapeutics. In his study, a simulation was carried out coupled with a set of population balance equations to describe the evolution of the crystal size distribution. His work provides an insight for design, development and optimization of such new and intensified crystallization units.

Neugebauer et al. [2] developed a dynamic model to study the corresponding effects between particle phase and fluidization medium in a fluidized bed layering granulation process. Their dynamic model, quite uniquely, considers bidirectional coupling of particles and fluidization medium. They also validated the performance of their model with experimental data. Kaur et al. [3] presented another study related to granulation which focused on a top-sprayed fluidized bed granulator. This process is also considered to have many applications especially in the pharmaceutical industry. First, they developed a number-based mathematical model using PBM. Next, they validated their model using a compartmental model.

Schmideder et al. [4] presented a study on dissolved air flotation and microflotation, which are primary purification steps in a range of bioprocesses utilizing microorganisms (e.g., algae and yeast). However, since the efficiency of these separation processes depends on the aggregation of microorganisms with microbubbles, they compared new or used existing aggregation models to investigate the suitability range of these models to predict separation efficiency in fermentation broths. Among the major outcomes of their investigation using computational fluid dynamics (the proposed aggregation models are coupled to the CFD model by applying a Lagrangian approach) and PBM is the demonstration of the heterogeneity of the fluid dynamics in the flotation tank.

Starting from the PBM framework as a powerful tool in science and engineering applications, Kuhn et al. [5] showed that the description of distributed properties subject to temporal and spatial variations with a PBM is not only limited to the engineering and natural sciences (as stated in this manuscript). Similar phenomena exist in the social domain (e.g., age and income). Processes of change and formation of public opinion are studied empirically and by means of different modeling approaches in a field called opinion dynamics. The work aimed to illustrate that opinion dynamics and PBM can mutually benefit by exchanging problems and methods. Therefore, they formulated a classic approach from opinion dynamics as a PBM, and concluded that problems from the social domain such as opinion dynamics can bring an array of stimulating insights to the PBM community and vice versa. In a broader perspective, they provide recommendations on how these methods and tools could be used across the mentioned disciplines.

2. Parameter Estimation/Model Calibration

In the area of parameter estimation/model calibration, there are three contributions that cover discrete-element method parameters, parameter identification and a systematic framework for parameter and state estimation.

Karkala et al. [6] considered the effectiveness of using dynamic yield strength (DYS) and shear-cell experiments to calibrate a few discrete-element method parameters, i.e., surface energy, and the coefficients of sliding and rolling friction. They performed experiments and parameter sensitivity analysis for two case studies on cohesive granules. They demonstrated that the combination of DYS and shear-cell simulations is beneficial, using data from their experimental system for validation. Golovin et al. [7] proposed a population balance model for a continuous fluidized bed spray agglomeration and validated it using experimental data. The main focus was on the description of the dynamic behavior in continuous operation mode in a certain neighborhood around steady-state. They employed various kernels and concluded that no kernel can match experimental data beyond a certain period of time with time independent parameters. However, they obtained improved model fit and parameter identification using a shifted time domain neglecting the initial start-up period. They used parametric bootstrap to illustrate confidence intervals and identifiability of the parameters. Dürr and Waldherr [8] look into the challenge with lack of data availability in multi-cellular systems where some properties may be impossible to measure due to economic or operational constraints. Therefore, they proposed an approach based on approximation of the underlying number density functions as the weighted sum of Gaussian distributions. This resulted in the ability to reduce the complexity of an infinite dimensional estimation problem to a finite dimension. They highlighted the application of their framework on two benchmark examples from literature and demonstrated that it has potential for model-based on-line reconstruction for multicellular systems.

3. Numerical Methods

Considering numerical methods related to solving PBM, two contributions are included in this Special Issue. Su et al. [9] proposed a local fixed pivot quadrature method of moments (LFPQMOM) for the solution of the population balance equation (PBE) for the aggregation and breakage process. According to their study, in theory, any number of moments can be tracked with the new method, but the computational expense can be relatively large due to many scalar equations that may be included. Bhonsale et al. [10] performed an analysis of uncertainty propagation methods applied to a breakage population balance model. This is because in data-driven or hybrid modeling, the variability in measured data influences the model parameters and the resulting model predictions. They performed various uncertainty propagation techniques and compared the results with those obtained from Monte Carlo simulations. They showed that linearization performs the worst in the scenario they considered (in the breakage population balance models), while sigma point and polynomial chaos methods have similar performance in terms of accuracy.

4. Stochastic Methods

Considering stochastic methods, two contributions are included in this Special Issue. Tran and Ramkrishna [11] proposed a method for direct computation of the average behavior of stochastic populations. They highlighted the application of their method using an example of antibiotic resistance between two bacterial species which is an ever increasing alarming issue in fighting disease. Their proposed strategy is not limited to one method and can be extended to other methods which may result in an efficient way to obtain the average with a shorter computational time and effort. They recommend testing this method on many other examples and suggest that it would help assess whether higher order terms in the Taylor expansion would be needed for reaching an increased accuracy level. Skenderović et al. [12] discussed the significance of droplet polydispersity on particle formation in metal oxide particle synthesis using the dual population balance Monte Carlo method (DPBMC). They applied their approach to particle synthesis from metal nitrate precursor solutions with flame spray pyrolysis (FSP) and compared model predictions to experiments from literature.

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