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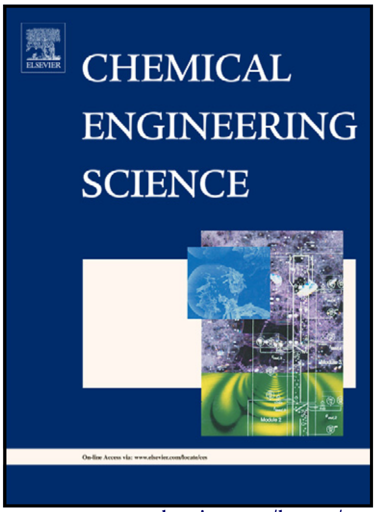

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High dimensional population balances for the growth of faceted crystals: Combining Monte Carlo integral estimates and the method of characteristics

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Abstract

A numerical scheme is proposed for the solution of population balance equations that describe the growth of faceted crystals. Therefore, two issues are discussed. First, a numerical scheme for solution of high dimensional population balance equations is proposed. The scheme is based on Monte Carlo integration for the integral distribution properties (number, area, volume) combined with the method of characteristics. Samples points are initially obtained from an arbitrary probability distribution via the Metropolis-Hastings algorithm. The evolution of these sample points is subsequently computed using the method of characteristics, while the sample points themselves are the basis of the Monte Carlo integration of the population to obtain e.g. total crystal volume to close the mass balance. The theoretical background of the Monte Carlo integration allows to estimate the error introduced in the mass balance depending on a particular choice of sampling points. The effectiveness of the scheme is verified for a analytically solvable 3-dimensional population. That case study is also employed to demonstrate that an adequate choice of the probability distribution for the generation of the initial sample points can improve the accuracy without increasing the computational effort. The second issue that must simultaneously be considered comprises the disappearance of faces during growth. Such conditions create a constraint for each face distance, measured from a chosen origin, which, prior to the disappearance of that face, had freely evolved according to its growth rate. This constraint is defined for general faceted crystals, and a procedure is proposed to correct the growth rate so that the constraint can be maintained in dynamic simulations. The application of this procedure is demonstrated in a second case study that simulates a 7-dimensional population balance equation.

Keywords: crystal growth, morphological changes, disappearing faces, morphological population balance, numerical solution

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