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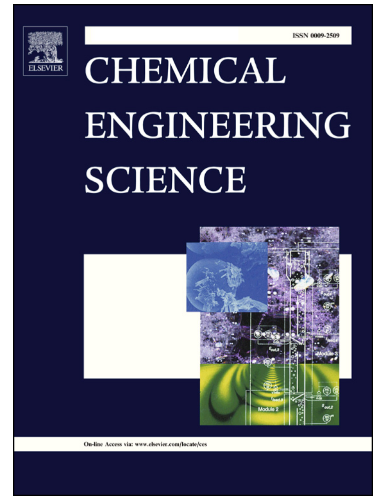

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An explicit adaptive grid approach for the numerical solution of the population balance equation

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Abstract

Many engineering applications, such as the formation of soot in hydrocarbon combustion or the precipitation of nanoparticles from aqueous solutions, encompass a polydispersed particulate phase that is immersed in a reacting carrier flow. From a Eulerian perspective, the evolution of the particulate phase both in physical and in particle property space can be described by the population balance equation (PBE). In this article, we present an explicit solution-adaptive numerical scheme for discretizing the spatially inhomogeneous and unsteady PBE along a one-dimensional particle property space. This scheme is based on a space and time dependent coordinate transformation which redistributes resolution in particle property space according to the shapes of recent solutions for the particle property distribution. In particular, the coordinate transformation is marched in time explicitly. In comparison to many existing moving or dynamic adaptive grid approaches, this has the advantage that the semi-discrete PBE does not need to be solved in conjunction with an additional system governing the movement of nodes in particle property space.

By design, our adaptive grid technique is able to accurately capture sharp features such as peaks or near-discontinuities, while maintaining the semi-discrete system size and adhering to a uniform fixed grid discretization in transformed particle property space. This is particularly advantageous if the PBE is combined with a spatially and temporally fully resolved flow model and a standard Eulerian solution scheme is applied in physical space. In order to accommodate localized source terms and to control the grid stretching, we develop a robust scheme for modifying the coordinate transformation such that constraints on the resolution in physical particle property space are obeyed.

As an example, we consider the precipitation of $BaSO_4$ particles from an aqueous solution in a plug flow reactor. Our findings demonstrate that for a given accuracy of the numerical solution the explicit adaptive grid technique requires over an order of magnitude fewer grid points than a comparable fixed grid discretization scheme.

Keywords: Population balance, Adaptive grid, Reacting flow

1. Introduction

Laminar or turbulent reacting flows with particle formation appear in many engineering applications such as the formation of soot in hydrocarbon combustion, the formation of clouds as a result of droplet condensation or the precipitation of nanoparticles from an aqueous solution. The prediction and analysis of these processes play an important role, for instance, in the reduction of pollutant emissions, the control of aerosols as well as the design of process conditions in chemical reactors. Often, the individual particles can be characterized by properties such as particle size, volume, shape or charge. These properties may change as the particles interact with each other and/or with the ambient fluid and, by consequence, the particles evolve both in physical space and in particle property space. From a Eulerian perspective, this evolution is described by the population balance equation (PBE) which governs the number density of particles per unit of volume in particle property space and per unit of mixture volume [1].

In the present article, we confine the attention to discretization-based methods for solving the spatially inhomogeneous and unsteady PBE. Alternative approaches such as the method of moments and stochastic solution schemes have been reviewed by Ramkrishna [2] and Rigopoulos [3], for instance. In the context of discretization-based methods, the PBE is commonly discretized on a *fixed* grid in particle property space and the resulting semi-discrete equations are solved by applying a standard Eulerian solution scheme [4]. Here, the semi-discrete system consists of scalar transport equations for so-called discrete number densities. Since these transport equations are formally identical to those of the reactive scalars which characterize the fluid phase, the PBE can be naturally incorporated into models for the laminar or turbulent carrier flow [3, 5–7].

While fixed grid discretization schemes are very mature, they frequently require an extremely fine grid throughout particle property space. This is particularly acute if the particle property distribution evolves over several orders of magnitude, potentially developing peaks or near-discontinuities. In commercial crystallizers, for instance, the particle size can span up to five orders of magnitude, ranging from the nucleation size ~ 1 nm to the final crystal size $\sim 100\,\mu$m. By consequence, the

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