



# Segregation dynamics of dense polydisperse fluidized suspensions modeled using a novel formulation of the direct quadrature method of moments



Luca Mazzei\*

Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE, UK

## AUTHOR - HIGHLIGHTS

- We test a novel version of DQMOM for dense multiphase flows.
- We estimate the order or magnitude of the diffusivity used in the model.
- We conduct a sensitivity analysis on the diffusivity.
- We model the segregation dynamics of polydisperse fluidized powders using the model.

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## ABSTRACT

Computational fluid dynamics (CFD) may be a useful design tool, provided that the mathematical models that we solve with it capture and describe well the most important features of the systems of interest. For fluidized beds, one of these features is the polydispersity of the powders: particles differ in size and alter their size distribution in time and space continuously. To model this key phenomenon, one needs to solve a population balance equation, that is, an equation that governs the evolution of the size distribution. The direct quadrature method of moments (DQMOM) allows doing so in commercial CFD codes at relatively low computational cost. This technique, successfully employed for describing dilute multiphase flows of particles that share the same velocity, still needs testing in the context of dense multiphase flows. Dense polydisperse fluidized powders can segregate or mix, depending on the process operating conditions, and to describe these phenomena one needs to let particles move with different velocities. In this work we use a recent version of DQMOM that has this feature: each quadrature class is advected with its own velocity. The transport equations of this model feature a diffusive-like contribution that allows the powders to mix at the particle length scale. We discuss how to assign a value to the diffusion coefficient and we carry out a sensitivity analysis on the latter; to do so, we simulate the mixing of powders initially segregated using different values for the diffusivity. Successively, after having estimated a suitable value for the latter, we simulate the system dynamics under conditions that should promote segregation, validating the results of the simulations experimentally.

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## 1. Introduction

Polydisperse multiphase systems are composed of a continuous phase (a gas or a liquid) within which other discontinuous phases are dispersed (particles, droplets or bubbles); each discontinuous phase is composed of elements continuously distributed over velocity and size, and possibly other properties, such as density. Even if virtually every industrial plant contains units that treat these systems (e.g., fluidized beds, bubble columns and crystallizers), designing them is still subject

to great uncertainties. This is because such systems undergo numerous physical and chemical phenomena that occur concurrently: chemical reactions take place, usually implicating all the phases and affecting their properties; also, elements of the discontinuous phases can break into subelements or aggregate, while new elements may nucleate. The behavior of the units and the quality of the product strongly depend on these competing phenomena, in turn influenced by phase interactions, system fluid dynamics and, indirectly, unit geometry and size.

To describe the behavior of polydisperse multiphase systems and design process units for treating them, researchers and engineers have resorted for several years to experimental correlations and pilot plants. These correlations, however, have limited applicability as they are valid only for the specific cases investigated; so, they cannot help

\* Tel.: +44 20 7679 4328; fax: +44 20 7383 2348.

E-mail addresses: [l.mazzei@ucl.ac.uk](mailto:l.mazzei@ucl.ac.uk), [luca.mazzei.a@gmail.com](mailto:luca.mazzei.a@gmail.com)

improve design and performance, or predict the effect of changing the size or geometry of a unit. Pilot plants, on the other hand, are costly and time-consuming and do not always lead to adequate scale up. In consequence, thanks to the high-speed computers and advanced numerical methods now available, the modeling and simulation of multiphase flows have rapidly gained importance. Due to the complexity of such flows, a relatively large number of modeling approaches have been developed in the literature (Fox, 2012). At the most fundamental level the particles are treated individually, so that the discrete structure of the dispersed material is entirely retained; here one models the behavior of each particle, accounting for its interaction with the surrounding fluid and other particles. This strategy is powerful but computationally extremely expensive. The information that these simulations provide is normally not of direct use to engineers and greatly exceeds their normal requirements. An alternative strategy is to model also the discontinuous phases as continua. Several Eulerian models of this kind have been developed (Drew and Passman, 1998); these, however, often present severe limitations.

One of the most important limitations, present also in many advanced models, is that these do not account for polydispersity, neglecting in particular that the discontinuous phases are made of elements with changing size distribution. They instead assume that the latter consist of classes of particles with equal and constant sizes. The constant-particle-size assumption significantly limits the model flexibility: classes may segregate or mix, and particles may change class, but variations in the diameters attached to each class are not allowed. Real systems are instead characterized by broad particle size distributions (PSDs) which evolve continuously owing to fluid–particle and particle–particle interactions. Particles can shrink, aggregate, break and nucleate; hence, their size distribution varies continuously in time and space. Predicting this evolution, which depends on the local conditions wherein a system operates, is key to accurately describing its behavior.

To account for polydispersity and be able to predict how PSDs evolve, one needs to solve a population balance equation (PBE), possibly along with customary multifluid balance equations for mass and/or linear momentum. Doing so is quite difficult, since the PBE dimensionality differs in general from that of classical fluid dynamic equations. In the last years numerous attempts to solve this equation, in particular within CFD codes, have been reported in the literature (in Fox, 2012 and Marchisio and Fox, 2007, for instance, one may find several references); nevertheless, *dense fluid–solid systems*, in which the phases strongly interact and do not share the same velocity field, have not been investigated extensively (Fan et al., 2004; Fan and Fox, 2008; Fox and Vedula, 2010; Mazzei, 2011; Mazzei et al., 2012), few works considering size-changing phenomena such as chemical reaction, aggregation or breakage.

Often engineers are only interested in few integral properties of the distribution function that describes the particle population. Such properties, called moments, may be important because they control the product quality or because they are easy to measure and monitor. The idea behind the method of moments is to derive transport equations for the moments of interest (Randolph and Larson, 1971). This method is attractive, for the number of equations to be solved is small; however, the moment transport equations are unclosed, because for any given set of moments that the modeler wishes to track, the equations normally involve higher-order moments external to the set (Marchisio and Fox, 2007). The quadrature method of moments (QMOM) and its direct version (DQMOM) overcome this issue by approximating the distribution function with a quadrature formula; assuming the functional form of the distribution allows to calculate, with a given approximation, the values of any higher-order moment external to the set tracked by the methods. QMOM tracks the moments of this

set by integrating their evolution equations; then, once these moments are known, it calculates the nodes and weights of the quadrature formula. DQMOM, conversely, directly tracks the latter, solving the evolution equations that govern them. The models are theoretically equivalent, as we shall discuss later on, but present different issues when one solves them numerically (Shohat and Tamarkin, 1943; Akhiezer, 1965; Wright, 2007; Mazzei et al., 2010a; Petitti et al., 2010; Mazzei, 2011; Mazzei et al., 2012).

In most versions of the quadrature-based moment methods reported in the literature, the PBE solved does not feature convection in physical space; written for well-mixed systems, for which the distribution function is uniform in such a space, these models account solely for particle growth, their PBEs featuring convection just in size space (e.g., Dorao and Jakobsen, 2006; Grosch et al., 2007; Aamir et al., 2009; Gimbut et al., 2009; Qamar et al., 2011). Some other models, written for nonuniform systems, account for convection in physical space, but often assume that all quadrature classes are advected with the same velocity field, so that particles share the same velocity (e.g., Petitti et al., 2010). This assumption prevents solids from segregating. Dense polydisperse fluidized powders may segregate or mix, depending on the process operating conditions, and in order to describe these phenomena one needs to let particles move with different velocities.

Few models catering for nonuniform dense polydisperse fluid–solid systems have this feature, and hence have the capability to describe segregation. Among the first to be developed are those of Fan et al. (2004) and Fan and Fox (2008); these let each quadrature class be advected with its own velocity field, whose evolution is governed by a coarse-grained dynamical equation. These DQMOM models, as Mazzei et al. (2010a) reported, have a significant limitation: they do not permit powders to micromix, that is to say, to mix at the length scale of the particles. Solely macromixing, that is to say, convection-induced mixing, is possible in such models. We shall address this aspect in detail later.

To overcome this problem, Mazzei (2011) recently developed a revised version of DQMOM in which the evolution equations for the quadrature weighted nodes and weights feature a diffusive flux that compensates for the error that one makes when calculating the convective flux of a property adopting the quadrature-based approximation of the distribution function that describes the particle population. In Mazzei (2011), we did not specify which value to assign to the diffusion coefficient. This, indeed, is an open issue, which we shall address in the present work.

This work aims to simulate the segregation dynamics of inert dense polydisperse fluidized powders. The paper is organized as follows. We introduce the problem that we intend to investigate. Next, we describe the mathematical model, in particular the DQMOM model recently developed in Mazzei (2011). Since we shall need them subsequently, we also report the evolution equations of the QMOM model, showing that the two are theoretically equivalent. Their equations feature a diffusive term which allows the powders to mix at the particle length scale (micromixing). We discuss how to assign a value to the diffusion coefficient appearing in the evolution equations of the models, conducting a sensitivity analysis on the latter; to do so, we simulate the mixing of nonuniform powders using different values for the diffusivity. Finally, after having estimated a suitable value for this coefficient, we simulate the system dynamics under conditions which should promote segregation, validating the predictions of the numerical simulations experimentally.

## 2. Problem description

We aim to simulate the dynamics of inert dense polydisperse fluidized powders under conditions that should promote segregation.

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