2013

Theoretical and Numerical Issues Concerning DQMOM When Simulating Polydisperse Fluidized Powders

Luca Mazzei
UniversityCollege, UK

THEORETICAL AND NUMERICAL ISSUES CONCERINING DQMOM WHEN SIMULATING POLYDISPERSE FLUIDIZED POWDERS

Luca Mazzei
Department of Chemical Engineering, UniversityCollegeLondon
Torrington Place
London, WC1E 7JE, UK
T: +44 (0)20 7679 4328; F: +44 (0)20 7383 2348; E: l.mazzei@ucl.ac.uk

ABSTRACT

To model the evolution of the particle size distribution in a polydisperse fluid bed, onemay solve a population balance equation. The direct quadrature method of moments permits to do so in CFD codes at relatively low computational cost. We analyze the model, discussing its limitations and how to overcome them. To test it, we simulate the mixing dynamics of inert polydisperse fluidized powders.

INTRODUCTION

Simulating the behavior of polydisperse fluidized mixtures is complex,sincethe particulate phase is characterized by a wide particle size distribution (PSD) and its dynamics are tightly coupled with those of the continuous phase. A so-calledpopulation balance equation (PBE) governs how the PSD evolves in time in each spatial point of a given domain. Solving thisequation by means of CFD codes ischallenging, insofar asits dimensionality is higher than that of customary balance equations. In the last years,many attempts to solve the PBE in CFD codes have been reported in the literature; references may be found in Fox (1) and Marchisio and Fox (2). However, *dense fluid-solid systems*, where phases strongly interact and do not share the samevelocity, have been investigated less extensively.

Often engineers are solely interested in few integral properties of the distribution function describing the particle population. Such properties are called moments. The idea behind the method of moments is to derive and solve only the transport equations for the moments of interest. The method is attractive, for thenumber of equations to be solved is quite small;but one issue arises: the moment transport equations are unclosed, becausefor any given set of moments that the modeler wishes to track, the equations normally involve higher-ordermoments external to the set. The direct quadrature method of moments (DQMOM) solves theissue by approximating the distribution function with a quadratureformula; assuming the functional form of the distribution permitsto calculate, with a given approximation, thevalues of any higher-order moment external to the set tracked by the method. DQMOM does not track the moments of the distribution, but solves the evolution equations of the nodes and weights of the quadrature formula;from these we can easily compute the approximate value of any moment.

Few models for dense polydisperse fluidized mixtures,in which each quadrature class is advected in real space with its own velocity field,have been developed. Among the first are those of Fan et al. (3) andFan and Fox (4); thesemodels, as

Mazzei et al. (5) reported,have a significant limitation: they do not allow powders to mix at the length scale of the particles (micromixing). The evolution equations of the quadrature nodes clearly reveal this: if growth,breakage, aggregation and alike size-changing phenomena are absent, the material derivatives of the nodes vanish (we shall clarify this point below). So, nodes cannot vary along pathlines, and powders that are initially nonuniform cannot homogenize in real space. Only macromixing, that is, convection-induced mixing, ispossible in such models.

To overcome this problem, Mazzei (6) recently developed a version of DQMOM in which theevolution equations for the quadrature nodes and weights feature a diffusive term; thisoffsets the error made when one calculates the convective flux of a property with the quadrature-basedapproximation of the distribution function. One expects this error to besmall, for a quadrature formula should approximate the convective flux reasonably well; but,even if this were true, such error would build up over time eventually leadingto wrong predictions. So, accounting for the deviation between real and quadrature-basedconvective fluxes is vital. In Mazzei(6) we *assume* that this deviation flux can be modeled as a diffusive flux, but do not specify which value to assign to the diffusion coefficient.

In this article, we briefly report our new model, discussing the shortcomings of the original version,we discuss how to decide which value to assign to the diffusion coefficient(and the range in which its value should reasonably lie) and wethenconduct a sensitivity analysis on it, simulating numerically the mixing dynamics of inert fluidized particles (for which all size-changing phenomena are absent) using different values for the diffusivity and comparing the numerical results withthe correct results,which one can obtain, in the simple case of mixing, analytically.

DQMOM MODEL

To describe the particle size distribution, we use a volume density function (VDF). Denoted by $f\left(\boldsymbol{x},s,t\right)$, we define it so that $f\left(\boldsymbol{x},s,t\right)ds\,d\boldsymbol{x}$ is the expected volume of particles present at time t in the volume $d\boldsymbol{x}$ about $\boldsymbol{x}$ with size in the range ds about s. DQMOM assumes that it is:

$$f=\sum_{r=1}^{\nu}\phi_r\left(\boldsymbol{x},t\right)\delta\left[s-s_r\left(\boldsymbol{x},t\right)\right] \tag{1}$$

This represents a quadrature formula involving 2ν functions: the weights ϕ_r and the nodes s_r. These are not assigned directly. To calculate them, we request that these conditions be met:

$$M_a=\int_0^{\infty}s^a f\,ds=\sum_{r=1}^{\nu}\phi_r\,s_r^a \quad \text{for} \quad 0\le a\le 2\nu-1 \tag{2}$$

where M_a is the moment of order a of the distribution and where a is integer.In other words, we require that the first 2ν integer moments of the real distribution

function be equal to those of the approximated distributionadopted by DQMOM.Sometimes, instead of dealing with the quadrature nodes, it is more convenient to deal with the quadrature weighted nodes, defined as $\sigma_r \equiv \phi_r s_r$.

In the new DQMOM model proposedin Mazzei (6), the evolution equations of the quadrature weights andweighted nodes read:

$$\partial_t \phi_r = -\partial_{\boldsymbol{x}} \cdot \phi_r \boldsymbol{v}_r + \partial_{\boldsymbol{x}} \cdot D_x \partial_{\boldsymbol{x}} \phi_r + c_r^{\phi} \quad , \quad \partial_t \sigma_r = -\partial_{\boldsymbol{x}} \cdot \sigma_r \boldsymbol{v}_r + \partial_{\boldsymbol{x}} \cdot D_x \partial_{\boldsymbol{x}} \sigma_r + c_r^{\sigma} \quad (3)$$

where D_x is a diffusion coefficient, c_r^{ϕ} and c_r^{σ} are source terms, whilst $\boldsymbol{v}_r$ is the velocity field associated with the rth quadrature class [thisis governed by a usual coarse-grained dynamical equation (7)]. The source terms are given by this set of linear algebraic equations:

$$(1-a)\sum_{r=1}^{\nu} s_r^a c_r^{\phi} + a\sum_{r=1}^{\nu} s_r^{a-1} c_r^{\sigma} = a(a-1) D_x \sum_{r=1}^{\nu} \phi_r s_r^{a-2} \partial_{\boldsymbol{x}} s_r \cdot \partial_{\boldsymbol{x}} s_r \text{ for } 0 \le a \le 2\nu - 1 \quad (4)$$

One can obtain the evolution equations of the quadrature nodes by combining Eqs. (3);this gives the following:

$$\partial_t s_r + \boldsymbol{v}_r \cdot \partial_{\boldsymbol{x}} s_r = \partial_{\boldsymbol{x}} \cdot \phi_r D_x \partial_{\boldsymbol{x}} s_r + c_r^s \quad , \quad c_r^s = c_r^{\sigma} - s_r c_r^{\phi} + D_x \partial_{\boldsymbol{x}} \phi_r \cdot \partial_{\boldsymbol{x}} s_r \quad (5)$$

In the original DQMOM version advanced in Fan et al. (3) andFan and Fox (4), diffusion was not accounted for (these models did not account for the deviation between real and quadrature-basedconvective fluxes; this is equivalent to setting the diffusion coefficient to zero). This means, from Eq. (5), that quadrature nodes cannot vary along pathlines, and accordingly a system initially nonuniform cannot homogenize in real space. So, only convection-induced mixing occurs, but mixing at the particle length scale (micromixing) cannot take place.Our model allows for micromixing. A consequence is that quadrature weights and weighted nodes are no longer conservative, as Eqs. (3) reveal.

ORDER OF MAGNITUDE OF THE DIFFUSION COEFFICIENT

We write the evolution equations of the quadrature weights (same considerations hold for the quadrature nodes and weighted nodes) in dimensionless form. Let t_c and x_c be the time and length scales in the bulk of the domain. The scales ofthe independent variables must render the derivatives of the scaled nondimensional dependent variables ofunit order of magnitude. As for the dependent variables, ϕ_r is dimensionless and of order unity; so, we only need to define scales for the velocity fields and for the quadrature nodes. Let these be v_c and s_c, respectively. Then, if we introduce the dimensionless variables $\overline{t} \equiv t/t_c$, $\overline{\boldsymbol{x}} \equiv \boldsymbol{x}/x_c$, $\overline{\boldsymbol{v}} \equiv \boldsymbol{v}/v_c$ and $\overline{s}_r \equiv s_r/s_c$, the first of Eqs. (3) gives:

$$\partial_{\bar{t}}\phi_r = -\frac{v_c t_c}{x_c}\left\{\partial_{\bar{x}}\cdot\phi_r\bar{\boldsymbol{v}}_r\right\} + \frac{D_x t_c}{x_c^2}\left\{\partial_{\bar{x}}\cdot\partial_{\bar{x}}\phi_r + \bar{c}_r^{\phi}\right\} \tag{6}$$

Two characteristic times appear: one associated with convection, x_c / v_c, and one with diffusion, x_c^2 / D_x. Their ratio φ is the inverse of a Peclet number. Since the equation is scaled, the term on the left-hand side and the bracketed terms on the right-hand side have unit order of magnitude; so, if $\varphi \ll 1$ the characteristic time must be x_c / v_c, whilst if $\varphi \gg 1$ it must be x_c^2 / D_x. Hence, the characteristic time depends onthe value of φ and, as one expects, the time scale is dictated by the term that dominates the quadratureweight rate of change.

The value of D_x in the evolution equations is related to the error that one makes when calculating the convective flux of any property using the quadrature-based approximationof the VDF (6). The larger the order ν of the quadrature formula, that is, the larger the number of quadrature classes used, the smaller the error. Moreover, the quadrature formula defined in Eq. (1) is Gaussian,having a higher accuracy than normal quadrature formulae. Thus, there surely exists a minimum value ν for which the error is small enough to render φ far less than unity. For quadrature formulae of this or higher order, the characteristic time t_c is x_c / v_c and Eq. (6) becomes:

$$\partial_{\bar{t}}\phi_r = -\partial_{\bar{x}}\cdot\phi_r\bar{\boldsymbol{v}}_r + \varphi\left\{\partial_{\bar{x}}\cdot\partial_{\bar{x}}\phi_r + \bar{c}_r^{\phi}\right\} \tag{7}$$

For short dimensionless times of order φ convection dominates and the diffusive and source terms affect negligibly the evolution of the quadrature weights. But for longer times the diffusive and source terms play an important role, which cannot be neglected; this is in particular true if we are interested in steady-state values, which by definition refer to long times.Accordingly, setting D_x to zero is a good approximation only for the very first instants of the dynamics.

The condition $\varphi \ll 1$ requires that $D_x \ll v_c x_c$. This gives an upper bound for D_x. A lower bound is instead set by the numerics.

To solve the DQMOM evolution equations in CFD we discretize them in space. The numerical scheme is diffusive, the numerical diffusion being represented by a coefficient D_n that depends on the scheme used and the grid coarseness. So, we do not really solve Eq. (7), but the following:

$$\partial_{\bar{t}}\phi_r = -\partial_{\bar{x}}\cdot\phi_r\bar{\boldsymbol{v}}_r + \varphi\left\{\left(1 + D_n / D_x\right)\partial_{\bar{x}}\cdot\partial_{\bar{x}}\phi_r + \bar{c}_r^{\phi}\right\} \tag{8}$$

If $D_n / D_x \gg 1$, the rate of diffusion is dictated by the numerics, not by the physics. So, this condition must be avoided. An additional reason for which $D_n / D_x \gg 1$ is unacceptable is this. Eq. (7) shows that the diffusive and source terms have the

same order of magnitude.For $D_n / D_x \ll 1$, however, this is untrue, as the relative importance of the source term decreases. In particular, for quite large values of D_n / D_x the source term becomes negligible compared to the diffusive term, and the quadrature weights are modelled – incorrectly – as conservative quantities. This problem arises not only when the numerical scheme is highly diffusive, but also when one sets D_x to zero. This is an additional reason, this time numerical, for which the coefficient of real diffusion cannot be set to zero. From this analysis we conclude that is must be $D_n \gg D_x \gg v_c x_c$.

SENSITIVITY ANALYSIS AND NUMERICAL SIMULATIONS

To test these ideas, we simulate the mixing dynamics of a powder that is initially nonuniform. We consider a system formed of two identical superposed layers of granular material (0.35 m in width and 0.15 m in height). Both layers are uniform in space and formed of polydisperse particles. The mean particle size in the top layer is larger than that in the bottom layer. All particles have equal density (2500 kg/m^3). We fluidize the system with a gas velocity (0.15 m/s) sufficiently high to achieve perfect mixing. Initially, the nodes and weights of the quadrature formula are uniform *in each layer*, i.e., their values are identical in each layer. We assume that, for a quadrature formula of order two, it is:

$$\text{Top layer: } s_1 = 240\,\mu\text{m} \quad , \quad \phi_1 = 0.380 \quad , \quad s_2 = 355\,\mu\text{m} \quad , \quad \phi_2 = 0.220$$

$$\text{Bottom layer: } s_1 = 75\,\mu\text{m} \quad , \quad \phi_1 = 0.262 \quad , \quad s_2 = 103\,\mu\text{m} \quad , \quad \phi_2 = 0.338$$

Once the powder has perfectly mixed, the quadrature nodes and weights will be uniform *in the entire bed*, and their values will differ from those reported above. This means, in particular, that the nodes will have changed along the pathlines, a result that can only be achieved if the diffusive terms in Eqs. (3) are accounted for. In this simple problem, we can calculate the new, steady-state values of the quadrature nodes and weights analytically. To do so, we firstly need to determine the values of the moments in each layer at time zero, then we need to calculate their average value over the entire fluidized bed and finally we need to calculatethe corresponding values of the quadrature nodes and weights; for further details we refer to Mazzei (6). The result is the following:

$$\text{Entire bed: } s_1 = 104\,\mu\text{m} \quad , \quad \phi_1 = 0.366 \quad , \quad s_2 = 316\,\mu\text{m} \quad , \quad \phi_2 = 0.234$$

Further details about this procedure and the system analyzed may be found in Mazzei (6); here for briefness we cannot report them. We would expect that DQMOM should yield these correct results provided $D_n \gg D_x \gg v_c x_c$.

As mentioned, for $D_n / D_x \ll 1$ the model essentially treats the nodes and weights of the quadrature formula as conservative quantities. This is incorrect, as Eqs. (3) show. We can calculate the wrong results that one would obtain in such a case by simply calculating the average values over the entire fluid bed of the weighted nodes and weights. The result is this:

Entire bed: $s_1 = 173\,\mu\text{m}$, $\phi_1 = 0.321$, $s_2 = 202\,\mu\text{m}$, $\phi_2 = 0.279$

We would expect that DQMOM should yield these wrong results for $D_n / D_x \gg 1$. To test this, we simulated the system described above in CFD adopting different values for the diffusivity. We used a uniform grid of square cells with a side length of 5 mm and, to discretize in space, a first-order upwind numerical scheme. For the operating and numerical conditions adopted, we estimate that $D_n \approx 10^{-4}$ m^2/s and $v_c x_c \approx 10^{-3}$ m^2/s. Thus, a significant separation of magnitude between these two values (which would be ideal in order to meet the condition $D_n \ll D_x \ll v_c x_c$) is absent. Increasing the separation of magnitude by reducing the value of D_n is not possible, because it would require using cells with a side length smaller by at least one order of magnitude, which would render the computational times much too long. Also, increasing the separation of magnitude by increasing the value of $v_c x_c$ is not possible, because it would require changing the system geometry and the operating conditions.Hence, we have to accept the values found, which allow to meet, at least partly, the condition $D_n \ll D_x \ll v_c x_c$.

The values of the quadrature nodes and weights predicted by DQMOM at steady state after mixing has taken place are reported in Table 1.

D_n / D_x	s_1 μm	ϕ_1	s_2 μm	ϕ_2
100	172	0.337	205	0.263
10	167	0.385	222	0.215
1	139	0.423	299	0.177
0.40	124	0.403	312	0.197
0.20	115	0.385	314	0.215
0.13	110	0.381	314	0.219
0.10	108	0.380	314	0.220

Table 1. Values of the quadrature nodes and weights predicted numerically after mixing has taken place for different values of D_n / D_x.

As we can see, for $D_n / D_x \gg 1$the values tend to the incorrect values previously calculated. Thus, the model incorrectly treats the quadrature weighted nodes and weights as conservative quantities. When the ratio D_n / D_x decreases, the values of the quadrature nodes and weights change, tending to the correct ones found above. These values are nearlyobtained for $D_n / D_x = 0.20$. From the table we see that whereas the nodes change monotonically, the weights do not. However, when the numerical diffusion becomes negligible compared to the real diffusion, both quantities are predicted reasonably well.

From these results, we might think that the smaller D_n / D_x the better, since the smaller the ratio, the more numerical diffusion is negligible. However, we cannot

take values for D_x too large, since we need to satisfy the condition $D_x \ll v_c x_c$. This ensures that convection dominates over diffusion. If we do not respect this condition, the consequence is that diffusion erases the gradients that convection generates in the domain (particle mixing must not be confused with the formation of bubbles and streamers, which occur naturally in gas-solid fluidized mixtures). In particular, diffusion would erase the gradients in void fraction, which would mean erasing the bubbles within a bubbling bed. To show this, in Figure 1 we report the spatial profiles of the void fraction predicted by the simulations for two different values of D_x.

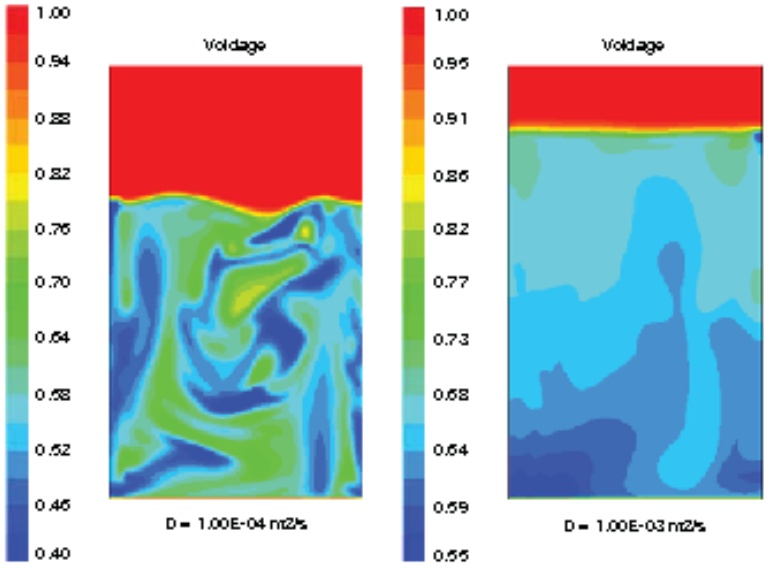

Figure 1. Spatial profiles of the voidage predicted numerically for two different values of the diffusion coefficient.

As we can see, for $D_x \ll v_c x_c$ the gradients are erased, the bubbles are lost and the height of the bed is consequently overpredicted.

CONCLUSIONS

The direct quadrature method of moments is a convenient method for solving the population balance equation within CFD codes. Nevertheless, because of the functional form that the method adopts for the volume density function, there is an error that the model makes in computing convective fluxes. This error must be accounted for, since otherwise the method predicts incorrectly that the nodes of the quadrature formula are constant along pathlines (for systems where particles are inert). In this article we have modeled the deviation between the correct and approximated fluxes as a diffusive flux, estimating the order of magnitude of the coefficient of diffusion. Thus, we have identified a range in which the coefficient must lie. To test these ideas, we have then simulated the mixing dynamics of a system of inert polydisperse particles using different values for the coefficient of diffusion. The results of the simulations have confirmed our conclusions, showing

that when the diffusion coefficient does not lie in the range identified, the results of the model are incorrect.

NOTATION

D_x	Diffusion coefficient
D_n	Numerical diffusion coefficient
f	Volume density function
M_a	ath integer moment of the volume density function
s	Particle size
s_r	rth node of quadrature formula
t	Time
$\overline{t}$	Dimensionless time
t_c	Characteristic time
$\boldsymbol{v}_r$	Velocity field for rth quadrature class
$\overline{\boldsymbol{v}}_r$	Dimensionless velocity field for rth quadrature class
v_c	Characteristic velocity
$\boldsymbol{x}$	Coordinate in real space
$\overline{\boldsymbol{x}}$	Dimensionless coordinate in real space
x_c	Characteristic length
c_r^{ϕ}	Quadrature weight source term for rth quadrature class
$\overline{c}_r^{\phi}$	Dimensionless quadrature weight source term for rth quadrature class
c_r^{s}	Quadrature node source term for rth quadrature class
c_r^{σ}	Quadrature weighted node source term for rth quadrature class
φ	Dimensionless parameter (inverse of Peclet number)
ϕ_r	rth weight of quadrature formula
σ_r	rth weighted node of quadrature formula

REFERENCES

1) Fox, R. O. 2012. Large-eddy-simulation tools for multiphase flows. Annu. Rev. Fluid Mech. 44, 47-76.
2) Marchisio, D. L., Fox, R. O. 2007. Multiphase Reacting Flows: Modelling and Simulation. CISM courses and lectures, 492. International Centre for Mechanical Sciences. Springer.
3) Fan, R., Marchisio, D. L., Fox, R. O. 2004. Application of the direct quadrature method of moments to polydisperse gas-solid fluidized beds. Powder Technol. 139, 7-20.
4) Fan, R., Fox, R. O. 2008. Segregation in polydisperse fluidized beds: Validation of a multi-fluid model. Chem. Eng. Sci. 63, 272-285.
5) Mazzei, L., Marchisio, D. L., Lettieri, P. 2010. Direct quadrature method of moments for the mixing of inert polydisperse fluidized powders and the role of numerical diffusion. Ind. Eng. Chem. Res. 49, 5141-5152.

6) Mazzei, L. 2011. Limitations of Quadrature-Based Moment Methods for Modeling Inhomogeneous Polydisperse Fluidized Powders. Chem. Eng. Sci. 66, 3628-3640.
7) Gidaspow, D. 1994. Multiphase Flow and Fluidization. Academic Press.