International Journal of Multiphase Flow 89 (2017) 413–416

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmulflow

Brief communication

Analytical solution for a three-dimensional non-homogeneous bivariate population balance equation—a special case

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ARTICLE INFO

Article history:
Received 20 August 2016
Revised 3 November 2016
Accepted 16 November 2016
Available online 2 December 2016

Keywords:
Analytical solution
Bivariate population balance equation
Method of manufactured solutions
Code verification

ABSTRACT

There has been a dramatic increase in the number of research publications using the population balance equation (PBE). The PBE allows the prediction of the spatial distribution of the dispersed phase size for an accurate estimation of the flow fields in multiphase flows. A few recent studies have proposed new efficient numerical methods to solve *non-homogeneous multivariate* PBE and implemented the same in computational fluid dynamics (CFD) codes. However, these codes are generally benchmarked against other numerical methods and applied without verification. To address this gap, an analytical solution for a three-dimensional non-homogeneous bivariate PBE is presented here for the first time. The method of manufactured solutions (MMS) has been used to construct a solution of the non-homogeneous PBE containing breakage and coalescence terms, and an additional source term appearing as a result of this method. The analytical solution presented in this work can be used for the rigorous verification of computer codes written to solve the non-homogeneous bivariate PBE. Quantification of the errors due to different numerical schemes will also become possible with the availability of this analytical solution for the PBE.

1. Introduction

The population balance equation (PBE) has attracted widespread interest in the field of multiphase flow modelling in recent years. There has been a dramatic increase in the number of research publications using the PBE to predict the spatial distribution of the dispersed phase size for an accurate estimation of the flow fields. The significance of modelling the polydispersity of the dispersed phase through solving the PBE has been found particularly useful in the case of higher dispersed phase concentrations, where particle aggregation and breakage effects are prominent, such as in turbulent flows (with liquid drops or gas bubbles as the dispersed phase). Although most of the studies have dealt with a monovariate[1] number density function (NDF) with the particle size as the internal coordinate,[2] a few recent works have coupled the PBE for a multivariate NDF with the flow equations, including a second internal coordinate such as chemical composition (Buffo and Alopaeus, 2016; Buffo et al., 2012; Renze et al., 2014). Increased computational power and improvements in the solution methods for the PBE, have made it possible to solve such multivariate PBEs numerically. The present work proposes an analytical solution to a non-homogeneous[3] three-dimensional bivariate PBE, which can be used for verifying the specialised computational fluid dynamics (CFD) codes written to numerically solve the PBE containing multiple internal and external[4] independent coordinates. Please note that *multivariate* is used in reference to the internal coordinate in the NDF and *dimension* refers to the external coordinate in this text.

Quadrature-based moment methods (QBMM) have made it computationally tractable to couple the multivariate PBE to the Eulerian–Eulerian flow equations. Methods such as the direct quadrature method of moments (DQMOM) (Marchisio and Fox, 2005) and the conditional quadrature method of moments

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[1] *Monovariate, bivariate* and *multivariate* are used to refer to the internal coordinates in this work.

[2] Internal coordinates include particle specific properties such as particle size, moisture content, composition, etc.

[3] When describing the PBE, the words *homogeneous* and *dimension* are used in reference to the physical space in this text. *Homogeneous* therefore means spatially homogeneous when characterising the PBE.

[4] External coordinates are the same as spatial coordinates.

http://dx.doi.org/10.1016/j.ijmultiphaseflow.2016.11.005

(CQMOM) (Cheng and Fox, 2010) have recently been implemented in open-source codes for this purpose (Buffo et al., 2013a; Renze et al., 2014). Code verification, which is a necessary step to assess the correctness of the computational method implemented for solving a partial differential equation (PDE), is however missing for the above implementations for non-homogeneous multivariate NDFs. Code verification ought to be performed against a benchmark solution for quantifying the accuracy of the numerical method and its order of convergence. Comparison with an analytical solution is the best benchmark possible as rigorous code verification analysis can be performed with it. Although analytical solutions for certain (spatially) homogeneous PBEs are available (Marchisio and Fox, 2005; McCoy and Madras, 2003), no such solution exists for the non-homogeneous PBE for monovariate or multivariate NDFs with the PBE containing breakage and aggregation (or coalescence) terms. The lack of an analytical solution for the latter has been the reason for the missing code verification for multivariate PBEs solved using DQMOM and CQMOM. For instance, Buffo (2012) performed code benchmarking for a *homogeneous* PBE and the numerical method was then applied to predict the distribution of bubble size and composition using a *non-homogeneous* multivariate PBE, and hence the flow, in a bubble column.

Validation of the numerical solution of a non-homogeneous bivariate PBE simulation against experimental results can be found in the literature (Buffo et al., 2013b) but code verification has never been presented. Discrepancies seen in the numerical results can occur due to numerical errors, which may not be detected due to the missing code verification step. Quantification of these errors due to the different numerical schemes is therefore essential in order to obtain full confidence in the correct implementation of the PBE model.

Higher-order discretisations for the convection term in the non-homogeneous PBE have been shown to result in a non-realisable moment set (also known as moment corruption) in certain QBMM, e.g. QMOM (Marchisio and Fox, 2013). Moment corruption can be analysed rigorously through a comparison of the time evolution of the numerical solution with an analytical solution for the non-homogeneous PBE. The propagation of the error in different moments can therefore be studied and compared for different advective discretisation schemes. This is currently not possible as analytical solutions are only available for the homogeneous PBE (McCoy and Madras, 2003), which does not bring the issue of moment corruption to light. The proposed analytical solution will allow for the detection and analysis of the moment corruption issue.

To address the above discussed limitations in the present scientific literature, an analytical solution to a three-dimensional non-homogeneous bivariate PBE is presented in this brief communication. The method of manufactured solutions (MMS) (Roache, 2002) has been used to generate this analytical solution. The proposed solution is sufficiently complex to test all terms in a transient, non-homogeneous PBE containing breakage and coalescence terms.

2. Method of manufactured solutions

The MMS is a reverse approach that ‘manufactures’ an exact solution to a given PDE (Roache, 2002). In order to ensure that the governing PDE is satisfied by the chosen solution, a suitable source term is added to it. The ‘manufactured’ solution must be analytic as well as non-trivial such that derivatives of all orders exist in the error (or Taylor) expansion of the discretised equation (Roache, 2002). This allows for the solution to “exercise” all terms in the error expansion, as stated by Roache (2002), and makes it complex enough to distinguish between different discretisations through the quantification of the errors. Trigonometric and exponential functions are best suited for this purpose. The manufactured solution need not be physically realistic as code verification is a purely mathematical exercise, however it must be complex enough to distinguish between different discretisations.

Jacobs et al. (2013) and Choudhary et al. (2016) have recently used MMS for verifying multiphase fluid flow solvers. Zhu et al. (2008) and Solsvik and Jakobsen (2016) used MMS to verify their solution methods for a homogeneous monovariate PBE. However, the complicated nature of the application of the MMS for the derivation of an analytical solution for the non-homogeneous multivariate PBE can be one of the reasons for the absence of this approach in the numerical verification of the non-homogeneous PBE solution codes.

It must be stressed that the inclusion of an artificial source term in the PDE (appearing as a result of the MMS) does not make the code verification any less useful. A verification exercise with an analytical solution obtained using MMS will help identify any code implementation issues so that a system without the artificial source term can also be correctly solved (Roache, 2002).

3. Analytical solution

A non-homogeneous PBE with breakage and coalescence terms can be written as (Ramkrishna, 2000):

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{u}n) = B_B - D_B + B_C - D_C + S, \tag{1}$$

where $n(\boldsymbol{\xi}, \mathbf{x}, t)$ is the NDF as a function of the *internal* and *external* coordinates, $\boldsymbol{\xi}$ and $\mathbf{x}$, respectively, and the time t. In the above equation, $\mathbf{u}$ refers to the velocity vector and S is the (artificial) MMS source term that has been added to the PBE. The ∇ operator applies to the external coordinates only. The terms B_B and D_B refer to the birth and death functions due to breakage, and B_C and D_C refer to the birth and death functions due to coalescence. Nucleation and growth are not considered in the present work.

A bivariate, three-dimensional NDF

$$n(\boldsymbol{\xi}, \mathbf{x}, t) = e^{-(\xi_1^2+\xi_2^2)} \sin^2 t\ \sin^2 x\ \sin^2 y\ \sin^2 z \tag{2}$$

is chosen as the ‘manufactured’ solution to the PBE in this work, where $\boldsymbol{\xi} = (\xi_1, \xi_2)$ and $\mathbf{x} = (x, y, z)$. The MMS source term S is then calculated using:

$$S(\boldsymbol{\xi}, \mathbf{x}, t) = S_1 + S_2 + S_3 + S_4 + S_5 + S_6. \tag{3}$$

The terms S_1 to S_6 are obtained as the contributions from the different terms in Eq. (1) and are described below.

The birth term due to breakage is written as:

$$B_B(\boldsymbol{\xi}) = \int_{\Omega_{\xi'}} \nu(\boldsymbol{\xi}') a(\boldsymbol{\xi}') P(\boldsymbol{\xi}|\boldsymbol{\xi}') n(\boldsymbol{\xi}') \mathrm{d}\Omega_{\xi'}, \tag{4}$$

where $\mathrm{d}\Omega_{\xi'} = \mathrm{d}\xi_1' \mathrm{d}\xi_2'$, the domain of integration $\Omega_{\xi'}$ is the entire positive $\mathbb{R}^2$ plane, $\nu(\boldsymbol{\xi}') = 2$ (for binary breakage) and the breakage rate $a(\boldsymbol{\xi}') = 1$. The daughter distribution function in this case is chosen as the product of two delta functions for symmetric breakage:

$$P(\boldsymbol{\xi}|\boldsymbol{\xi}') = \delta\left(\xi_1 - \frac{\xi_1'}{2}\right)\delta\left(\xi_2 - \frac{\xi_2'}{2}\right). \tag{5}$$

Since $P(\boldsymbol{\xi}|\boldsymbol{\xi}')$ is a probability density function, it is chosen to satisfy the property $\int_{\Omega_\xi} P(\boldsymbol{\xi}|\boldsymbol{\xi}')\mathrm{d}\Omega_\xi = 1$.

In the present bivariate population balance problem both internal variables are assumed to be extensive, as shown by the form of the above symmetric breakage daughter distribution function. This assumption is, however, by no means restrictive on the application of the MMS to verify the PBE solution methodology. The daughter distribution function can be modified for an intensive internal variable (such as chemical composition), if required.