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Application of the least-squares method for solving population balance problems in $\mathbb{R}^{d+1}$

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Abstract

In multiphase chemical reactor analysis the prediction of the dispersed phase distribution plays a major role in achieving reasonable results. The combined CFD–PBE (population balance equations) are computationally intensive requiring efficient numerical methods for dealing with them. This paper presents the formulation and validation of a spectral least squares method for solving the steady state population balance equations in $\mathbb{R}^{d+1}$, with d the physical spatial dimension and 1 the internal property dimension. The least-squares method consists in minimizing the integral of the square of the residual over the computational domain. Spectral convergence of the L_2-norm error of the solution and of the moments of the solution are verified for the zero- and one-dimensional cases using model problems with analytical solutions.

Keywords: Chemical reactors; Population balance; Multiphase reactors; Multiphase flow; Least-squares method

1. Introduction

Population balance modeling is an active field of research due to its application to several engineering and scientific problems. This method is commonly used to study precipitation, polymerization, particle size distribution, dispersed phase distribution in multiphase flow problems, and so on. In particular in multiphase flow problems, the dispersed phase distribution presents a strong effect in the hydrodynamic properties and phase distribution. For that reason, considerable efforts have been made in order to develop polydispersed multi-fluid models with an inherent population balance module that will be able to consider the effects of the variations in the size and shape distributions of the dispersed phase. In particular, the present status on PBE modeling of bubbly flows has been examined (Jakobsen et al., 2005).

Using a population balance approach the dispersed phase is commonly treated using a density function, DF, for instance $f(\mathbf{r}, \xi, t)$ where $\mathbf{r}$ is the spatial vector position, ξ is the property of interest of the dispersed phase, and t the time. Thus, $f(\mathbf{r}, \xi, t)\,\mathrm{d}\xi$ can represent for example the average number of particles per unit volume around the point x in the time t, with the property between ξ and $\xi+\mathrm{d}\xi$. The evolution of this density function must take into account the different processes that control particle population such as breakage, coalescence, growth and convective transport of the particles. The resulting equation is a nonlinear partial integro-differential equation which requires to be solved by a suitable numerical method, although analytical approximations can sometimes be derived for some particular cases, see for example Patil and Andrews (1998).

The method of moments is an efficient method to solve the PBE, but it is only applicable to a limited number of problems and gives no information about the shape of the distribution. For example, Frenklach (1985) applied the method of moments to a coagulation process where the coagulation rate was constant. For an arbitrary coagulation rate function, this formulation results in an excess of unknowns compared to the number of equations whichh is denoted as a closure problem (Hulburt and Katz, 2003). One way to avoid this problem is to assume the shape of the density function, and so the parameters of the density function are related, closing off the set of moments equations (Williams, 1986). A different alternative is to express the density function as a truncated series of some orthogonal polynomials (Hulburt and Katz, 2003). McGraw (1997) suggested a modification of the method of moment

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which consists in using a quadrature approximation in order to avoid the closure problem. McGraw (1997) based his method on the product difference (PD) algorithm suggested by Gordon (1968), calling this approach quadrature method of moments (QMOM). Marchisio et al. (2003) and Marchisio et al. (2004a) used this approach to study particulate systems. Later, McGraw and Wright (2002) proposed a new moment closure method, the Jacobian matrix transformation (JMT) which avoids the use of the PD algorithm. Similarly, Marchisio et al. (2004b) extended the QMOM method to multifluid applications calling this approach the direct quadrature method of moments (DQMOM). Bove et al. (2005) presented the parallel parent and daughter classes (PPDC) which used the PD algorithm for reducing the computational cost of the QMOM. It is important to mention that the PD algorithm is a numerical ill-conditioned method for computing the Gauss quadrature rule (e.g. Lambin and Gaspard, 1982). In general, the computation of the quadrature rule based on the power moments of the density function is quite sensitive to small errors as the number of moments used becomes large (e.g. Golub and Welsh, 1969; Gautschi, 1994). Therefore, the applicability of QMOM is limited to no more than 12 moments, although in certain applications it is claimed that only a few moments are enough for obtaining reliable results (McGraw et al., 1997).

A different way of avoiding the closure problem is discussed by Frenklach (2002) in the method of moments with interpolative closure (MOMIC). In this case, the natural logarithmic of the moments is expressed by a polynomial in the moment order, and thus, the required moments are interpolated or extrapolated. Further discussion about the closure for the method of moments can be found in Diemer and Olson (2002).

An alternative strategy is to employ projection methods, such as finite element methods (FEM), in which the solution is approximated as a linear combination of the basis functions over a finite number of sub-domains. Chen et al. (1996) developed a wavelet-Galerkin method for solving PBEs for the treatment of particle-size distribution in problems of a continuous, mixed-suspension and mixed-product removal crystallizer with effects of breakage. Niemanis and Hounslow (1998) applied FEM to the steady-state PBE, finding more accurate solutions than using the sectional methods and using less computational power. Liu and Cameron (2001) proposed the use of a wavelet-based method for the treatment of problems involving particle nucleation, growth and agglomeration. Niemanis and Hounslow (2002) showed an a posteriori error estimate of the FEM applied to PBE. A posteriori error estimate is an important characteristic of the projection methods, which allows to quantitatively assess the quality of an obtained numerical solution. This characteristic is not commonly presented in the previous discussed methods. Due to the fact that for some applications such as chemical reactor simulations the computational cost of the solver of the PBE requires to be reduced, high-order polynomial approximation methods could be an option, improving the behavior of FEM solvers. The global approximation of the solution, compared with the local one of FEM or sectional methods, permits to reduce the final computational cost since less points are required for the same accuracy. These methods, including FEM, can be presented in the framework of the methods of weighted residuals (MWR). Depending on the election of the trial and test functions different methods can be obtained (Canuto et al., 2000). Subramain and Ramkrishna (1971) presented a Tau method for solving the distribution of the population of microbial cells that present growth and breakage processes. Mantzaris et al. (2001) discussed the Galerkin, Tau and pseudo-spectral methods as a tool for solving multivariable cell population balance models that present growth and breakage. Recently, Dorao and Jakobsen (2005a, 2006) discussed the applicability of the least squares method (LSM) (Jiang, 1998a; Bochev, 2001; Proot and Gerritsma, 2002; Pontaza and Reddy, 2003) for solving the population balance equation.

The LSM consists in finding the solution which minimizes the L^2 norm of the residual over the computational domain. The LSM can also be considered a special case of the MWR where the trial and test functions are equal to the residual equation (Finlayson, 1972). The interest on the LSM has increased quite a lot during the last decade as a consequence of its properties:

- Independent of the underlining equation, least squares always leads to symmetric positive-definite systems of linear algebraic equations, which can be efficiently solved.
- For first order problems, e.g. an advective transport equation, the LSM does not require any special numerical treatment like the up-wind discretization in the case of finite difference. Thus, no numerical diffusion is introduced.
- The evaluation of the accuracy of the approximate solution is many areas of engineering and applied science is rather important. The LSM meets the need for a posteriori error analysis by supplying an error indicator in the form of the residuals that are minimized by the procedure. In particular, this is a very reliable indicator which can be used for example for grid refinement.
- Finally, the LSM is formulated in a very general setting. Thus, the programming can be done in a very systematic way and new applications requires a minimum work reducing drastically cost and programming errors in code development.

Dorao and Jakobsen (2005a, 2006) applied the least-squares spectral method to the population balance equation involving breakage and coalescence processes using Legendre polynomials for the particle space discretization and Crank–Nicolson for the time discretization. Thus, the solver shown spectral convergence in the property space while algebraic convergence rate for time. Later, Dorao and Jakobsen (2005b) discussed the space–time least-squares formulation for solving the PBE. In this space–time formulation, time is treated as an additional dimension, which allows high-order accuracy both in space and in time (e.g. De Maerschalck, 2003; Pontaza and Reddy, 2004). In this way, space–time can be solved at once, or per time-step on a space–time slab in a kind of semi-discrete formulation.

The main goal of this paper is to extend the previous mathematical framework for solving the PBE including the physical