Spectral Solutions of a Combined Multifluid–population Balance Model Describing Bubbly Flow

A Numerical Study of weighted Residual Methods

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Abstract: Fluid particle breakage and coalescence phenomena are important for optimal operation for industrial process units like the bobble column reactors. The population balance equation (PBE) can be applied to describe the evolution of populations of countable entities such as the bubbles in the bubble column. In recent literature, the least-squares methods has been adopted for the approximate solution of population balance (PB) models. Adopting a weighted residual method such as the least-squares method, the distribution function resolved instead of obtaining only a few moments of the distribution function. The performance of the least-squares method for PB problems should be compared to other techniques in the family of weighted residual methods. The aim of the present study is to evaluate the orthogonal collocation, tau and last-squares methods for the solution of a combined multifluid-PB model describing bubbly flows.

1 INTRODUCTION

Despite the simple construction of the bubble columns and their widespread use for chemical reactions and separation in the process industries, our understanding of the complex flows in these vessels is still very limited. The complexity of the hydrodynamics in the bubble columns relates to the evolution of phenomena such as breakage, coalescence, growth and convective transport of the bubbles. In the mathematical modeling framework, the PBE (Ramkrishna, 2000; Jakobsen, 2008; Randolph and Larson, 1988; Sporleder et al., 2012) is considered a concept for describing the evolution of populations of countable entities such as the bubbles in the bubble column. Adopting the PB modeling technique to bubbly flows, the dispersed gas phase is treated as a population of bubbles distributed not only in physical space but also in an abstract property space. The quantity of basic interest in PB modeling is the statistical density function representing the behavior of the population of bubbles. The evolution of the statistical density function must take into account the different processes that control the population of the bubbles in the vessel, such as breakage, coalescence, growth and convective transport. Thus the PBE provides a statistical description of the dispersed phase where the

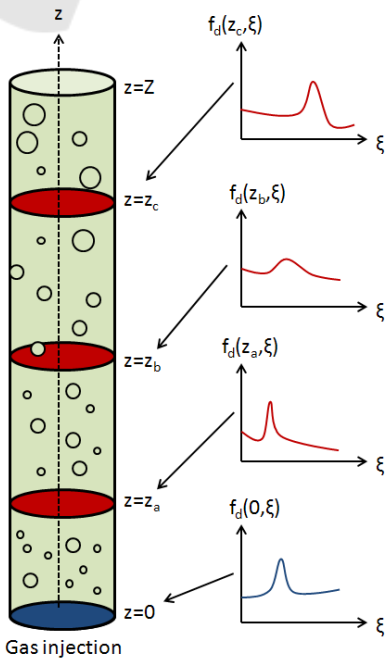

Figure 1: Sketch of a bubble column reactor. The parameter ξ is a characteristic property of the bubble, for example the bubble diameter. Because of the different interaction processes, the distribution of the bubbles evolves.

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density function may be denoted by $f(\mathbf{r},\xi,t)$ where $\mathbf{r}$ is the spatial position vector, ξ is the property of interest of the dispersed phase, and t is the time. Moreover, $f(\mathbf{r},\xi,t)\,\mathrm{d}\xi$ represents the average number of particles per unit volume around the point $\mathbf{r}$ $(\mathbf{r},\mathbf{r}+\mathrm{d}\mathbf{r})$ in the time t, with the property between ξ and $\xi+\mathrm{d}\xi$. The resulting PBE is characterized mathematically as a non-linear integro-partial differential equation which must be solved by a suitable numerical method.

In recent publications, the least-squares method has been adopted for the solution of PB problems, e.g. (Dorao and Jakobsen, 2006b; Dorao and Jakobsen, 2007b; Dorao and Jakobsen, 2008; Dorao and Jakobsen, 2009; Dorao and Jakobsen, 2007a; Dorao and Jakobsen, 2006a; Nayak et al., 2011; Sporleder et al., 2011; Zhu et al., 2009a; Zhu et al., 2009b; Patruno et al., 2009; Patruno, 2010; Borka and Jakobsen, 2012a). The least-squares method has also been applied to other chemical reactor problems such as the pellet equations and fixed packed bed reactors (Rout et al., 2011; Rout and Jakobsen, 2012; Solsvik and Jakobsen, 2012; Sporleder et al., 2011). However, the least-squares technique is a method in the family of weighted residual. Thus, it is of interest to reveal the properties of the least-squares method compared to other methods in the weighted residual framework like the orthogonal collocation and tau methods.

The aim of the present study is to compare the performance of different solution techniques in the family of weighted residual methods. The solution methods is evaluated for a combined multifluid-PB model describing bubbly flow. The evaluation should consider residual measures, computational time, implementation issues, and complexity of the algebraic theory of the methods.

2 THE MODEL

The combined multifluid-PB model considered in the present study is based upon the work of (Nayak et al., 2011; Borka and Jakobsen, 2012a; Borka and Jakobsen, 2012b; Borka and Jakobsen, 2012c). The steady-state model holds one dimension in physical space and one dimension in the property space (bubble diameter). The model equations is outlined in the sequel.

The main advantages of the novel model by (Nayak et al., 2011) is that both the PBE and the momentum equation of the dispersed gas phase is in terms of the internal coordinate ξ. Hence, the inner coordinate space physics can be resolved provided that a sufficient numerical method is available. In particular, the least-squares, tau, Galerkin and orthogonal collocation methods in the weighted residual framework can be applied to solve the model proposed by (Nayak et al., 2011).

In the following, the multifluid–PB model is outlined for bubbly flows in a cold-flow column.

2.1 The dispersed Phase

The two-dimensional (one dimensiona in the physical space and one dimension in the property space) PBE is presented by:

$$\begin{aligned}
&\frac{\partial}{\partial z}\left[v_z(\xi,z)\,f_{d,m}(\xi,z)\right]+\frac{\partial}{\partial \xi}\left[v_\xi(\xi,z)\,f_{d,m}(\xi,z)\right]\\
&=-b(\xi)\,f_{d,m}(\xi,z)\\
&+V(\xi)\int_{\xi}^{\xi_{\max}} h(\xi,\zeta)b(\zeta)\frac{f_{d,m}(\zeta,z)}{V(\zeta)}\,\mathrm{d}\zeta\\
&-f_{d,m}(\xi,z)\int_{\xi_{\min}}^{(\xi_{\max}^3-\xi^3)^{1/3}} c(\xi,\zeta)\frac{f_{d,m}(\zeta,z)}{\rho_d(z)V(\zeta)}\,\mathrm{d}\zeta\\
&+\frac{\xi^2V(\xi)}{2}\int_{\xi_{\min}}^{(\xi^3-\xi_{\min}^3)^{1/3}} \frac{c([\xi^3-\zeta^3]^{1/3},\zeta)}{[\xi^3-\zeta^3]^{2/3}}\\
&\times\frac{f_{d,m}(\zeta,z)}{\rho_d(z)V(\zeta)}\frac{f_{d,m}([\xi^3-\zeta^3]^{1/3},z)}{V(\xi)-V(\zeta)}\,\mathrm{d}\zeta
\end{aligned}\tag{1}$$

in which $f_{d,m}$ is the mass density function [kg/m^3/m]. The bubbles are transported in physical space according to velocity v_z and in the property space according to velocity v_ξ. Moreover, the internal coordinate is the bubble diameter. The breakage rate and daughter size redistribution function proposed by (Coulaloglou and Tavlarides, 1977), and the coalescence model by (Prince and Blanch, 1990) are adopted. The breakage frequency yields:

$$b(z,\xi)=\frac{k_1\varepsilon^{1/3}}{\xi^{2/3}}\exp\left[-\frac{\sigma k_2}{\rho_l\varepsilon^{2/3}\xi^{5/3}}\right]\tag{2}$$

where k_1 and k_2 are empirical parameters, which depend on the system properties. The daughter size redistribution function is given as:

$$\begin{aligned}
h(\xi,\zeta)=&2P(\xi,\zeta)=2\frac{2.4\left(\frac{\pi}{2}\xi^2\right)}{V(\zeta)}\\
&\times\exp\left(-4.5\frac{[2V(\xi)-V(\zeta)]^2}{V(\zeta)^2}\right)
\end{aligned}\tag{3}$$

The coalescence model by (Prince and Blanch, 1990) is defined as the product of a collision volume rate $h_c(\xi,\zeta)$ and the coalescence probability $\lambda_c(\xi,\zeta)$:

$$c(\xi,\zeta)=h_c(\xi,\zeta)\lambda_c(\xi,\zeta)\tag{4}$$

The expression for the coalescence probability is given as:

$$\lambda_c(\xi,\zeta) = \exp\left[-\frac{\left[\frac{r_c^3(\xi,\zeta)\rho_l}{16\sigma}\right]^{1/2}\varepsilon^{1/3}\ln\left[\frac{h_0}{h_f}\right]}{\left[r_c(\xi,\zeta)\right]^{2/3}}\right] \quad (5)$$

where the equivalent radius is defined as:

$$r_c(\xi,\zeta) = \frac{1}{4}\left[\frac{1}{\xi}+\frac{1}{\zeta}\right]^{-1} \quad (6)$$

The collision volume rate is given as:

$$h_c(\xi,\zeta) = \frac{\pi}{4}[\xi+\zeta]^2\left[\beta[\xi]^{2/3}+\beta[\varepsilon\zeta]^{2/3}\right]^{1/2} \quad (7)$$

The bubble growth velocity is estimated as:

$$v_\xi(z,\xi) = -\frac{\xi v_z}{3\rho_d(z)}\frac{\partial p_d(z)}{\partial z} \quad (8)$$

The momentum equation of the dispersed phase is given as:

$$\begin{aligned}&\frac{\partial}{\partial z}\left[f_{d,m}(\xi,z)v_z(\xi,z)v_z(\xi,z)\right] = \\ &-\frac{\partial}{\partial\xi}\left[f_{d,m}(\xi,z)v_\xi(\xi,z)\right] \\ &-\frac{f_{d,m}(\xi,z)}{\rho_d(z)}\frac{\partial p_d(z)}{\partial z}+f_{d,m}(\xi,z)g+f_{\text{drag}}(\xi,z)\end{aligned} \quad (9)$$

The dispersed phase fraction:

$$\alpha_d(z) = \int_0^\infty \frac{f_{d,m}(\xi,z)}{\rho_d(z)}\,d\xi \quad (10)$$

The gas-phase pressure is assumed equal to the liquid-phase pressure: $P = P_d = P_l$. The ideal gas law gives the relationship between the pressure and the dispersed phase density:

$$p(z) - \frac{p^0}{\rho_d^0}\rho_d(z) = 0 \quad (11)$$

The drag force is defined as:

$$\begin{aligned}f_{\text{drag}} = &-\frac{3}{4}\rho_l\frac{C_D}{\xi}\frac{f_{d,m}(\xi,z)}{\rho_d(z)}|v_r(\xi,z)-v_l(z)| \\ &\times\left[v_r(\xi,z)-v_l(z)\right]\end{aligned} \quad (12)$$

where

$$C_D = \max\left(\min\left[\frac{16}{\text{Re}p}(1+0.15\text{Re}_p^{0.687}),\frac{48}{\text{Re}_p}\right],\frac{8}{3}\frac{\text{Eo}}{\text{Eo}+4}\right) \quad (13)$$

$$\text{Re}_p = \frac{\rho_l|v_z(z,\xi)-v_l(z)|\xi}{\mu_l} \quad (14)$$

$$\text{Eo} = \frac{g(\rho_l-\rho_g)\xi^2}{\sigma} \quad (15)$$

2.2 The Continuous Phase

The liquid continuity equation:

$$\frac{d}{dz}\left[\alpha_l(z)\rho_l v_l(z)\right] = 0 \quad (16)$$

or integrated:

$$\alpha_l(z)\rho_l v_l(z) = \alpha_l(z=0)\rho_l v_l(z=0) \quad (17)$$

The momentum equation:

$$\begin{aligned}&\alpha_l(z)\rho_l v_l(z)\frac{d}{dz}v_l(z) = \\ &\alpha_l(z)\left[-\frac{dp(z)}{dz}-\frac{1}{2}\rho_l\frac{f_w(z)}{D}v_l(z)^2\right] \\ &-\int_0^\infty f_{\text{drag}}(\xi,z)\,d\xi+\alpha_l(z)\rho_l g\end{aligned} \quad (18)$$

The summation of the phase area fraction must be unity:

$$\alpha_d+\alpha_l = 1 \quad (19)$$

The wall friction factor is calculated as:

$$f_w(z) = \left[0.79\ln\left[\text{Re}_l(z)\right]-1.64\right]^{-2} \quad (20)$$

3 NUMERICAL METHODS

Basically, spectral methods are based upon using a representation of the solution function over the entire computational domain via a truncated series expansion (Finlayson, 1972):

$$f_{\text{ex}}(\xi) \approx f^{\mathcal{P}}(\xi) = \sum_{j=0}^{\mathcal{P}}\alpha_j\varphi_j^{\mathcal{P}}(\xi) \quad (21)$$

in which $\varphi_j^{\mathcal{P}}(\xi)$ denotes the basis function and α_j denotes the basis coefficients. A nodal basis is obtained if the truncated series expansion (21) is given in terms of Lagrangian basis polynomials $\ell_j^{\mathcal{P}}(\xi)$:

$$f(\xi) \approx f^{\mathcal{P}}(\xi) = \sum_{j=0}^{\mathcal{P}} f_j^{\mathcal{P}}\ell_j^{\mathcal{P}}(\xi) \quad (22)$$

in which the basis coefficients are meaningful in the sense that they correspond to the solution function values at the collocation points.

The methods of weighted residual is presented by the following generalized inner product:

$$\begin{aligned}&\int_\Omega \mathcal{R}(\xi; f_0^{\mathcal{P}}, f_1^{\mathcal{P}}, ..., f_{\mathcal{P}}^{\mathcal{P}})w_i(\xi)\,d\Omega = 0 \\ &\text{for} \quad i = 0,1,\ldots,\mathcal{P}\end{aligned} \quad (23)$$

where w_i are weighting functions and $\mathcal{R}$ is the residual. The particular choice of the weighting function defines the particular solution approximation technique in the family of weighted residual methods:

- the least-squares method

$$w_i = \frac{\partial}{\partial f_i^{\mathcal{P}}} \mathcal{R}(\xi, f_0^{\mathcal{P}}, f_1^{\mathcal{P}}, ..., f_{\mathcal{P}}^{\mathcal{P}}) \tag{24}$$

- the tau method

$$w_i = \ell_i^{\mathcal{P}}(\xi) \tag{25}$$

- the orthogonal collocation method

$$w_i = \delta(\xi - \xi_i) \tag{26}$$

The tau (Lanczos, 1938) and least-squares (Jiang, 1998; Bochev and Gunzburger, 1998; Pontaza, 2003) methods have not obtained the same popularity as the orthogonal collocation method (Villadsen and Steward, 1967; Villadsen, 1970; Villadsen and Michelsen, 1978; Michelsen and Villadsen, 1981) in the chemical reactor engineering society. However, the tau method is similar to the Galerkin method (Galerkin, 1915). The essential difference between the Galerkin and the tau methods is the treatment of the boundary conditions. Theory of the least-squares method from a chemical engineering point of view is given by (Dorao, 2006; Zhu, 2009; Sporleder, 2011). Furthermore, the algebra and implementation issues using the least-squares method for the solution of a PB problem is provided by (Solsvik and Jakobsen, 2013).

4 RESULTS

The solution of the PBE (1) is presented in figure 2. The PB model has been solved with the orthogonal collocation, tau and least-squares methods.

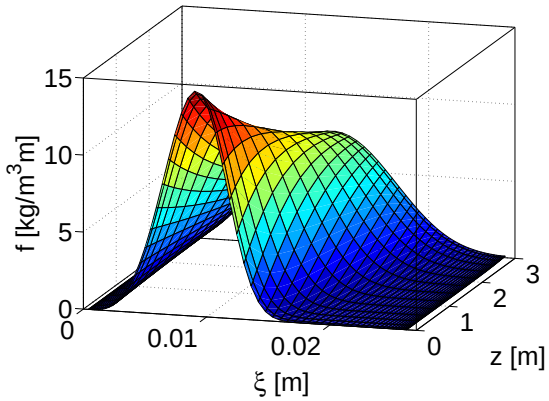

Figure 2: Solution of a PB problem. The bubble size distribution along the bubble column height.

Two residual measure definitions have been employed to evaluate the accuracy of the solution methods. The residual measure definitions are based on (i) the problem operator form and (ii) the algebraic system form. The former residual definition measure the residual of the governing equation, while the latter definition gives the residual of the algebraic equation system that is actually solved. Noticeable, for the orthogonal collocation method the problem operator form and the algebraic system form coincide. Figure 3 shows the residual versus the number of iterations adopting the residual measure definition based on the algebraic system form. Based on this particular residual measure, the tau method is significantly favorable above the orthogonal collocation and least-squares methods. The orthogonal collocation and least-squares methods obtain the same accuracy, but with differences in the number of iteration to reach convergence, in which the least-squares method requires less iteration to reach its minimum residual value. In figure 4 the residual measure definition based on the problem operator form is adopted. For this particular residual measure definition, the tau and orthogonal collocation show the same performance. On the other hand, the least-squares method obtains a significant larger value of the residual measure. Thus, the least-squares method does not fulfill the governing equation as well as the orthogonal collocation and tau methods. The least-squares method requires further attention to reveal the significantly larger resid-

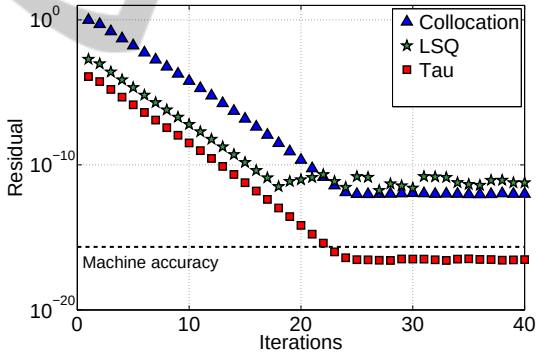

Figure 3: Residual (algebraic system form) as a function of the number of iterations.

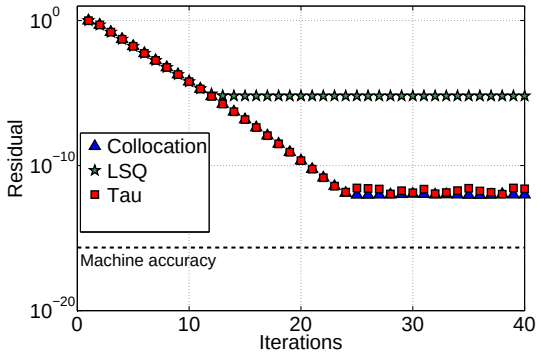

Figure 4: Residual (problem operator form) as a function of the number of iterations.

ual measure on the problem operator form compared to the orthogonal collocation and tau methods.

The orthogonal collocation method is favorable considering the simplicity of implementation compared to the tau and leas-squares methods. Moreover, the orthogonal collocation method uses less computational costs per iteration than the relatively more computational demanding tau and least-squares methods.

5 CONCLUSIONS

The accuracy of the orthogonal collocation, tau and least-squares method can be evaluated on different residual measure definitions. Dependent on the residual measure definition adopted, the relatively performance of the numerical methods may change significantly. However, the simulation results of the present PB problem indicate that the orthogonal collocation and tau method are favorable above the least-squares method considering accuracy. Nevertheless, the orthogonal collocation method uses less computational costs per iteration than the tau and least-squares methods. Furthermore, the orthogonal collocation method holds the simplest algebraic theory, and is thus associated with the simplest implementation issues.

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