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Numerical simulations of drop size evolution in a horizontal pipeline

A.C. Bourdillon, P.G. Verdin*, C.P. Thompson

School of Energy, Environment and Agrifood, Oil & Gas Engineering Centre, Cranfield University, Bedfordshire, MK43 0AL, United Kingdom

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ABSTRACT

A population balance model using a standard method of moments $(S - \gamma)$ in an Eulerian–Eulerian framework has been used for oil and brine two-phase flow simulations in pipelines. Results have been compared to both numerical and experimental data from the literature. The effects of the forces constituting the momentum transfer term at the interphase between droplets and the continuous phase (drag, lift, turbulent dispersion and virtual mass), turbulence modelling, break-up and coalescence parameters are analysed; they are shown to be important for droplet mean diameter evolution. It has been demonstrated that a correct combination of models and parameters improves (47% for the best case) simulated results when compared to experimental data. Interactions between the different components of the whole model are discussed and their corresponding effects on the droplet diameter predictions are explained. In particular, the addition of the lift force tends to push the droplet toward the walls of the computational domain where turbulence and shear stress are the strongest, therefore leading to an increased break-up rate. Based on the findings of this study, recommendations for further population balance-based modelling with a standard method of moments are provided.

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Introduction

During the transport of oil and water through pipes, interactions between the two fluids occur continuously. Considering oil as the continuous phase and water as the dispersed phase, these strong interactions can give birth to droplets being transported with the continuous phase. Such droplets can potentially interact with each other and with the pipe wall, leading to a complex physical behaviour. The correct prediction of droplets movement, size and shape evolution is necessary to evaluate the deposition rate along with other critical parameters influencing the flow such as separation and pressure gradients.

The population balance method (PBM) solving the population balance equations (PBEs) currently stands as the reference method in this field of study (Ramkrishna, 2000). PBE equations characterise the evolution of the number of particles in a given region of the domain through time. These equations require numerical models for closure. For this purpose, several approaches, such as Monte Carlo methods (Friesen and Dabros, 2003; Zhao et al., 2010; Marchisio et al., 2004), have been used in the past. However, when using these methods, a high number of droplets is required to achieve an accurate averaging of their global evolution. Methods of classes have come as alternative solutions to overcome the computational expense induced by Monte Carlo approaches (Hounslow et al., 1988; Litster et al., 1995; Ramkrishna, 2011). Within each class, the PBEs are solved directly for the number density function. For instance, within a given range of droplet sizes, the particle size distribution (PSD) is discretised into an equivalent number of classes where the PBEs are solved. The number of classes necessary to accurately represent a population of droplets can therefore become very large. This is considered as the major drawback of the method of classes.

In addition, the use of such method can be difficult. A mother droplet that belongs to a specific class at a specific time may produce for instance two or more child droplets during a break-up event that will belong to other classes in the future.

Significant work has been performed over the past few years to solve the PBEs at a relatively low computational cost. The most promising approach is the method of moments, first introduced by Hulburt and Katz (1964). This method consists in solving the PBEs by tracking the moments of the particle size distribution. Several itemisations of the method have emerged recently such as the standard method of moment (SMOM) (Hulburt and Katz, 1964; Marchisio et al., 2002), the direct quadrature method of moments (DQMOM) (McGraw, 1997) and the extended quadrature method of moment (EQMOM) (Marchisio and Fox, 2013).

A standard method of moments has been used in the current study. The equations of the moments contain unclosed integral terms and therefore, additional modelling is required by assuming an initial (log-normal) distribution of droplets. Such a method has been successfully validated by Lo and Rao (2007). The $S - \gamma$ standard method

^{*} Corresponding author. Tel:+44 1234 750111x5214.

E-mail address: p.verdin@cranfield.ac.uk, patrick_verdin@yahoo.fr (P.G. Verdin).

of moments model described in Lo and Rao (2007) is used here to perform numerical simulations of brine droplets in oil in a horizontal pipeline. This work has been performed with the commercial CFD software StarCCM+ V8.02 (CD-Adapco, 2012). The study focuses on the identification of key parameters influencing the droplet behaviour during their transport. For this purpose, several drag models have been implemented and tested. The lift, turbulent dispersion and virtual mass force have been discussed. Parameters influencing droplet behaviour in turbulence, break-up and coalescence models parameters have also been investigated. Simulation results of droplet diameter prediction have been compared and validated against both numerical and experimental results from the literature.

Mathematical models

Models and physical effects taken into account in the simulations performed with StarCCM+ will now be described. Continuity, momentum and turbulence equations derived here are part of the segregated solver. The population balance modelling is performed with the available $S - \gamma$ model. Break-up and coalescence models used in this work are also part of the software. Different drag models have however been implemented; their influence on the results is discussed in the following sections.

Continuity, momentum and turbulence equations

For the Eulerian–Eulerian model, all phases are assumed to be in an equilibrium state. Each phase has its own velocity, energy and material properties. However, the conservation equations of each phase need closure. This is achieved through the definition of the phase interaction at each phase interface in each control volume. The continuity equation for an Eulerian–Eulerian model, in a general form, is written as:

$$\frac{\partial \alpha_i \rho_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{u}_i) = \sum_{j \neq i} \left(K_{ij}^{mass} - K_{ji}^{mass} \right) + S_i^{mass}.$$
(1)

Subscripts *i* and *j* denote the continuous and dispersed phases. The terms α_i , ρ_i , $\mathbf{u_i}$ and S_i^{mass} refer to the volume fraction, the density, the velocity vectors and the mass source term of phase *i*, respectively. The transfer rates of mass (K_{ij}^{mass} and K_{ji}^{mass}) from one phase to the next are both positive. Hence, for keeping the mass balance, the following two relationships have to be satisfied during the computation:

$$\sum_i \alpha_i = 1 \; ; \; \sum_i S_i^{mass} = 0,$$

The momentum equations are:

$$\frac{\partial \alpha_i \rho_i \mathbf{u}_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{u}_i \mathbf{u}_i) = -\alpha_i \nabla p + \alpha_i \rho_i \mathbf{g} + \mathbf{M}_i + \mathbf{F}_i^{int} + \nabla \cdot [\alpha_i (\tau_i + \tau_i^t)] + \sum_{j \neq i} (K_{ij}^{mass} \mathbf{u}_j - K_{ji}^{mass} \mathbf{u}_i) + \mathbf{S}_i^{mom},$$
(2)

where *p* stands for the pressure field, **g** is the gravitational acceleration vector, F_i^{int} represents the internal forces acting on phase *i*, and τ_i and τ_i^t are the molecular and turbulent stress tensors, respectively. The term **M**_i represents the sum of forces transmitted from one phase to the next. This term is usually composed of different forces such as drag (\mathbf{F}_{ij}^d), lift (\mathbf{F}_{ij}^ℓ), virtual mass (\mathbf{F}_{ij}^{vm}) and turbulent dispersion (\mathbf{F}_{ij}^{td}). The forces acting on the continuous phase due to the dispersed phase must be equal in absolute value to the force acting on the dispersed phase:

$$\mathbf{F}_{ij} = -\mathbf{F}_{ji}.\tag{3}$$

The forces constituting the interphase momentum transfer term (\mathbf{M}_i) will be derived in the following sections.

The realizable $k - \varepsilon$ turbulence model (Shih et al., 1994) was selected as the population balance solver is accessible only through the $k - \varepsilon$ turbulence formulation. Eqs. (4) and (11) below give the transport equation for the turbulent kinetic energy term (k) and the transport equation for the turbulent dissipation term (ε), respectively.

$$\frac{\partial \alpha_i \rho_i k_i}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{u}_i k_i) = \nabla \cdot \left[\alpha_i \left(\mu_i + \frac{\mu_i^t}{P_{r,k}^t} \right) \nabla k_i \right] + \alpha_i S_{k,i} + \alpha_i \left[E_{k,i} + E_{b,i} - \rho_i ((\varepsilon_i - \varepsilon_0) + E_{Y,i}) \right] + \sum_{j \neq i} (K_{ij}^{mass} k_j^{(ij)} - K_{ji}^{mass} k_i).$$

$$(4)$$

The terms μ_i and μ_i^t denote the molecular and the turbulent dynamic viscosity, respectively. The dimensionless term P_r is the Prandtl number. The production term E_k , in Eq. (4), represents the generation of turbulent kinetic energy due to the mean velocity gradient. E_Y stands for the dissipation of turbulent kinetic energy due to the contribution of fluctuating dilatation and ε_0 is the ambient turbulence value in the source terms that counteracts turbulence decay. E_b is the production of turbulent kinetic energy due to buoyancy effects. Finally, S_k is the source term for the turbulent kinetic energy. These terms are expressed as:

$$E_k = \mu^t R^2 - \frac{2}{3} \rho k \nabla \cdot \mathbf{u} - \frac{2}{3} \mu^t (\nabla \cdot \mathbf{u})^2, \qquad (5)$$

$$R = |\mathbf{R}| = \sqrt{2\mathbf{R} : \mathbf{R}^T} = \sqrt{2\mathbf{R} : \mathbf{R}},\tag{6}$$

$$\mathbf{R} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}), \tag{7}$$

$$E_b = \beta \frac{\mu^t}{P_{r,k}^t} (\nabla T \cdot \mathbf{g}), \tag{8}$$

$$\beta = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p,\tag{9}$$

$$E_{\rm Y} = \frac{2k\varepsilon}{u_{\rm Sound}}.$$
(10)

R stands for the modulus of the mean strain rate tensor, β is the thermal expansion coefficient and *T* is the temperature. The transport equation for the turbulent dissipation term (ε) can be written as:

$$\frac{\partial \alpha_{i}\rho_{i}\varepsilon_{i}}{\partial t} + \nabla \cdot (\alpha_{i}\rho_{i}\mathbf{u}_{i}\varepsilon_{i}) = \nabla \cdot \left[\alpha_{i}\left(\mu_{i} + \frac{\mu_{i}^{t}}{P_{r,\varepsilon}^{t}}\right)\nabla\varepsilon_{i}\right] \\
+ \alpha_{i}\left[C_{\varepsilon 1}R\varepsilon + \frac{\varepsilon_{i}}{k_{i}}(C_{\varepsilon 1}C_{\varepsilon 3}E_{b,i}) - \frac{\varepsilon_{i}}{k_{i} + \sqrt{\upsilon\varepsilon_{i}}}C_{\varepsilon 2}\rho_{i}(\varepsilon_{i} - \varepsilon_{0})\right] \\
+ \sum_{j\neq i}(K_{ij}^{mass}\varepsilon_{j}^{(ij)} - K_{ji}^{mass}\varepsilon_{i}) + \alpha_{i}S_{\varepsilon,i},$$
(11)

where the coefficients of the model are defined as:

$$C_{\varepsilon 1} = max \left[0.43, \frac{\frac{Rk}{\varepsilon}}{5 + \frac{Rk}{\varepsilon}} \right], \tag{12}$$

$$C_{\varepsilon 2} = 1.9,\tag{13}$$

 $C_{\varepsilon 3} = 1 \text{ if } E_b \ge 0, \quad 0 \text{ if } E_b < 0.$ (14)

The constants used in the terms $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and $C_{\varepsilon 3}$ follow the definition of the realizable $k-\varepsilon$ model.

The turbulent dynamic viscosity is written as:

$$\mu^t = \rho \zeta_\mu \frac{k^2}{\varepsilon},\tag{15}$$

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