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Validation of Euler-Euler and Euler-Lagrange Approaches in the Simulation of Bubble Columns

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In the pharmaceutical industry bubble columns bioreactors (Altenbach-Rehm, 1999) have been used extensively for a wide variety of different systems, including shear-sensitive fermentation cultures. The main advantages of bubble columns are lack of any agitation equipment, the reduced power demands, the elimination of any sealing arrangements for the moving shaft and in general, the straightforward operation of this reactor type. Disadvantages include the limitation to systems with low viscosity and moderate oxygen supply, as well as the uncontrolled coalescence of the gas-phase.

Thus, the aim of this work is to computationally study, design and optimize pharmaceutical bubble column reactors and to assess the reliability of two different simulation methods for the prediction of the flow in bubble columns. Subsequently, the method can be extended to stirred systems, such as multiphase stirred tanks, which are widely used in pharmaceutical processing.

Two numerical approaches are used to reproduce the gas-liquid flow in the test rig, i.e., a three-dimensional two-phase Euler-Lagrange model (Lain, 2002) and an Euler-Euler model (Pfleger and Becker, 2001). The first approach treats the bubbles as point-volume discrete particles interacting with the carrying liquid phase. The bubble flow is calculated by solving the equations of motion taking into account all the forces on each single parcel. In the Euler-Euler model the bubbles are treated as a dispersed phase characterized by a bubble-size distribution in each cell of the computational domain. The RANS transport equations are solved for both phases, considering the exchange of source terms between liquid and gas. The turbulence in the liquid phase is resolved by the standard $\kappa - \varepsilon$ model and the advanced $\kappa - \zeta - f$ model. Different computational grids are employed in order to study the numerical effects on the description of the vortical flow structures in the bubble column. The simulation results are finally compared with experimental data and an analysis of the different numerical models is presented.

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1. Test case definition

The considered test case is commonly referred to as the "Becker case" (Becker, 1994). The locally aerated flat bubble column has height, width and depth equal to 2 m, 0.5 m and 0.08 m, respectively (see Figure 1). The liquid level is set to 1.5 m and the gas is distributed from the bottom of the column through five 40 mm porous disks. The gas is fed only from the leftmost disk located 0.15 m from the left wall, while the other four disks are closed. Typical instantaneous snapshot of rising bubble swarm and LDA measurements of long-time averaged liquid velocity field on mid-depth plane could be also seen in Figure 1 (Sokolichin and Eigenberger, 1999). In the simulations the bubble diameter is set equal to 1.6 mm with a gas flow rate of 1.6 l/min (Hu and Celik, 2007).

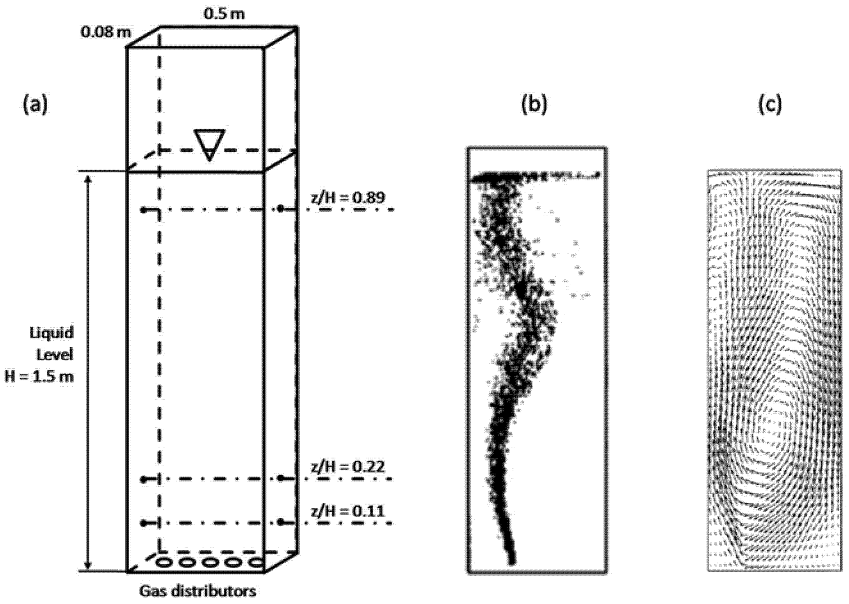

Figure 1. (a) Geometry of the flat bubble column from Becker (1994). (b) A typical instantaneous picture of rising bubble swarm: binary and inverted photographs (Sokolichin and Eigenberger, 1999). (c) Long-time averaged liquid velocity field on mid-depth plane: LDA measurement from Sokolichin and Eigenberger (1999).

2. Numerical method

2.1 Euler-Lagrange Approach

The Euler-Lagrange approach refers to a simulation method where the equation of motion for the continuous phase (i.e., the liquid phase) is solved on an Eulerian frame of reference. The disperse phase is tracked explicitly within a Lagrangian frame of reference and Newton's equation of motion is solved for each individual particle.

One of the first applications of this simulation method for bubbly flows is documented in the work of Delnoij (1997) and recent works focused on the refinement of this technique.

Several novel concepts for the computation of multiphase flow simulation include:
- to use a more sophisticated treatment of the liquid phase, i.e., using Large-Eddy (LES, e.g. Darmana, 2006) and develop strategies for the parallelization of the code to allow the simulation of larger systems.
- to use unsteady Reynolds-Averaged-Navier-Stokes (URANS, e. Lain, 2002) methods.
- to accurately model the liquid-phase fluctuations by, e.g., solving a Langevin equation (refer to van Dijk, 2007, for an recent example).
- to improve the numerical algorithm for mapping the interaction forces between Lagrangian particles and the continuous phase, i.e., so called Lagrangian-to-Euler mapping (Hu and Celik, 2007).
- to improve the interpolation of Eulerian quantities at discrete particle positions, i.e., so called Euler-To-Lagrangian mapping (Deen, 2004).

In our work, we have included the most promising strategies developed by different researchers in the open-source CFD-package “OpenFOAM” (OpenCFD, 2008). While the details of our implementation are presented in the paper of Radl (2009), we outline here only the momentum equations for the continuous phase:

$$\frac{\partial \overline{\mathbf{u}}_L}{\partial t} + \nabla \cdot \left(\overline{\mathbf{u}}_L \overline{\mathbf{u}}_L \right) = -\nabla \overline{p}' + \frac{1}{\varepsilon_L} \cdot \nabla \cdot \left[\varepsilon_L \cdot \nu_{eff} \cdot \left(\nabla \overline{\mathbf{u}}_L + \nabla \overline{\mathbf{u}}_L{}^T - \frac{2}{3} \cdot \mathbf{I} \cdot \left(\nabla \cdot \overline{\mathbf{u}}_L \right) \right) \right] + \frac{\mathbf{\Phi}_L}{\varepsilon_L \cdot \rho_L} \qquad (1)$$

This is the filtered Navier-Stokes equation in the variables $\overline{u}_L$ and $\nabla\overline{p}'$ which are the filtered velocity and the filtered kinematic pressure, i.e., the pressure divided by the liquid-phase density, respectively. The liquid-phase void fraction ε_L and the gas-liquid interaction forces $\boldsymbol{\Phi}_L$ are obtained by mapping from the dispersed phase directly. To account for the sub grid scale turbulent fluid motion, we use a standard single-phase Smagorinsky model to calculate the turbulent viscosity and subsequently the effective viscosity ν_{eff}. The Smagorinsky constant has been chosen according to the work of Hu and Celik (2007) and was set equal to $C_S = 0.032$. A universal wall function (de Villiers, 2006) is used to calculate the turbulent viscosity at the wall, i.e., the boundary layer near the wall was not resolved. The computational grid consisted of 64 x 10 x 192 cells in x-, y- and z-direction respectively. For the disperse phase, i.e., the bubbles, we solve Newton’s equation of motion for each bubble taking into account the gravity force, the pressure gradient force, the drag force, the lift force and the added mass force, as presented in Radl (2009).

2.2 Euler-Euler Approach

In the Euler-Euler approach both continuous (liquid) and dispersed phase (gas bubbles) are solved on an Eulerian frame of reference (Pfleger and Becker, 2001). The simulations are in this case obtained with the commercial CFD code Fire v2008 (AVL, 2008). The momentum source terms on the gas phase are represented by the drag force (Pfleger and Becker, 2001) and the turbulent dispersion (AVL, 2008).

Transport equations for turbulence are solved for the continuous liquid phase. Two different models are tested in the current work: the standard κ–ε model and the advanced κ–ζ–f model. The κ–ε model is actually the most diffused RANS model for the simulation of turbulent flows. The standard law-of-the-wall for mean velocity has also been used (AVL, 2008).

The κ–ζ–f (Hanjalic, 2004) is a general low-Reynolds number eddy-viscosity model based on Durbin's elliptic relaxation concept (1991). The formulation is similar to the standard κ–ε model, though it includes non-local pressure-strain effects and near-wall turbulence anisotropy. The particularity of the model is that the eddy viscosity ν_t is related to the velocity scale ratio ζ, normalized from the velocity scale $\overline{v}^2$ as $\zeta = \overline{v}^2 / \kappa$.

$$\nu_t = C_\mu \zeta \frac{\kappa^2}{\varepsilon} \tag{2}$$

The velocity scale $\overline{v}^2$ represents the velocity fluctuations normal to the streamlines and can provide a scaling for the representation of the turbulent damping close to the wall. For this reason the κ–ζ–f model does not require the adoption of wall functions. In addition to the standard κ and ε equations, the turbulent quantities are obtained from the transport equation for ζ

$$\rho \frac{D\zeta}{Dt} = \rho f - \rho \frac{\zeta}{k} P_k + \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\zeta}\right)\frac{\partial \zeta}{\partial x_j}\right] \tag{3}$$

and from the elliptic equation of the Helmholtz type for the relaxation function f, with the terms T and L representing the turbulent time and length scales (Durbin, 1991).

3. Results and discussions

Results for the mean liquid-phase flow field (averaged over 115 s) with the Euler-Lagrange approach are shown in Figure 2. The results of our simulations for the velocity profile in the middle plane of the column at three different heights z/H (see Figure 1, a) are compared in Figure 3 (a) to experimental data of Sokolichin and Eigenberger (1999). As can be seen, we find exceptionally good agreement in the lower area (z/H=0.11) where the bubbles enter the column. The sharp peak in the liquid velocity flow field observed experimentally can be well reproduced with our simulations. Also in the other areas of the bubble column the simulation results are consistent with the experimental data. However, there are quantitative differences on the left hand side where the bubbles rise along the side of the column. Here the simulations show lower near-wall velocities compared to the experimental data. The deviation of the results of the Euler-Lagrange simulations near the wall may be attributed to the use of the universal wall function of de Villiers (2006).

For the Euler-Euler approach two different meshes have been used, consisting of 58000 (Mesh 1) and 11200 (Mesh 2) tetrahedral cells, respectively. The first grid was similar to the one used for the LES simulations, while the second was made of very coarse cells with average dimensions of 15x30x12 mm. According to the diagrams in Figure 3, the κ–ε approach is generally worse than the κ–ζ–f model, which mostly provides good results in the near-wall region. The velocity peak appears to be always overestimated, but an improvement of the turbulent dispersion force could perhaps limit this effect. The κ–ε model seems to be completely unable to predict the flow with the coarse mesh 2, while the results of the κ–ζ–f approach are in acceptable agreement with the experimental data. The double velocity peaks in mesh 1 could be caused by to the restriction of simulation time to 180 real seconds. Longer computations could possibly smooth the mean flow velocities.

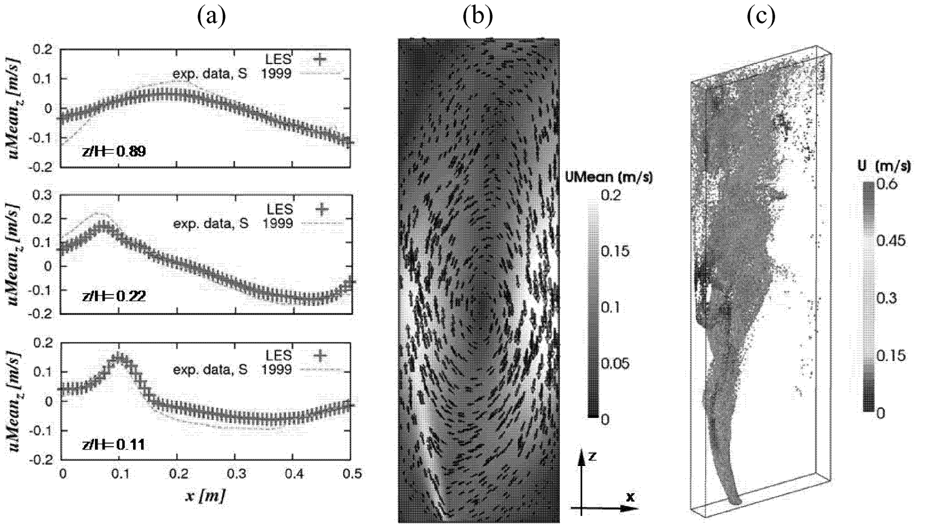

Figure 2. (a) Profiles of mean vertical velocity uMean$_z$ for different heights in the bubble column. (b) Vector plot of mean velocity field uMean. (c) Typical instantaneous distribution of gas bubbles (diameter 3x-scaled, coloured by velocity).

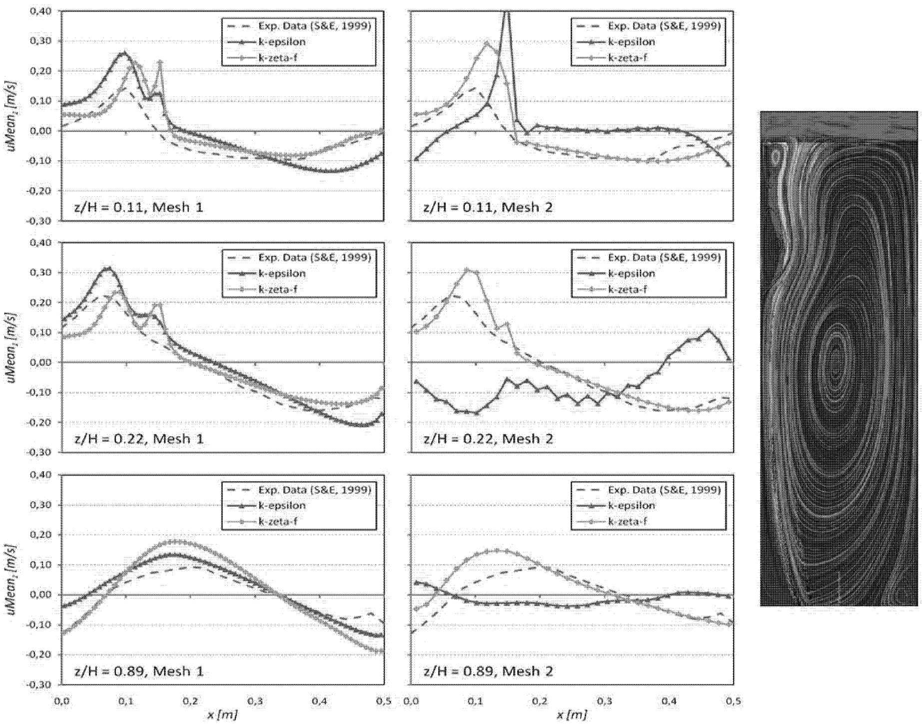

Figure 3. Profiles of mean vertical velocity for different heights z and for different meshes 1 and 2 (left). Streamlines of mean velocity field uMean (right).

4. Conclusions

As expected, the Euler-Lagrange LES code produced better results than the unsteady RANS approach and may be considered as the most advanced method for the simulation of dispersed multiphase flows. Nevertheless, the Euler-Euler calculations with the advanced $\kappa-\zeta-f$ turbulence model showed promising results, even in a five-time coarser computational mesh. This aspect could definitely represent an advantage in terms of time costs for the industrial application of bubbly flows.

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