Finite element simulation of turbulent bubbly flows

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A finite element approach for solving gas-liquid flows with mass transfer and chemical reactions is presented. The incompressible Navier-Stokes equations coupled with a modified $k-\varepsilon$ turbulence model for computation of the eddy viscosity are solved by a discrete projection scheme from the family of Pressure Schur Complement methods. Additionally, the simplified two-fluid (Euler-Euler) model based on an analogy of the Boussinesq approximation is adopted for the description of the two-phase flow. A robust solution strategy based on nested iterations is proposed for the numerical treatment of the resulting system of PDEs, which are discretized by high-resolution finite element schemes designed on the basis of algebraic flux correction in order to stabilize the convective terms. The performance of the developed mathematical model is illustrated by a number of numerical results obtained from simulations on three-dimensional unstructured meshes.

1. Introduction

Chemical engineering processes, where contacting the gaseous and liquid phases is required in the most efficient way, are generally realized in bubble columns and airlift loop reactors. This way, depending on the process realized in the given equipment, mass transfer between the present phases and (or) chemical reactions are taking place. It is clear, that approximate estimations are essential for the designation of these aerated (production) units. Principally, qualitatively good primary estimations can be extracted from scale-up studies based on experimental measures, but the development of avdanced CFD models offers an increasingly high potential of their utilization. A comprehensive summary of recent results and approaches can be found in the proceedings of the priority research program *Analysis, Modelling and Numerical Calculation of Multiphase Flows* [3]. The complexity of the involved phenomena of two-phase flow is reflected by the fact, that publications including the detailed description of discretization and implementation have been very scarce. Taking into account, that the developed models describing the liquid-gas flow phenomenon are subject to underlying fluid-flow solver extended with an appropriate turbulence model, the implementation is in most of cases realized in the framework of commercial CFD software which is typically based on robust but insufficiently accurate and/or efficient numerical algorithms. In the work presented here we address the implementation algorithm for the numerical solution of all the acting governing equations supplemented with the most basic form of auxiliary model equations in order to concentrate on the computational aspects. The implementation of the $k-\varepsilon$ turbulence model with special emphasises on the positivity preserving discretization and the numerical treatment of convective terms is addressed in [8] and forms the inevitable support for the work presented here.

2. Mathematical model

The complete mathemetical model presented in this paper consists from two parts, from the hydrodynamic core and the simplified two-fluid model based on an analog of Boussinesq approximation for natural convection problems. Therefore, the validity of the adopted model is

restricted to bubbly flows characterized with moderate gas holdups (up to 10%). Under such circumstances the "incompressible" Navier-Stokes equations are enriched with an extra buoyancy force term, by what the gas-liquid mixture is characterized as a weakly compressible fluid. Then, (according to Sokolichin *et al.* [4], [5]) by replacing the effective density $\tilde{\rho}_L$ by the liquid density ρ_L except for the gravity force one can obtain the Navier-Stokes equations for the liquid phase in the following form:

$$\frac{\partial \mathbf{u}_L}{\partial t} + \mathbf{u}_L \cdot \nabla \mathbf{u}_L = -\nabla p_* + \nabla \cdot (\nu_T \mathcal{D}(\mathbf{u}_L)) - e\mathbf{g},$$
$$\nabla \cdot \mathbf{u}_L = 0, \qquad p_* = \frac{p - p_{\text{atm}}}{\rho_L} + \mathbf{g} \cdot \mathbf{x} - gh, \qquad e = \frac{\tilde{\rho}_L}{\rho_L} \tag{1}$$

where $\mathcal{D}(\mathbf{u}) = \nabla \mathbf{u} + \nabla \mathbf{u}^T$ and the effective viscosity $\nu_T = C_\mu \frac{k^2}{\varepsilon}$ is a function of the turbulent kinetic energy k and its dissipation rate ε. The evolution of these quantities is described by two scalar transport equations

$$\frac{\partial k}{\partial t} + \nabla \cdot \left(k\mathbf{u}_L - \frac{\nu_T}{\sigma_k} \nabla k \right) = P_k + S_k - \varepsilon, \tag{2}$$
$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \left(\varepsilon \mathbf{u}_L - \frac{\nu_T}{\sigma_\varepsilon} \nabla \varepsilon \right) = \frac{\varepsilon}{k}(C_1 P_k + C_\varepsilon S_k - C_2 \varepsilon), \tag{3}$$

where the production terms $P_k = \frac{\nu_T}{2} |\nabla \mathbf{u} + \nabla \mathbf{u}^T|^2$ and $S_k = -C_k e \nabla p \cdot \mathbf{u}_{\text{slip}}$ are due to the shear and bubble-induced turbulence (BIT), respectively. The involved constants $C_\mu = 0.09$, $C_1 = 1.44$, $C_2 = 1.92$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$ for the standard $k - \varepsilon$ model are known with high precision, whereas the BIT parameters $C_k \in [0.01, 1]$ and $C_\varepsilon \in [1, 1.92]$ are highly problem-dependent [4]. After decomposition of the interphase force term responsible for momentum exchange between the present two phases and using the assumptions introduced by Sokolichin *et al.* [4], [5], the momentum balance of the gas phase reduces to:

$$0 = -\alpha \nabla p - \alpha C_W \mathbf{u}_{\text{slip}}, \qquad C_W = C_D \frac{3}{8} \frac{\rho_L}{r} |\mathbf{u}_{\text{slip}}| \approx 5 \cdot 10^4 \ \frac{kg}{m^3 s}. \tag{4}$$

In the presence of turbulence, the motion of the gas phase is subject to the bubble path dispersion which can be included into the hydrodynamic model as an extra contribution to the slip velocity. The rate of such dispersion depends on the turbulent viscosity ν_T and on the turbulent Schmidt number σ_G. Then, for this drift velocity $\mathbf{u}_{\text{drift}}$ holds:

$$\mathbf{u}_{\text{drift}} = -\frac{\nu_T}{\sigma_G} \frac{\nabla n}{n} \tag{5}$$

which then together with the liquid velocity $\mathbf{u}_L$ and slip velocity $\mathbf{u}_{\text{slip}}$ gives the direct expression for the gas velocity $\mathbf{u}_G$ istead of obtaining it from the momentum equation:

$$\mathbf{u}_G = \mathbf{u}_L + \mathbf{u}_{\text{slip}} + \mathbf{u}_{\text{drift}}. \tag{6}$$

The gas density ρ_G is assumed to satisfy the ideal gas law $p = \rho_G \frac{R}{\eta} T$, which enables us to express the gas holdup e and the interfacial area a_S per unit volume as follows [6]

$$e = \frac{\tilde{\rho}_G R T}{p \eta}, \qquad a_S = (4\pi n)^{1/3} (3e)^{2/3}.$$

The effective density $\tilde{\rho}_G = e\rho_G$ and the number density n satisfy the following continuity equations:

$$\frac{\partial \tilde{\rho}_G}{\partial t} + \nabla \cdot (\tilde{\rho}_G \mathbf{u}_G) = -m_{\text{int}}, \tag{7}$$
$$\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{u}_G) = 0. \tag{8}$$

In (7) the term appearing on the right hand side is equivalent to the rate of mass transfer of materials between the phases (absorption, desorption), which can be due to physical or reaction-enhanced absorption. Its value depends on the driving force of the individual species present in both phases (modeled by extra transport equations) and on the interfacial area a_S, which for the case of neglected bubble coalescence and breakup (as it is in the present work) is considered as a constant, otherwise modeled on the basis of population balance models.

Summarizing the presented *drift-flux* model one should mention the range of its validity, which is constrained to bubbly flows with moderate holdups and superficial velocities. Processes realized outside these operation conditions need the incorporation of additional effects and forces into the model. However, by the influence of unclearness of these auiliary features the developed model out and away looses of its generality then gains by it. Furthermore, following the computational aspects the performance of the implemented general model with the less of empiricism is rather interesting.

3. Numerical algorithm

The implementation of the model presented in the previous part is in general performed on the basis of the finite element method, which offers the treatment of non-Cartesian geometries, with internal obstacles as well. The incompressible Navier-Stokes equations are solved in the framework of the open-source software package FEATFLOW (see *http://www.featflow.de*), where the Multilevel Pressure Schur Complement (MPSC) method is utilized as the decoupling technique for the velocity and pressure [7]. Within the mentioned MPSC method the individual velocity components are solved in an iterative loop consisting of separate defect correction subloops after which the incompressibility constraint is achieved by projection of the intermediate velocity onto the subspace of divergence-free functions (for details see [7]). A tender spot regarding to the numerical unstable convective terms in case of convection-dominated flows is handled by construction of high-resolution finite element schemes by making use of algebraic flux correction (see [1], [2]). The integration of such nonlinear combinations of high- and low-order methods into the numerical scheme offers the overcome of over- and under-shoots, which for *a priori* nonnegative physical quantities is clearly non-acceptable.

The mathematical models consisting of coupled subproblems are treated sequentially, which gives rise to a nested iteration loop system, where the outermost iteration loop k is responsible for the coupling of the most relevant blocks and for achieving convergence of the selected quantities. The such developed block-iterative algorithm decomposes the outermost iteration loop into three blocks:

- the Navier-Stokes equations
- the transport equations associated with the $k-\varepsilon$ turbulence model
- the computation of the gas velocity - $\mathbf{u}_G$, the transport equations of the effective density - $\tilde{\rho}_G$, number density - n and the present species.

In fact, the solution of the Navier-Stokes equations is handled in a nested outer iteration loop l (MPSC with a fixed point defect correction loop m due to the nonlinear convection term) updating the intermediate flow field given by $\mathbf{u}^{k+1,l+1}$ and $p^{k+1,l+1}$. Equivalently, the solution of the strongly coupled system of the $k-\varepsilon$ equations is performed by an other outer iteration loop l, where both of the transport equations are solved in a fixed point defect correction loop m due to the updated implicit source terms. However, the explicit source terms are assigned to their new values in the outermost iteration loop k. Regarding to the third block of the solution, operator splitting tools are employed to separate convection-diffusion and absorption-reaction 'transports' at each time step. In this particular case it means, that the scalar quantities are transported without sources/sinks, but afterwards are exposed to a nodal ODE system taking into account

their accumulation or consumption. Then, the solution to system (1)-(7) supplemented by the convection-reaction-diffusion equations for effective concentrations is integrated in time from t_n to $t_{n+1} = t_n + \Delta t_n$ as follows:

1. Solve the Navier-Stokes equations (1) for $\mathbf{u}_L$ and p.
2. Use L_2-projection to recover the pressure gradient ∇p.
3. Calculate the gas velocity $\mathbf{u}_G$ from the slip relation (6).
4. Solve the continuity equation (7) for the gas phase and for the number density n (8).
5. Convert $\tilde{\rho}_G$ and n into the gas holdup e and a_S; evaluate m_{int}.
6. Solve the transport equations for effective concentrations of species.
7. Solve the ODE systems for absorption-reaction.
8. Enter the inner loop of the $k-\varepsilon$ model (2)–(3); update the turbulent eddy viscosity ν_T.
9. Insert ν_T and e into (1) and evaluate the residual.
10. If converged, then proceed to the next time step otherwise go to 1.

4. Numerical examples

The validation of the mathematical model, developed algorithm and its implementation was realized in three consequent stages, starting from the simpler problems activating just the basic tools till the performance of the whole model. In this organisation of validation of the model, firstly the notoriously known backward facing step problem was processed in order to validate the implemented turbulence $k-\varepsilon$ model. This problem is characterized with the Reynolds number $Re = \frac{UH}{\nu} = 44,000$ (where U is the inflow velocity, H is the step height, and ν is the kinematic viscosity of the fluid). For more detailed description of this benchmark problem the reader is referred to [2]. In Figure 1 is shown the comparison and a good agreement with the results obtained by Ilinca *et al.* [9] for the same simulation conditions and Reynolds number.

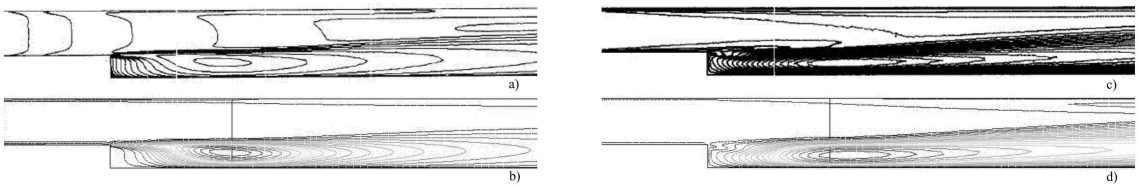

Figure 1: Backward facing step simulation results ($Re = 44,000$). Contour lines of *a),b)* - turbulent kinetic energy; *c),d)* - turbulent eddy viscosity. *a),c)* - reference solution [9].

The next stage of validation was concerned the two-phase flow inside a locally areated flat bubble column. In this particular case the problem set-up was in accordance with the one experimentally and computationally investigated by Becker *et al.* [10]. The bubble column of size $50cm$, $150cm$ and $8cm$ was represented by a Cartesian computational mesh of 6912 hexahedral elements. The unsymmetrically placed gas sparger of size $6cm$ at the bottom of the column fed by the volumetric rate of 1.6 l/min is responsible for the flow pattern consisting of a large and almost stationary vortex formed to the right of the sparger, which pushes the bubble stream toward the left wall (Figure 2). Further movement of the bubble swarm results in a meandering motion in the upper part of the column which is also in a good agreement with

the observations of Becker *et al.* [10]. Even though the performance of the standard $k-\varepsilon$ model is in this case satisfactory, in general, the incorporation of extra source terms regarding to the bubble-induced turbulence should be necessary, so without experimentally supported data the computational results should be taken with appropriate care.

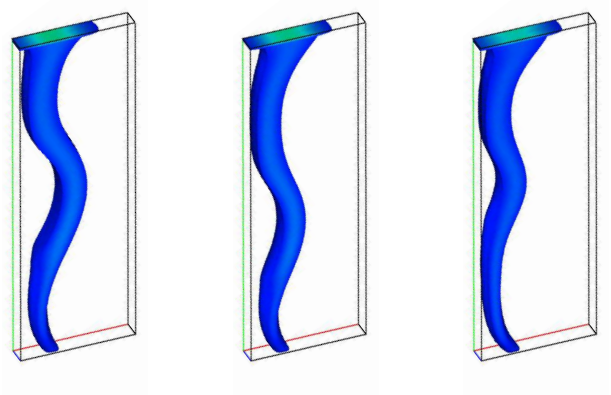

Figure 2: Gas holdup distribution for the locally aerated flat bubble column.

The last stage concerning the validation of the full model includes except of two-phase flow, the modeling of concentration fields associated with the present species and what is more the mass transfer of gas into the liquid was taken into account. The simulations carried out in this stage are basically based on the same geometric configurations presented for the flat bubble column but are two dimensional. The sink term in the gas holdup equation (7) was attributed to physical absorption into the first and reaction-enhanced absorption in the second case. From the chemical point of view, in the first case the physical absorpion of CO_2 in pure water, while in the second case the reaction-enhanced absorption of CO_2 into the aqueous solution of NaOH was investigated. Depending on the examined process the behaviour has changed dramatically, what is shown in Figure 3. From the mentioned figure it is clear, that the fast chemical reaction taking place in the second case completely transfers the introduced gas almost within the one tenth of the column length from the inlet. However, the predicted behaviour of the modelled bubble columns in these two particular cases is quite reasonable; for its justification a further research based on experimental data is required. The incorporation of an appropriate subgrid reaction model [11] should also has its justification, especially due to the assumed fast chemical reaction.

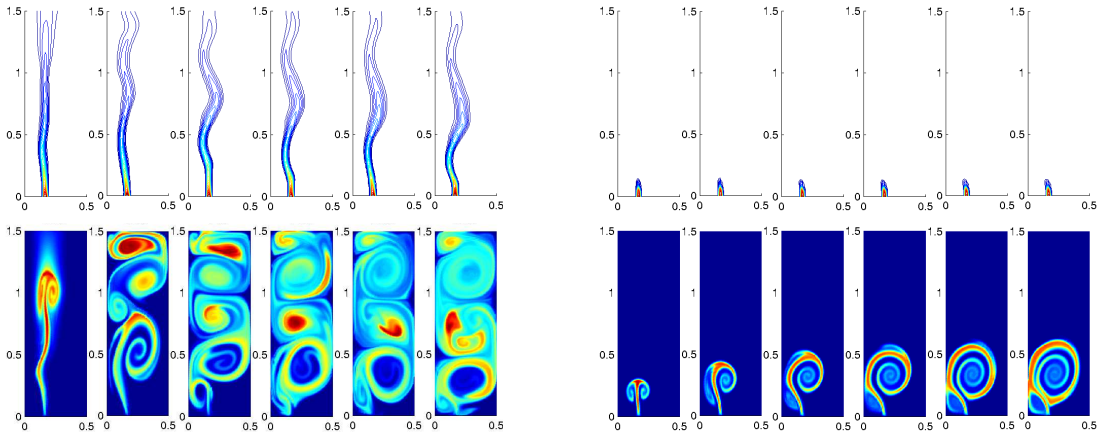

Figure 3: Physical absorption (left) and reaction-enhanced absorption of CO_2 (right) represented by gas holdup distribution (top) and dissolved CO_2 concentration (bottom).

5. Conclusions

The drift-flux model for buoyancy-driven bubbly flows was coupled with scalar transport equations describing the absorption of gas followed (and enhanced) by chemical reactions in the liquid phase. Turbulence effects were taken into account by means of a modified $k-e$ turbulence model which was found to produce reasonable results. Further research is needed to improve the modeling of the bubble size distribution and bubble-induced turbulence as well. Based on the recent advances in the field of Large Eddy Simulation (LES) the latter indicate that it might be a good candidate for this purpose.

An unstructured grid finite element method was proposed for the numerical solution. The discretization of the troublesome convective terms was performed by a nonlinear positivity-preserving scheme equipped with a multidimensional flux limiter of FCT or TVD type. Nested iterations were used to provide the coupling of model equations, to get rid of nonlinearities and to solve the linear systems. The interplay of the hydrodynamics, mass transfer and chemical reaction was illustrated by numerical examples.

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