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CFD Simulation of Bubble Columns using the VOF Model: Comparison of commercial and Open Source Solvers with an Experiment

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Bubble columns are a well known type of reactor in the field of chemical engineering. Usually gas is dispersed (through a distributor or a membrane) in the bottom of a column filled with a liquid. The buoyancy driven flow yields excellent mixing behavior and a large inner surface area without the need of moving parts, fixed baffles or any type of filling material in the column. Bubble columns are typically used as fermenters, in gas stripping, loop-type bubble columns, mixers and other applications.
In this paper transient ab-initio simulations, using a commercial and an open source CFD (Computational Fluid Dynamics) program, of rising bubble swarms are compared to experimental results. The simulations make use of two available implementations of a VOF (Volume of Fluid) model that is capable of describing the phase distributions of completely immiscible gas and liquid phases using a finite volume approach. It is shown that the computational cost can be small enough (even when using a higher grid density) to get results, in good agreement with the experiments and in short time, for applications in chemical engineering (e.g. design of unit operations).

1. Simulation

1.1 Geometry and grid

A laboratory scale bubble column was simulated. The geometry of the bubble column is shown in Fig 1. The inner volume of the column is 200x200x2000mm. For all considerations in this paper the unaerated column is filled with water up to 1000mm. In the lower part of the column a separator plate can be installed to run the bubble column in looping configuration where only 50% of the gas distributor in the bottom is permeable. The "wind-box" below the gas distributor was

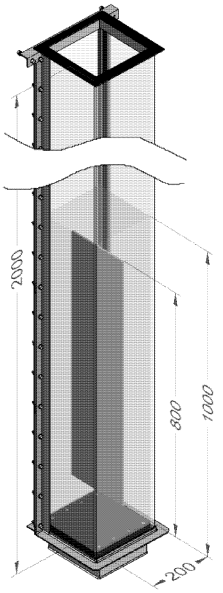

Fig 1: Geometry of the bubble column

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included in the simulation domain to get a physically correct inlet pressure distribution. A constant inlet pressure at the gas-distributor plate would be an oversimplification of the boundary conditions. The aluminum distributor plate has 7x7 equidistant holes with a diameter of 3mm. The holes are completely resolved in the finite volume grid which exclusively consists of hexahedral cells with an equi-angle-skew factor below 0.3. The effects of two different grid densities (360000 and 2600000 cells) in otherwise identical geometries were considered in the simulations.

1.2 Model and numerical background

For the simulations of sharp fluid-fluid interfaces using a finite volume approach the VOF (Volume of Fluid) Model is very suitable (Akhtar et.al., 2007).

In contrast to the VOF model an Euler-Euler model can be used, that describes two completely interpenetrating phases. Two complete sets of conservation equations are solved. Euler-Euler models are suitable for simulation of fluidized solid phases or mixing liquid phases. A big drawback of the Euler-Euler approach is the interaction of the phases and bubble-sizes that are left to be defined by the user. Bubble coagulation and dispersion (ab-initio) are hard to impossible to model using Euler-Euler approaches.

The VOF model assumes two or more completely immiscible fluids. Here we will limit the number of fluids to 2, as we are only considering air and water (and no other phases). A scalar indicator α is used to define the volume of one fluid V_1 in every control volume (the content of the other fluid V_2 is simply 1-α):

$$\alpha = \frac{V_1}{V} \tag{1}$$

The above indicator is a scalar function in 3 dimensional space that needs to be discretized (in space and time) in order to be usable in a direct finite volume solver. Apart from the usual discretizations of the continuity-, Navier-Stokes- and energy-equations a few exemplary steps are outlined below that yield a suitable mathematical setup. Below some of the inner workings of the VOF Model implemented in the OpenFOAM Solver are described (Ubbink, 1997 and Rusche, 2002). The Fluent Solver probably works in a similar way but is regarded as a black-box, due to lacking documentation, with only a few knobs to turn for the user.

First a discretization of the Gauss theorem is derived that is applicable in a general way for finite volumes bounded by n flat faces (i.e. suitable for polyhedral cells in unstructured grids).

$$\int_V \nabla \vec{\phi} dV = \oint_{dV} d\vec{S} \cdot \vec{\phi} = \sum_{f=1}^{n} \left(\int_f d\vec{S} \vec{\phi} \right) = \sum_{f=1}^{n} \vec{A}_f \cdot \vec{\phi}_f \tag{2}$$

Following equation considers the fluxes through the faces of the finite volume cell:

$$\oint_{\partial V} \alpha d\vec{S}\vec{u} \approx \sum_{f=1}^{n} \alpha_f \cdot \vec{A}_f \cdot \vec{v}_f = \sum_{f=1}^{n} \alpha_f F_f \tag{3}$$

To get a bounded solution (i.e. $0 \le \alpha \le 1$) and at the same time sharp interfaces a so called compressive differencing scheme is used, that introduces a weighting factor (β).

$$\alpha_f = \beta \cdot \alpha_P + (1-\beta)\alpha_n \tag{4}$$

Expressed in form of cells and nearest neighbors the discretized indicator function suitable for a direct finite volume solver is:

$$\alpha_P \cdot \alpha_P^{t+\delta t} = \sum_{nb=1}^{n} a_{nb} \cdot \alpha_{nb}^{t+\delta t} + S_{\alpha P} \tag{5}$$

To avoid the numerical diffusion in the convection equations the temporal discretization is done using the Crank-Nicholson scheme that is second order accurate in time. Implicit time stepping causes numerical diffusion in direction of the flow, explicit time stepping introduces diffusion normal to the direction of flow.

1.3 Discretization methods and solver settings

Following table shows the methods chosen for discretization of the scalar VOF indicator α and the temporal discretization in the used solvers. All other field-variables were at least discretized with 2nd order accuracy.

Variable	OpenFOAM-1.4.1	Fluent 6.3.26
α	interfaceCompression	Geo-Reconstruct
t	1st/2nd order implicit	Crank-Nicholson

The explicit time stepping scheme in Fluent was avoided due to its instability with the used models. The size of the biggest time step in Fluent was limited by the stability and number of sub-iterations of the Geo-reconstruct scheme. In OpenFOAM a dynamic limiter was set to the maximum Courant number in the computational domain (Co < 1).
No turbulence model was used in the simulations. Using a turbulence model caused an extremely slow rise of the air bubbles due to turbulent viscosity limiting the terminal rising velocity of the bubbles. Using a turbulence model gives unphysical results for both VOF and Euler-Euler models (see also Chen, 2001).
Where applicable surface tension (between air and water: η=0.07N/m) and contact angle (between water and all walls: Θ=30°) were set. All simulation runs were started at t=0 with an initially stationary water column of 1m height. Compressibility effects were neglected in the simulations. The inlet was defined as a velocity inlet in Fluent and as a fixed U-value in OpenFOAM. The outlet was defined as a pressure outlet in Fluent and as a zero gradient boundary condition of pressure in OpenFOAM. The walls and the

separator walls were set to no slip in Fluent and a fixed U-value of (0 0 0) in OpenFOAM. The material properties of water and air were those at 298K.

1.4 Investigation of influential parameters on simulation results

The following images (Fig. 2, 3 and 4) show the same cross section through the middle of the bubble column. The influence of various parameters on the simulation results is presented. The bright areas show values of the phase indicator α between 0.4 and 0.6 (i.e. the interface between gas and liquid).

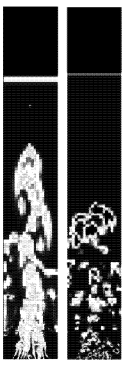

Fig. 2

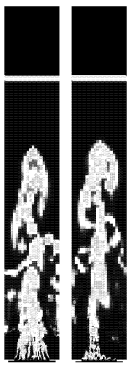

Fig. 3

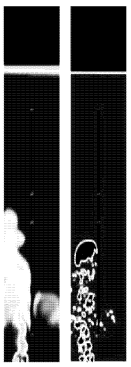

Fig.4

Fig. 2: Influence of used solver (left: OpenFOAM, right: Fluent, both at t=1.5s, superficial gas velocity: 0.04m/s, both meshes: 360000 cells)
Fig. 3: Influence of contact angle using OpenFOAM (left: not active, right: active at Θ=30°, both at t=1.5s, superficial gas velocity: 0.04m/s, both meshes: 360000 cells)
Fig. 4: Influence of temporal discretization when using the Fluent solver (left: 1st Order implicit, right: 2nd Order implicit, both at t=0.8s, looping-type bubble column with internal separator, superficial gas velocity: 0.01m/s, both meshes: 2600000 cells). These numerical experiments clearly show that the choice of solver and discretization methods (both spatial and temporal) have the biggest influence on the results. Lower order discretizations lead to "smeared" surfaces and physically incorrect results.

2. Comparison and Conclusion

For the comparisons of experimental and simulation results the loop-type configuration is presented. The superficial gas velocity is set to v=0.01m/s. The same finite volume grid containing 2600000 cells was used for Fluent and OpenFOAM. The results are displayed in Fig. 5, 6, 7 and 8. The cross sectional area is located in the middle of the column. The left part of each figure is the simulation result of Fluent, in the middle is a synchronized black and white picture captured by a Redlake Motion Pro high speed camera (@2000fps), the right part is the simulation result of OpenFOAM. The bright areas correspond to values of the VOF indicator α between 0.4 and 0.6. The cumulated simulation time for t=0.8s using Fluent is 480 CPU days and 13.6 CPU days for OpoenFOAM. Both simulations were run on the same hardware (Dual 1.9GHz Power5+ processors). The operating system used for Fluent was AIX 5.3. Linux 2.6.18 was used for OpenFOAM. Fluent was parallelized 4x, OpenFOAM 2x.

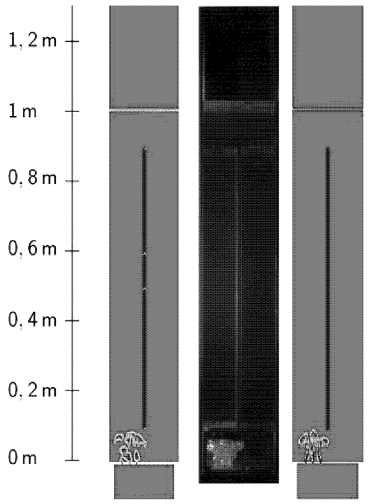

Fig. 5: Fluent, Experiment, OpenFOAM t=0.2s

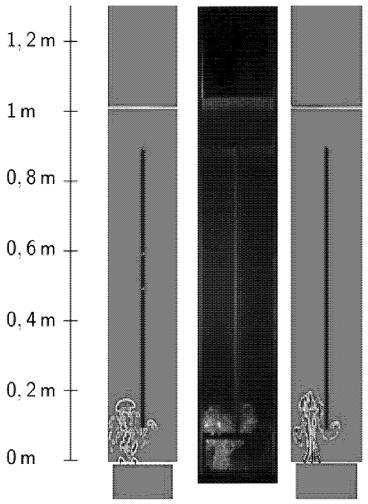

Fig. 6. Fluent, Experiment, OpenFOAM t=0.4s

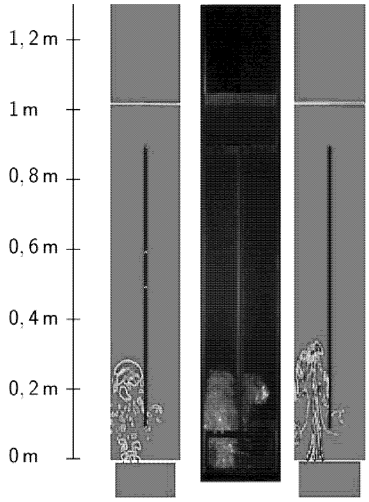

Fig. 7: Fluent, Experiment, OpenFOAM t=0.6s

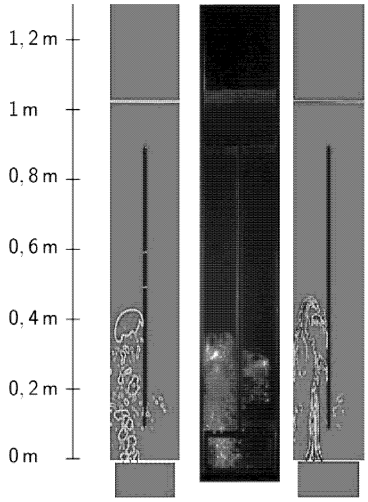

Fig. 8: Fluent, Experiment, OpenFOAM t=0.8s

The comparisons show that both solvers produce a good prediction of the gas hold-up in the bubble column, which can be measured by the height of the liquid level. Both solvers overpredict the rising velocity of the leading bubbles. Due to time constraints (and licensing costs) the numerical experiments with Fluent were stopped. Using OpenFOAM it was possible to simulate five seconds of real time for the looping-type bubble column at two different gas flow rates yielding results in very good agreement to

the experiments. Gas hold up and gas distribution in the downcomer are predicted correctly (see Fig. 9, left: experiment, right: OpenFOAM, t=4.9s), yet the simulation of the smaller bubbles would need an even higher grid density and adaptive refinement around interfaces (see Theodorakakos, 2004).

Symbols

f	Centre of the cell face
$\vec{A}_f$	Face area vector (m)
n	Number of faces of the control volume (1)
F_f	Volumetric flux rate (m^3/s)
V	Total volume of the control volume (m^3)
V_i	Volume of Fluid i in the control volume (m^3)
$S_{\alpha P}$	Source term
α	Volume of fluid indicator function (1)
α_P, α_N	Cell index, nearest neighbor index (1)
δt	Time step size (s)
$\vec{\varphi}$	Arbitrary vector function
$d\vec{S}$	Surface area vector (m^2)
∂V	Surface area of the control volume (m^2)

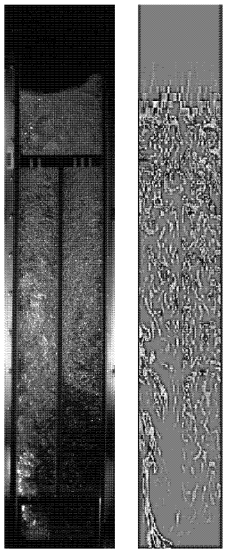

Fig. 9

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