CFD SIMULATION OF BUBBLE COLUMNS USING A VOF MODEL

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ABSTRACT

Bubble columns are a well known type of reactor in the field of chemical engineering. In bubble columns is dispersed (through a distributor or a membrane) at 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, multiphase reactors, in gas stripping, loop-type bubble columns, mixers and other applications. The important factor in mass transfer between liquid and gas phase is the enhancement via continuous surface renewal and intrinsically hindered concentration boundary layer formation. In this work loop-type bubble columns are analyzed, with a focus on the physically correct prediction of the onset of the circulating flow and the gas entrainment in the loop for varying gas flow rates and gas distribution plates.

For this purpose, transient ab-initio simulations - using OpenFOAM-1.6 - of rising bubble swarms are compared to experimental results from a high speed camera (2000 frames per second). The simulation uses an implementation 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 [1]. Five seconds of real time for the looping-type bubble column at two different gas flow rates were simulated yielding results in very good agreement with the experiments. The comparisons show that the simulation runs produce a good prediction of the overall gas hold-up in the bubble column, which can be measured by the height of the liquid level. However, the rising velocity of the leading bubbles is overpredicted to some extent yielding a shorter-than-observed residence time of these bubbles. Gas hold up and gas distribution in the downcomer are predicted correctly. It was observerd that the simulation of the smaller bubbles would need an even higher grid density and adaptive refinement around interfaces [2].

INTRODUCTION

Bubble columns are a well known type of reactor in the field of chemical engineering. In a typical bubble flow reactor gas is dispersed at the bottom of a column through a distributor. The buoyancy driven two-phase 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 reactors, mixers and other applications.

In this work transient ab-initio simulations of rising bubble swarms, using an open source CFD (Computational Fluid Dynamics) program, are compared to experimental results. Simulation runs were done using two different implementations of a VOF (Volume of Fluid) model, a finite volume approach, that is capable of describing the phase distributions of completely immiscible gas and liquid phases. It is found that the computational cost is affordable (even when using a higher grid density) to get results, in good agreement with the experiment. This suggests that a CFD approach can be successfully applied for applications in chemical engineering (e.g. design and improvement of unit operations).

1 SIMULATION

1.1 Geometry and grid

A laboratory scale bubble column with inner dimensions of 200x200x2000 mm was simulated. The un-aerated column was filled with water up to 1000 mm. In the lower part of the column a vertical separator plate was installed to run the bubble column in looping configuration where only half of the gas distributor area in the bottom is aerated.

The superficial gas velocity was set to v=0.04 m/s. The ”wind-box” below the gas distributor was included in the simulation domain to get a physically correct inlet pressure distribution. A constant inlet pressure at the gas-distributor plate was regarded as an oversimplification of the boundary conditions. The aluminum distributor plate had 7x7 equidistant holes with a diameter of 3 mm. The orifices were completely resolved in the finite volume grid which consists of hexahedral cells with an equi-angle-skew factor below 0.3. The effects of three different grid densities (800,000, 2,700,000 and 21,600,000 cells) in identical geometries were tested in the simulations.

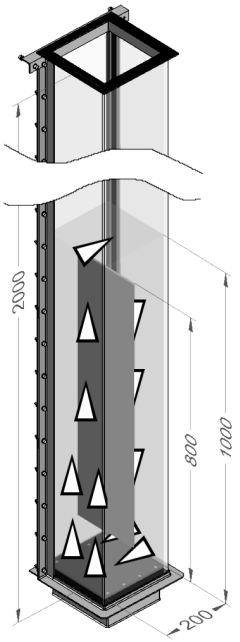

Figure 1: Geometry with installed separator showing a typical looping type flow pattern in the bubble column

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 suitable (Akhtar et.al., 2007). As an alternative to the VOF model an Euler-Euler model can be used, that describes two completely inter-penetrating 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 considerable drawback of the Euler-Euler approach is the interaction of the phases and bubble-sizes that need to be defined by the user. Bubble coalescence and dispersion (ab-initio)

are difficult 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 two, as we are only considering air and water. A scalar indicator γ is used to define the volume of one fluid V_1 in every control volume (the relative content of the other fluid V_2 is simply 1-γ) and thus $\gamma = V_1/V$.

The indicator introduced above 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).

For incompressible flow the (conservative) transport equation of γ can be written as:

$$\frac{\partial \gamma}{\partial t} + \nabla \gamma \vec{u} = 0 \tag{1}$$

A discretization of the Gauss theorem is derived, that is applicable in a general way for finite volumes bounded by n flat faces (and is suitable for polyhedral cells in unstructured grids):

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

The fluxes through the faces of a finite volume cell are given by:

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

To get a bounded solution (i.e. $0 < \gamma < 1$) and sharp interfaces a so called compressive differencing scheme (see Ubbink 1997 and Olsson et.al. 2004) is used, that introduces a weighting factor (β),

$$\gamma_f = \beta \cdot \gamma_P + (1 - \beta) \cdot \gamma_N. \tag{4}$$

A form of the indicator function that is suitable for finite volume solvers can be given by:

$$a_P \cdot \gamma_P^{t+\delta t} = \sum_{nb=1}^{n} a_N \cdot \gamma_N^{t+\delta t} + S_{\gamma P}. \tag{5}$$

To minimize the numerical diffusion in the convection equations the temporal discretization is done using the Crank-Nicholson scheme that is second order accurate in time. More precisely: time stepping is weighted by 0.9 Crank-Nicholson scheme and 0.1 Euler to avoid numerical instabilities. Implicit time stepping may cause numerical diffusion in direction of the flow, explicit time stepping introduces diffusion normal to the direction of flow.

1.3 Discretization methods and solver setting

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

Variable	Meaning	Algorithm
γ_1	VOF-indicator	interfaceCompression
t	time	Crank-Nicholson (w=0.9)

Table 1: Discretization settings of two important field variables

A dynamic limiter was adjusted to control the time step in order to keep the maximum Courant number in the computational domain below 0.9. No turbulence model was used in the simulations. Using a turbulence model caused an unphysically slow rise of the air bubbles due to the 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). Surface tension (between air and water: η=0.07N/m) and contact angles (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 fixed U-value in OpenFOAM. The outlet was defined as a zero gradient boundary condition of pressure in OpenFOAM. The walls and the separator walls were set to a fixed U-value of (0 0 0). The material properties of water and air used in the simulations correspond to a temperature of 298 K.

2 COMPARISON AND CONCLUSION

It is shown that the grid dependent rising velocity of the leading bubble converges quickly with increasing grid density. In the simulation the rising time is under-predicted slightly because compressibility effects and mechanical properties of the used air-valves are neglected. The building-up of the final pressure at the start of the experiment leads to a slower than ideal rise of the bubbles. The specific surface area is also grid-dependent but already is in the range of published results.

Using OpenFOAM six seconds of real time for the looping-type bubble column were simulated yielding results in good agreement with the experiments of the authors and published results (Nakao, 1983). The gas distribution in the down-comer is predicted correctly (see figure 4, left: simulation result: isosurface for γ_1=0.75, right: synchronous still image from high speed camera), yet the simulation of the smaller bubbles would need an even higher grid density and adaptive refinement around interfaces (see Theodorakakos, 2004). A simulation to evaluate the convergence of the specific surface at very high grid densities (173M cells) is in preparation. Future plans for experiments are PIV-measurements of the liquid phase using flourescent seeding. First tests have shown a great potential of this method.

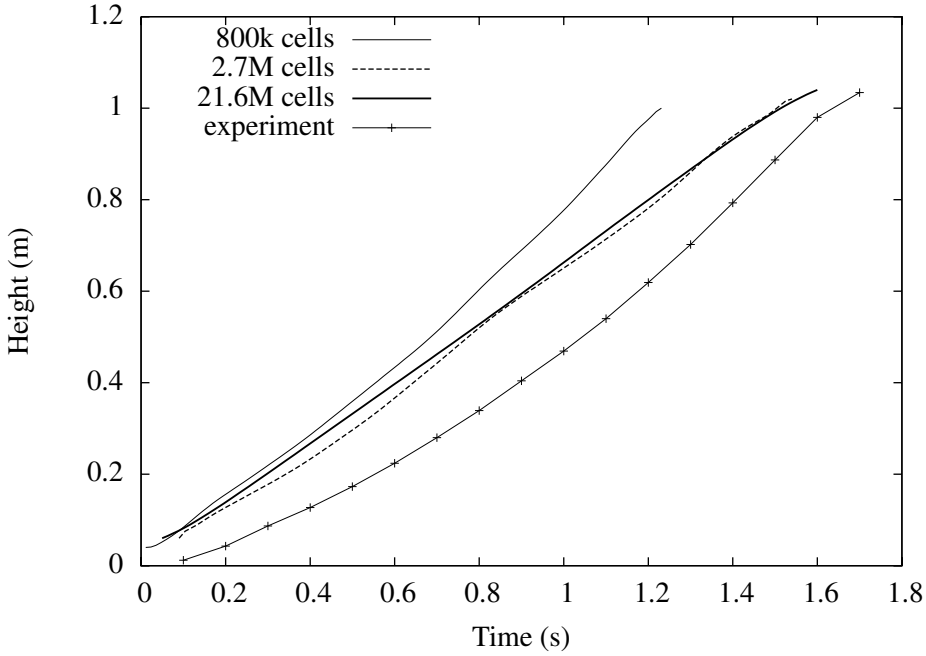

Figure 2: Comparison of the position of the leading bubble in simulation and experiment

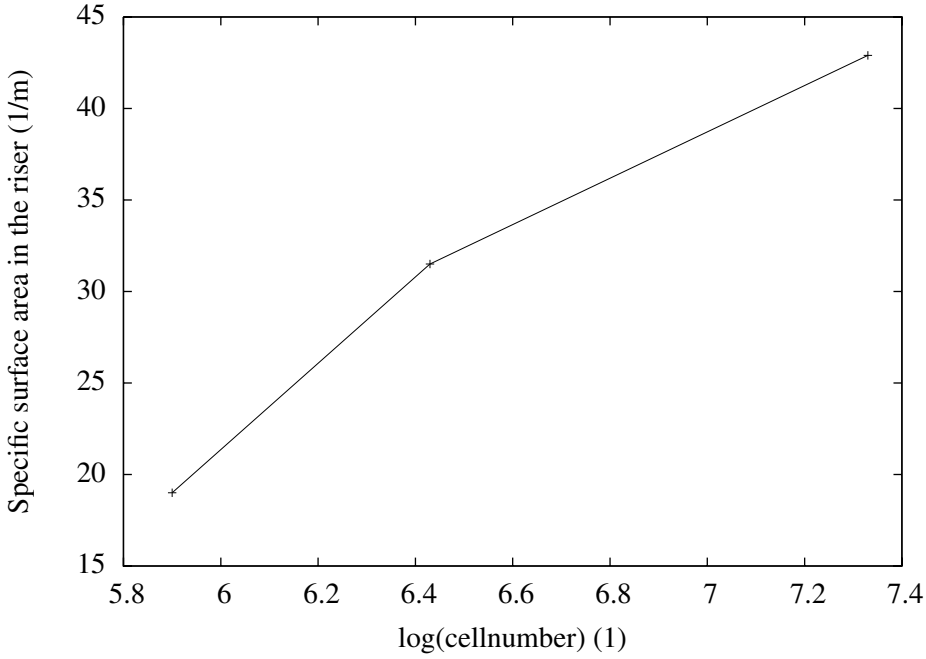

Figure 3: Simulated specific surface area in the riser at t=2.45 s.

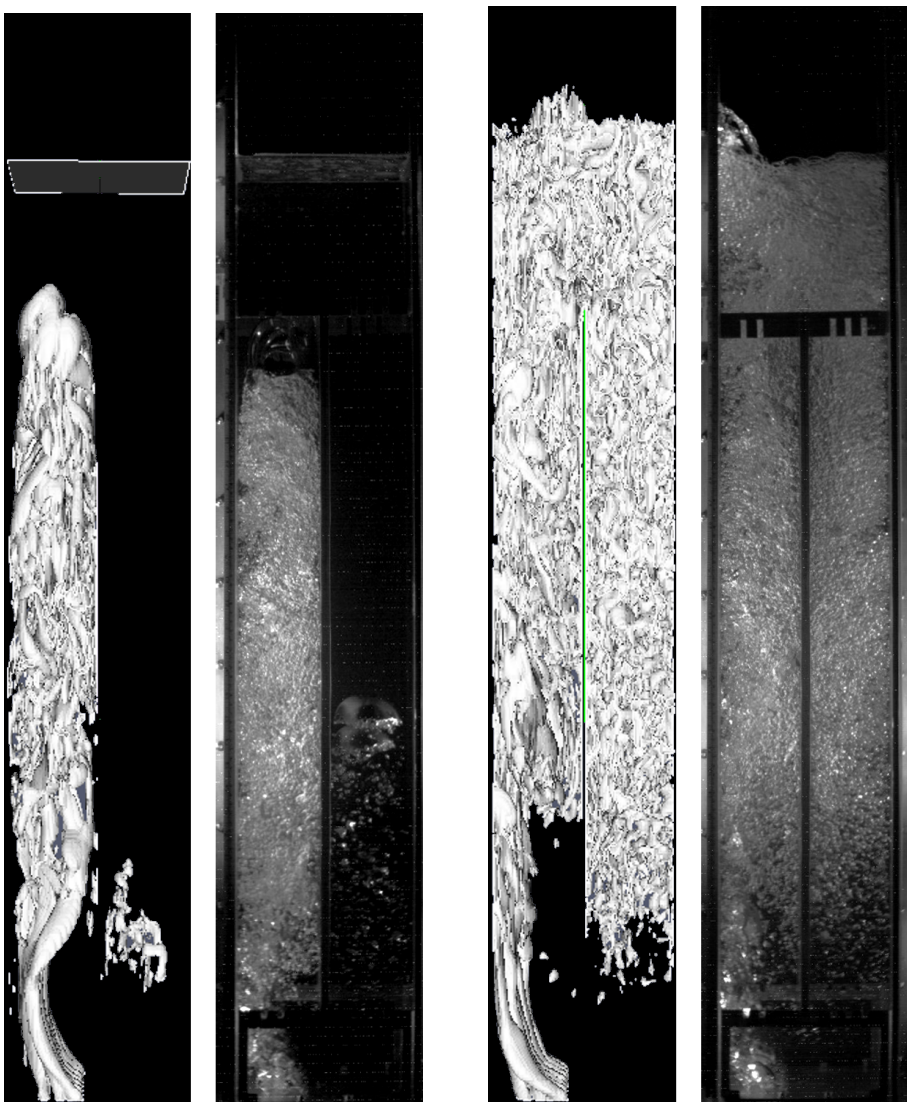

Figure 4: Comparison of simulation result (left) with experiment (right)

NOMENCLATURE

$a_{P,N}$	General matrix coefficients of cell (P) and neighbours (N) (1)
f	Center of the cell face
$\vec{A}_f$	Face area vector (m)
$\vec{u}_f$	Velocity vector at face center (m/s)
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)
$S_{\gamma P}$	Source term
γ	Volume of fluid indicator function (1)
γ_P	VOF of Cell (1)
γ_N	VOF of the nearest neighbor cells (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)

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