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Computational Analysis of a Vortex Ingesting Bioreactor for Hydrogen Production

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In this work, the fluid dynamics behaviour of a bioreactor specifically designed for a fermentative hydrogen production process is investigated by Computational Fluid Dynamics (CFD) simulations. The geometrical features of the bioreactor, which is a dual impellers baffled stirred tank provided with a draft tube, and the gas-liquid characteristics of the vortex ingesting operating mode make the modelling and the numerical solution tasks particularly challenging. The computational strategy is based on the two-phase formulation of the Reynolds Averaged Navier-Stokes equations in an Eulerian framework for both the continuous and the dispersed phase. The results of the simulations are compared with available experimental data collected in a parallel investigation under the same operating conditions and a identical bioreactor geometry. The reliability of the predicted overall hydrodynamics behaviour and the accuracy of the turbulent two-phase mean velocity field are evaluated and critically discussed. The results confirm that the proposed CFD approach is a suitable tool for the design and optimization of stirred bioreactors.

1. Introduction

The production of biological hydrogen is included among the environment friendly processes (Boran et al., 2009) and the viability of hydrogen production from organic substrates by anaerobic fermentation of either suspended-cells or attached-growth of appropriate bacteria is nowadays well-established (e.g. Levin et al., 2004; Wang and Wan, 2009). The engineering issues for moving towards the production scale concern the bioreactor design and the selection of the operating conditions (Noebauer and Schnitzhofer, 2011). With respect to the investigations carried out on biochemical and biotechnological aspects (e.g. Paulo et al., 2013), the bioreactor design and scale up have been less extensively considered, although in the past few years significant efforts have been devoted to the study of the microbial conversion of organic substrates to bioenergy (Ngo et al., 2011). Recently, Computational Fluid Dynamics (CFD) has been identified as a viable approach to the bio-hydrogen reactors design and optimization (Ding et al., 2010; Wang et al., 2010), as an alternative to the semi-empirical and trial and error approaches, which are still widely adopted (Nanqui et al., 2011).
It is well known that the fermentative bio-hydrogen production process is affected by a number of critical factors, including mixing of the liquid phase, medium composition, pH and temperature. On the fluid dynamics side, typically turbulent multiphase flow conditions have to be tackled and for this reason the bioreactor design would take advantage of comprehensive modelling techniques, which are able to account for the local distribution of the fluid dynamics variables interacting with the chemical and biochemical factors.

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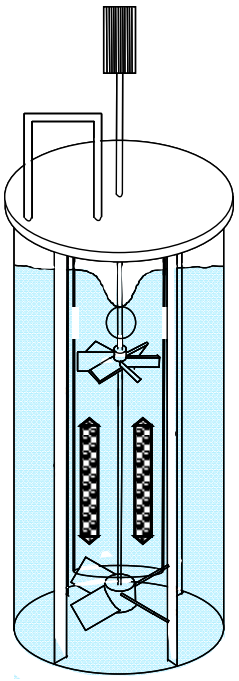
In this work, the currently available CFD techniques for turbulent gas-liquid flows modelling are applied to the investigation of a specific bioreactor, which has been designed for the purpose of transferring the results recently obtained by Cappelletti et al. (2012) in glass vials of about 100 mL to a larger scale.
Particular consideration is given to the requirements of the H_2 production process identified by Cappelletti et al. (2012) for the generation of biohydrogen under batch and attached-growth conditions from molasses and cheese whey by selected Thermotoga strains, which are strict anaerobic bacteria. In order to devise a viable production process, a novel, dual impeller vortex ingesting stirred bioreactor has been designed. This configuration allows to fulfil all the process hydrodynamics requirements, including the gas recirculation for stripping the dissolved gaseous fermentation products, which was found to improve H_2 production (e.g. Massanet-Nicolau et al., 2010; Ngo et al., 2011). In the following, the modelling procedure and the results of the CFD simulations carried out under different operating conditions are presented and discussed.

2. The Model Bioreactor

The bio-hydrogen reactor modelled in this work was purposely devised in order to propose an attached growth process as an alternative to the dispersed biomass configuration. A cylindrical fully baffled stirred tank provided with a flat base and a lid was selected. The agitation was provided with a dual impeller consisting in a lower 4-bladed 45° pitched blade turbine (4b-PBT) and an upper 6-bladed 45° pitched blade turbine (6b-PBT). The structured supports for the microorganism were inserted inside a draft tube. This novel stirred tank design allows an external loop for the product gas, which is suitable for being coupled with a membrane module for H_2 recovery. In this way, it is possible to have a flux across the membrane without introducing any compressor/fan for moving the gas. For the fluid dynamics investigation, the external gas circulation took place inside a simple external tube. As the model fluids demineralised water and air have been adopted. The main geometrical characteristics and dimensions of the model bioreactor are reported in Figure 1.



Main geometrical dimensions

T [m]	0.232	vessel diameter
H [m]	2T	vessel height
W [m]	T/10	baffle width
D_1 [m]	0.40T	diameter of the 4b-PBT
C_1 [m]	0.60T	distance of the 4b-PBT from the bottom
D_2 [m]	T/3	diameter of the 6b-PBT
C_2 [m]	1.35T	distance of the 6b-PBT from the bottom
D_{DT} [m]	0.40T	diameter of the draft tube
L [m]	1.36T	height of the draft tube

Figure 1: Geometrical characteristics of the model bioreactor

3. The CFD model

The stirred bioreactor fluid dynamics behaviour was investigated under fully turbulent single phase and gas-liquid conditions. The CFD simulations were based on the numerical solution of the Reynolds averaged Navier-Stokes (RANS) equations in single-phase conditions and on the relative Eulerian formulation in the two-phase case, which were already successful applied to the prediction of either single phase (Coroneo et al., 2011) or two phase flows (Montante and Magelli, 2007; Montante et al., 2007) in turbulent stirred tanks.

For the gas-liquid conditions, separate flow fields for the liquid phase and the bubbles were obtained simultaneously, by solving the continuity and momentum equations for each phase.

The continuity and momentum equations for a generic phase q, based on the Eulerian treatment, are

$$\frac{\partial}{\partial t}\left(\alpha_q\right)+\nabla\cdot\left(\alpha_q\mathbf{u}_q\right)=0\,, \tag{1}$$

$$\frac{\partial}{\partial t}\left(\alpha_q\rho_q\mathbf{u}_q\right)+\nabla\cdot\left(\alpha_q\rho_q\mathbf{u}_q\mathbf{u}_q\right)=-\alpha_q\nabla p+\nabla\cdot\boldsymbol{\tau}_q+\mathbf{R}_{pq}+\alpha_q\rho_q\left(\mathbf{F}_g+\mathbf{F}_{lift,q}+\mathbf{F}_{vm,q}\right), \tag{2}$$

where α_q is the volumetric fraction of the phase q, $\mathbf{u}$ is the velocity vector, p is the pressure, $\boldsymbol{\tau}$ is the Reynolds stress tensor, while $\mathbf{F}_g$, $\mathbf{F}_{lift}$ and $\mathbf{F}_{vm}$ are the gravitational, lift and virtual mass forces, respectively.

The inter-phase momentum transfer term, $\mathbf{R}_{pq}$, was modelled via the bubble drag coefficient, C_D, as

$$\mathbf{R}_{pq}=\frac{3}{4}\frac{\alpha_s\rho_s}{d_b}C_D\left|\mathbf{u}_p-\mathbf{u}_q\right|\left(\mathbf{u}_p-\mathbf{u}_q\right), \tag{3}$$

where C_D was calculated by assuming the bubbles as rigid spheres of fixed diameter.

Preliminary simulations were performed for a simpler single phase flow case, with the bioreactor filled with water up to the lid. This preliminary condition was investigated in order to assess the effect of the geometrical complexity of the computational domain and of the turbulence modelling on the reliability of the results. In particular, the standard k-ε and the Reynolds Stress (RSM) turbulence models were considered for closing the RANS equations in single phase conditions. The preliminary evaluation of the turbulence model effects was necessary since, as a difference with the case of standard geometry fully baffled stirred tanks, the flows inside the draft tube, similarly to the case of unbaffled tanks, could be critically dependent on the turbulent model closure (Ciofalo et al., 1996).

As for the two-phase flow, the standard k-ε model with the physical properties of the gas-liquid mixture was adopted and the two phases shared the same k and ε values. Different simulations were performed, based either on a mono-dispersed or on a bi-dispersed bubble size, in order to highlight the effect of this assumption on the simulation results. In the latter case, one continuous phase and two dispersed phases were considered.

The model equations were solved on a computational domain whose main elements are depicted in Figure 2, discretised by about 2×10^6 cells. For the single phase flow, the external tube for the recirculation was removed from the computational domain and replaced with a closed lid. The simulations were started from still fluid conditions, and the liquid level was equal to the vessel height for the single phase case and to 1.6T for the two phase case.

In order to tackle the moving impellers and the stationary walls, the computational domain was divided into three regions and the equations were solved with respect to an appropriate reference frame. The so-called “Sliding Mesh” approach was adopted for coupling the stationary and the rotating domains. The simulations were run with a fixed time step size corresponding to an impeller rotation of 6°, thus overall 60 time steps were required for completing one full impeller rotation. The number of internal iterations for each time step was varied depending on the specific case for ensuring constant values of the residuals. Convergence and pseudo-steady state attainment were guaranteed by almost constant and very low residual values and by identical flow variables after two subsequent complete impeller revolutions. In order to perform an appropriate comparison with the ensemble averaged experimental velocity fields, which were collected by the Particle Image Velocimetry (PIV) technique (Montante et al., 2013), the results of several impeller revolutions calculated after obtaining a fully developed flow field were time averaged. The simulations were run on the parallel version of the commercial code Fluent 6.3 on a

eight core computer, after partitioning the computational domain in eight sub-domains. Further details of the numerical solution method are omitted here for the sake of shortness.

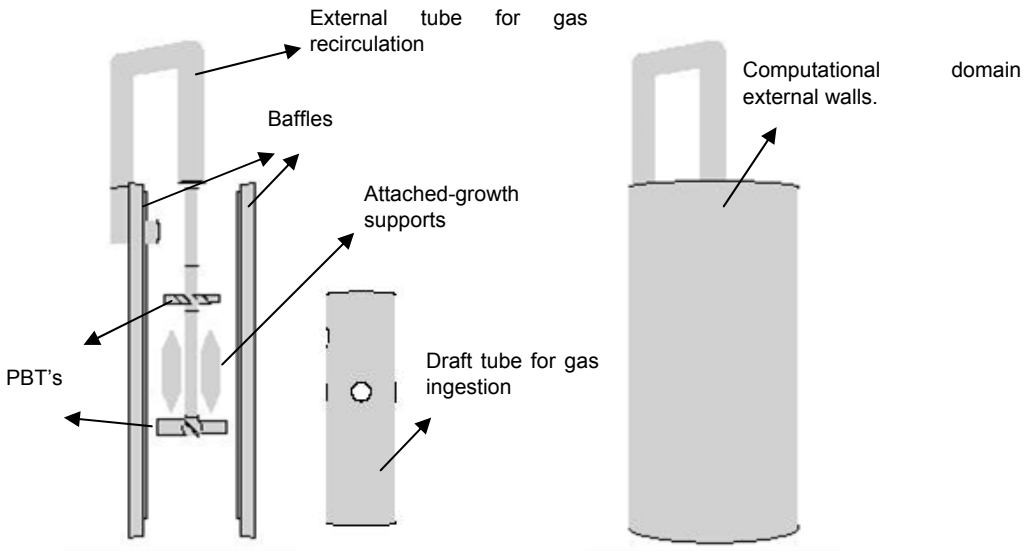
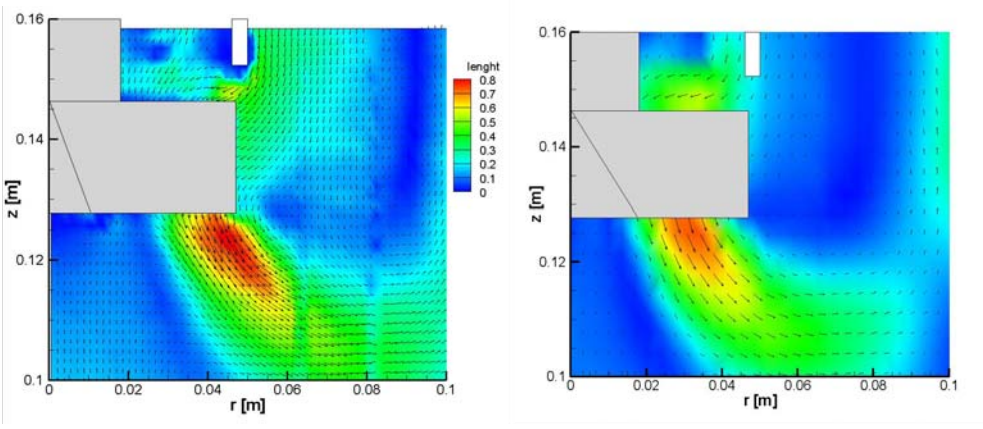


Figure 2: Main geometrical elements included in the computational domain.

4. Results and discussion

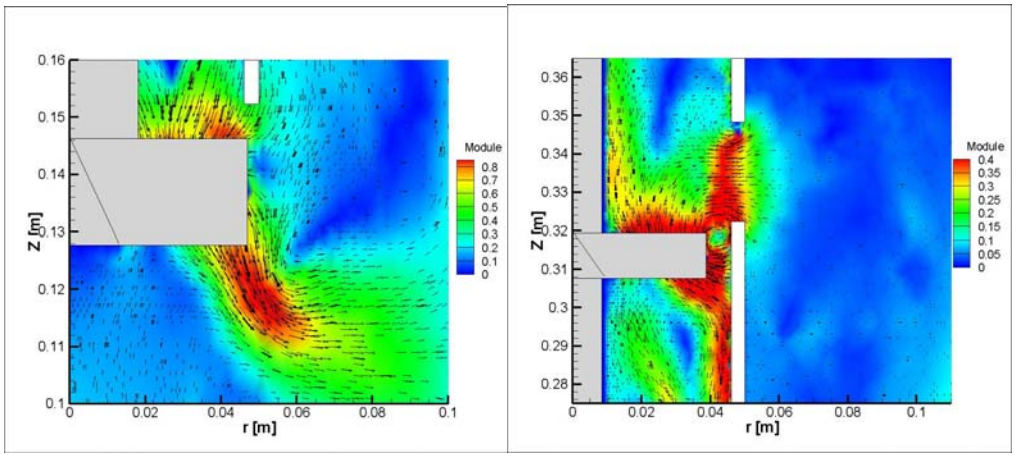
The evaluation of the appropriateness of the computational approach is based on the experimental PIV data collected in a parallel investigation, whose specific results are provided in Figure 3. The reported experimental 2D liquid velocity vector plots superimposed to the colour maps of velocity magnitude are relevant to a portion of the reactor, placed in the vertical plane midway between two consecutive baffles and below the lower impeller. As can be observed, the liquid velocity field in the two-phase case maintains the main characteristics of the single phase flow, although a reduction of the velocity magnitude due to the bubble action and the variation of the discharge flow position is clearly visible.



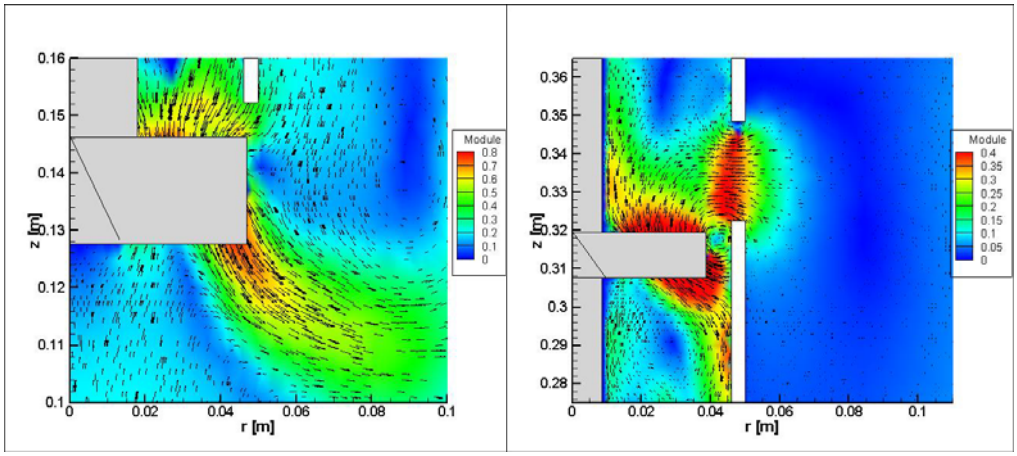
Single phase flow ***Two-phase flow***

Figure 3: Liquid flow field measured by Particle Image Velocimetry. N=360 rpm.

Due to the highly swirling flow inside the draft tube, the effect of the turbulence modelling has been investigated at first for the single phase case, corresponding to the vessel filled with water up to the lid, thus preventing air entrainment. The results of the calculations obtained around the two impellers by either the Reynolds Stress model or the standard k-ε model are summarized in Figure 4 (a) and (b), respectively.



(a) Turbulence model: Reynolds Stress Model.



(b) Turbulence model: standard k-ε.

Figure 4: Effect of turbulence modelling on the single phase flow field predictions

As can be observed, in both cases the predicted liquid flow field agrees fairly well with the experimental results and the main differences between the two turbulence model predictions are obtained below the impeller.
In order to perform a quantitative evaluation of the computed results, the velocity components in specific locations have been compared, as shown in Figure 5, where the profiles of the axial (a) and radial (b) velocity components are shown at a specific elevation (z/T=0.4) located below the lower Pitched Blade Turbine. Also, the power consumption due to agitation as obtained by strain gauge measurements and by the two models have been compared and the results are shown in Figure 6, where the accuracy of the simulations in both cases is apparent. Overall, the comparison of experimental and simulation results for the single phase case has led to conclude that although a slightly better accuracy is obtained by adopting the RSM, the adoption of the k-ε model is viable. Therefore, due to the complexity of the overall problem, the k-ε model has been preferred to the RSM for the two-phase flow investigation due to its numerical robustness and lighter computational costs.
The two-phase flow simulations had the challenging aim to correctly predict the vortex ingesting operating mode of the bioreactor. It was already pointed out that this is a particularly demanding tasks, since the phenomenon of

surface aeration should be modelled from fundamental principles (Patwardhan and Joshi, 1998), although recently successful results were obtained adopting an Eulerian-Eulerian approach by Torrè et al. (2007) for a partially baffled stirred tank. Also the vortex formation and shape were well captured by either an Eulerian model or a Volume of Fluid model in recent investigations (e.g. Cartland Glover and Fitzpatrick, 2007; Motamedvaziri and Armenante, 2012).

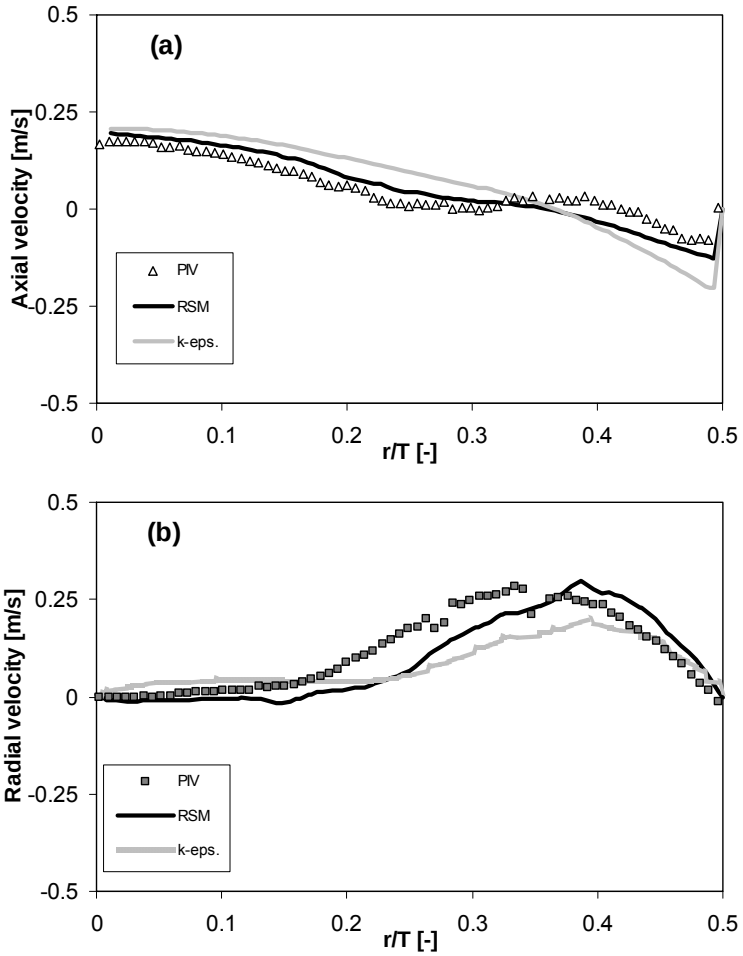


Figure 5: Comparison of predicted and measured axial (a) and radial (b) velocity profiles (single phase flow).

The vortex ingesting operation of the present bioreactor was aimed at allowing an external gas recirculation, which final aim is to strip the gaseous fermentation products and to carry them into the external loop where a membrane separation module will be placed for pure H_2 recovery. Therefore, the main overall parameter to catch is the gas flow rate flowing into the external tube during the vortex ingesting operating mode. As expected, due to the lack of a fundament model for the surface aeration mechanism, the capability of the simulation to predict accurately the measured gas flow rate under the different agitation conditions was found to be deeply dependent on the bubble size assumption. Overall, a satisfactory gross behaviour of the reactor operating mode was however obtained. As a matter of fact, under the investigated condition the experimental gas flow rate was equal to 50L/s while the simulation results ranged from 30L/s to 70L/s depending on the bubble size.

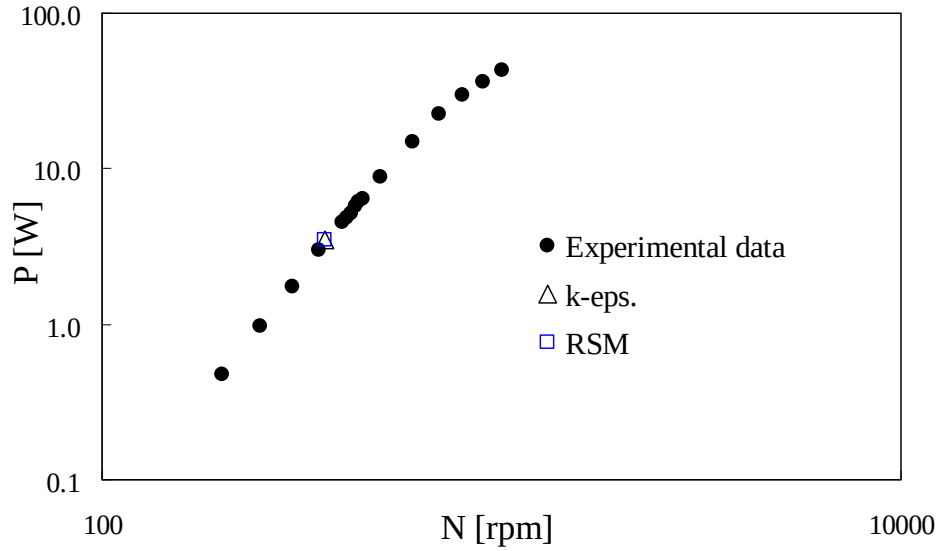


Figure 6: Power consumption vs impeller speed.

As an example of the different level of gas entrainment predicted as a function of the bubble size, in Figure 7 the colour maps of the liquid volume fraction inside the draft tube are shown for either monodisperse or bidispersed bubbles.

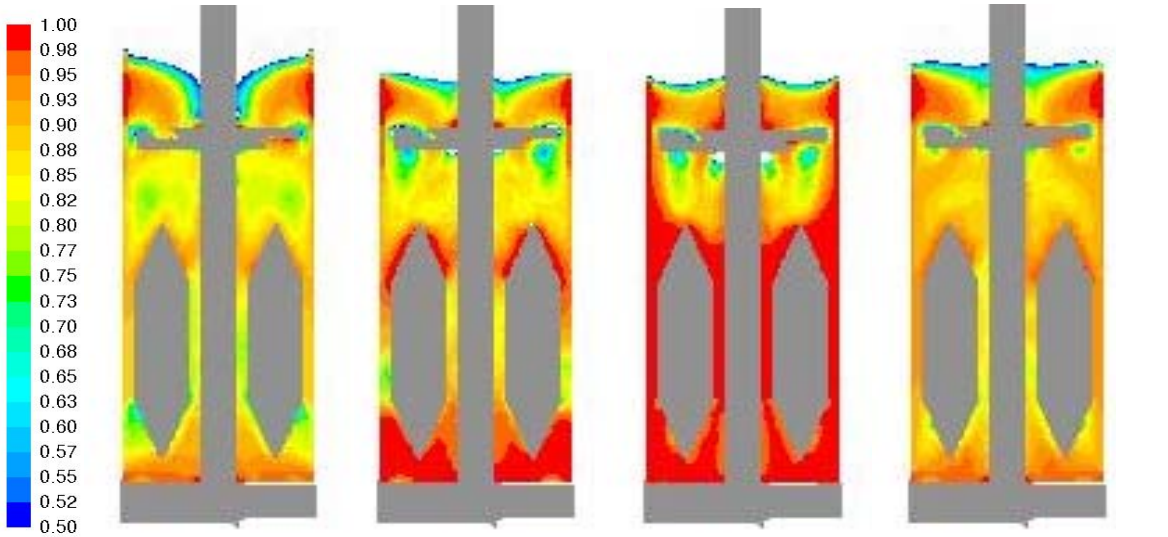


Figure 7: Effect of the bubble size on the liquid volume fraction inside the draft tube.

As can be observed, apart from the expected increase of the liquid hold-up at increasing bubble size, a different gas-liquid interface shape is predicted, although the range of bubble size assumed in the different simulations was not dramatically different.

As for the flow field predictions, the results obtained under the assumption of mono-sized bubbles of 0.50mm and of two bubble classes of 0.25mm and 1.1mm are shown in Figure 8 and 9 respectively. As can be observed, the liquid flow field in the lower part of the vessel matches fairly well the experimental results (Figure 3) in both cases, although for two bubble classes case, the position of the discharge flow of the impeller is closer to the PIV data. As for the bubbles flow field, the pumping action of the upper impeller is properly predicted while a specific quantitative evaluation of the results will be address in future works.

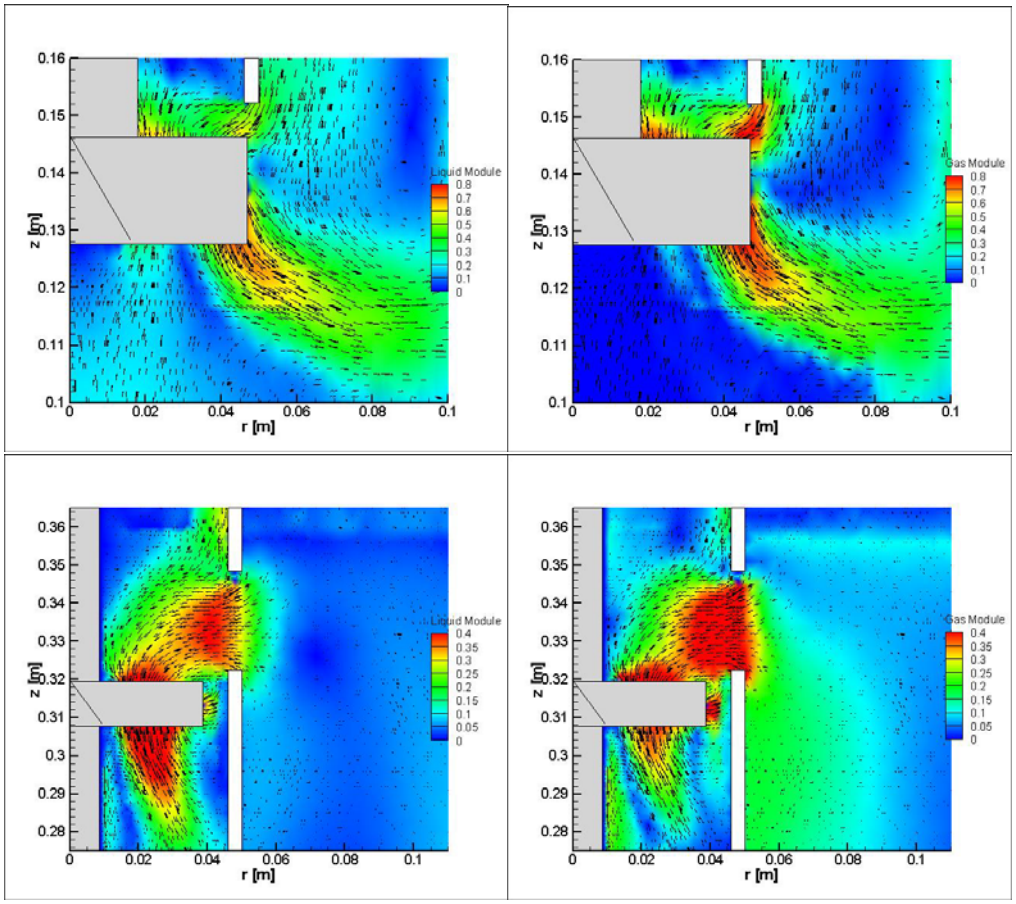


Figure 8: Liquid (left) and bubbles (right) flow field predictions under the assumption of monodispersed bubbles. (d_b=0.5mm).

5. Conclusions

A vortex-ingesting stirred bioreactor designed for the production of H_2 by anaerobic fermentation of waste organics has been investigated by CFD simulations based on an Eulerian-Eulerian approach. Overall the fluid dynamics and operational features of the bioreactor are correctly predicted with an increasing level of accuracy at increasing number of bubble classes. The results show that the CFD strategy already developed for simpler gas-liquid stirred vessels can be usefully applied to the design of bioreactors for hydrogen fermentation production, provided that further developments of the model for including fermentation kinetics and mass transfer are performed. The overall process of H_2 production by fermentation has been already implemented in the present hydrodynamic model by defining a volumetric reaction kinetic on the bags volumes, defined as porous regions with the same pressure drops as the real support adopted for the biomass growth. As for the gas flow rate, after stripping the hydrogen is allowed to escape from the reactor with the inert recirculated gas previously predicted by

the fluid dynamics simulation. The results obtained with this approach however will be evaluated in future investigations.

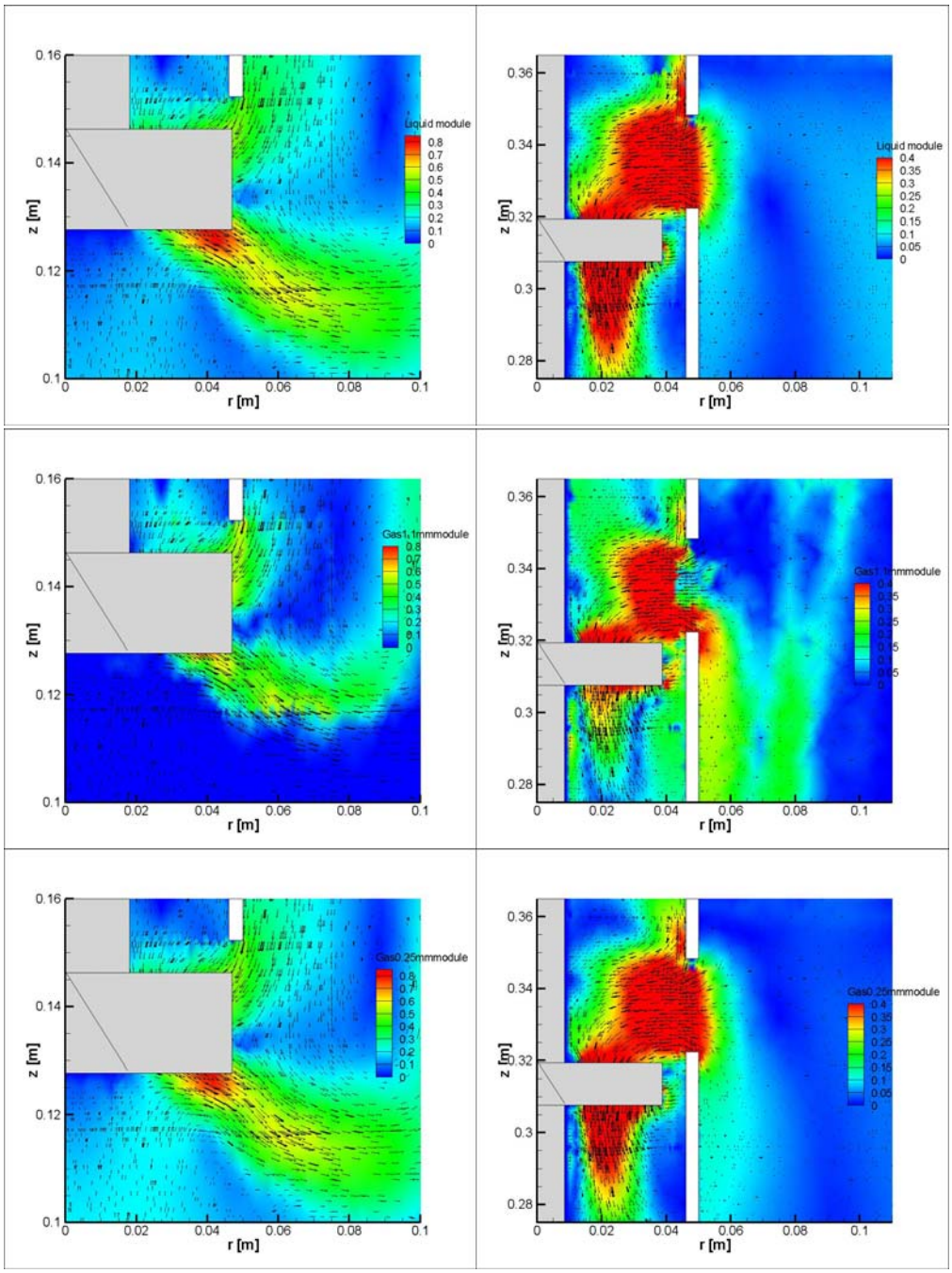


Figure 9. Liquid (upper) and bubbles (d_{b1}=0.25mm center; d_{b2}=1.10mm lower) flow field predictions under the assumption of bi-dispersed bubbles.

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