CHEMICAL ENGINEERING TRANSACTIONS
VOL. 32, 2013
Chief Editors: Sauro Pierucci, Jiří J. Klemeš
Copyright © 2013, AIDIC Servizi S.r.l.,
ISBN 978-88-95608-23-5; **ISSN** 1974-9791
A publication of
AIDIC
The Italian Association
of Chemical Engineering
www.aidic.it/cet
DOI: 10.3303/CET1332121

Computational Analysis of a Vortex Ingesting Bioreactor for Hydrogen Production

Giuseppina Montante*[a], Mirella Coroneo[b], Javier A. Francesconi[c], Alessandro Paglianti[b], Franco Magelli[a]

[a]Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, viale Risorgimento 4, 40136 Bologna, Italy
[b]Dipartimento di Ingegneria Civile Chimica Ambientale e dei Materiali, Università di Bologna, via Terracini 28, 40131 Bologna, Italy
[c]INGAR (CONICET-UTN), Avellaneda 3657 (3000), Santa Fe, Argentina
giuseppina.montante@unibo.it

In this work, the fluid dynamics behaviour of a model 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 under the same operating conditions and an 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.

1. Introduction

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). These aspects have been less extensively investigated with respect to the biochemical and biotechnological aspects, 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 design and the scale-up of bio-hydrogen reactors (Ding et al., 2010), which are still mainly based on semi-empirical and trial and error approaches (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 technique, which are able to account for the local distribution of the fluid dynamics variables interacting with the chemical and biochemical factors. In this work, the attention is focused on the application of currently available CFD techniques for turbulent gas-liquid flows modelling to the investigation of a specific bioreactor, which has been designed to transfer the results recently obtained by Cappelletti et al. (2012) in glass vials of about 100 mL to a larger scale.

In particular, the requirements of the H_2 production process identified by Cappelletti et al. (2012) from molasses and cheese whey by selected *Thermotoga* strains, which are strict anaerobic bacteria, under batch and attached-growth conditions are considered. In order to devise a viable production process, a novel, dual impeller vortex ingesting stirred bioreactor has been designed. This configuration allows to fulfil

Please cite this article as: Montante G., Coroneo M., Francesconi J., Paglianti A., Magelli F., 2013, Computational analysis of a vortex ingesting bioreactor for hydrogen production, Chemical Engineering Transactions, 32, 721-726 DOI: 10.3303/CET1332121

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 CFD model

The CFD simulations of the stirred bioreactor were based on an Eulerian treatment of the gas-liquid system. The continuity and momentum equations for each phase were solved for obtaining separate flow fields for the liquid phase and the bubbles, simultaneously. The continuity and momentum equations for a generic phase q, based on the Eulerian treatment, are:

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

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

where α_q is the volumetric fraction of the phase q, **u** is the velocity vector, p is the pressure, τ is the Reynolds stress tensor, F_g, F_{lift} and F_{vm} are the gravitational, lift and virtual mass forces, respectively. The inter-phase momentum transfer term, R_{pq}, was modelled via the drag coefficient, C_D, as:

$$R_{pq}=\frac{3}{4}\frac{\alpha_s\rho_s}{d_b}C_D\left|u_p-u_q\right|\left(u_p-u_q\right) \tag{3}$$

where the drag coefficient C_D was calculated by assuming the bubbles as rigid spheres of fixed diameter. Different cases where considered either based on mono-dispersed or bi-dispersed bubbles, in order to highlight the effect of this assumption on the simulation results. As for the Reynolds stress tensor modelling, the standard k-ε model with the physical properties of the gas-liquid mixture was adopted; therefore, the two phases shared the same k and ε values. The model equations were solved in a computational domain whose main elements are depicted in Figure 1, discretised by about 2×10^6 cells.

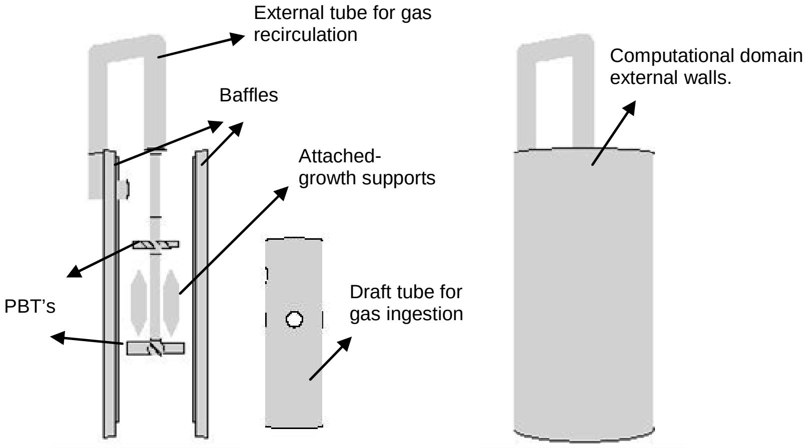


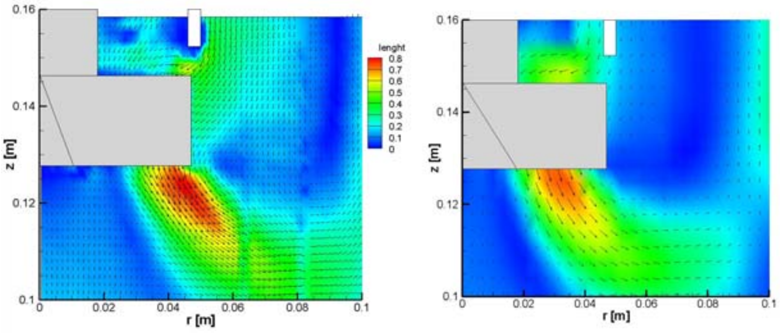
Figure 1: Main geometrical elements included in the computational domain.

The simulations were started from still fluid conditions, with the liquid level fixed at H=1.6T. The model was implemented in the commercial code Fluent 6.3. 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 computational domain was partitioned in eight sub-domains and the parallel version of the code was run on a eight core computer.

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. The details of the numerical solution method are omitted here for the sake of shortness.

3. Results and discussion

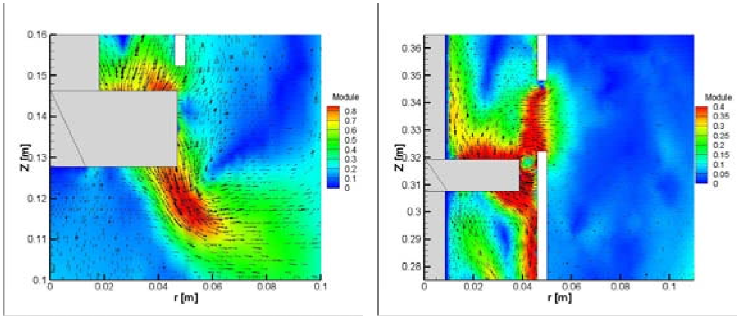
In the following, the hydrodynamics characteristics of the bioreactor working under single phase and vortex ingesting conditions will be discussed. The evaluation of the appropriateness of the computational approach is based on the experimental Particle Image Velocimetry (PIV) data collected in a parallel investigation, of which specific results are provided in Figure 2. The 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 between two consecutive baffles and below the lower impeller. As can be observed, the liquid velocity field maintains its main characteristics although a reduction of the velocity magnitude due to the bubble action and the variation of the discharge flow position is clearly visible.



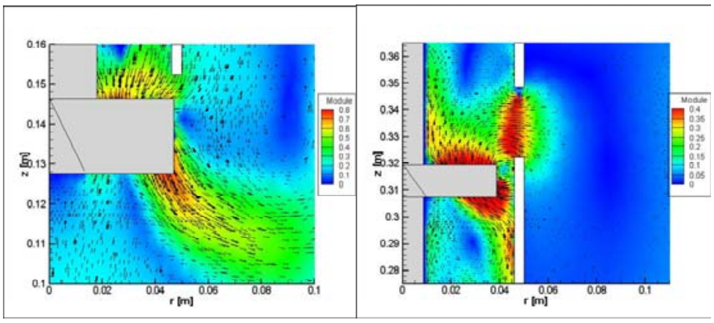
Single phase flow ***Two-phase flow***

Figure 2: 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 3 (a) and (b), respectively.



(a) Turbulence model: Reynolds Stress Model.



(b) Turbulence model: standard k-ε.

Figure 3: 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 shown in Figure 2. The main differences between the two turbulence model predictions are obtained below the lower 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 4, where the profiles of the axial and radial velocity components are shown at a specific elevation located below the lower Pitched Blade Turbine.

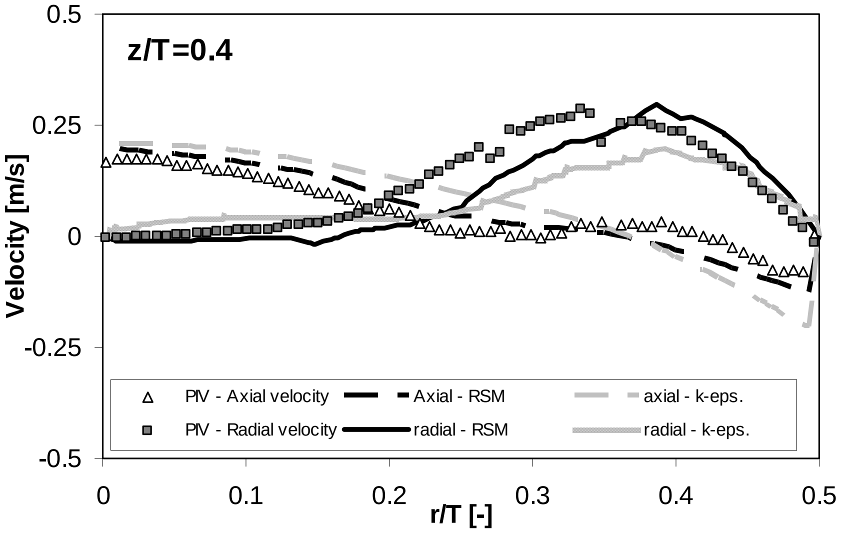


Figure 4: Comparison of predicted and measured axial and radial velocity profiles (single phase flow).

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 5, where the accuracy of the simulations in both cases is apparent.

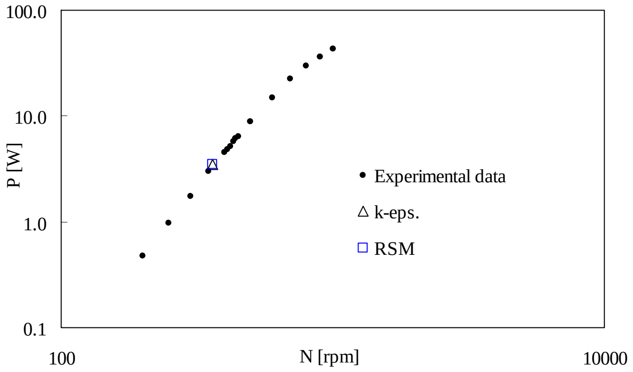


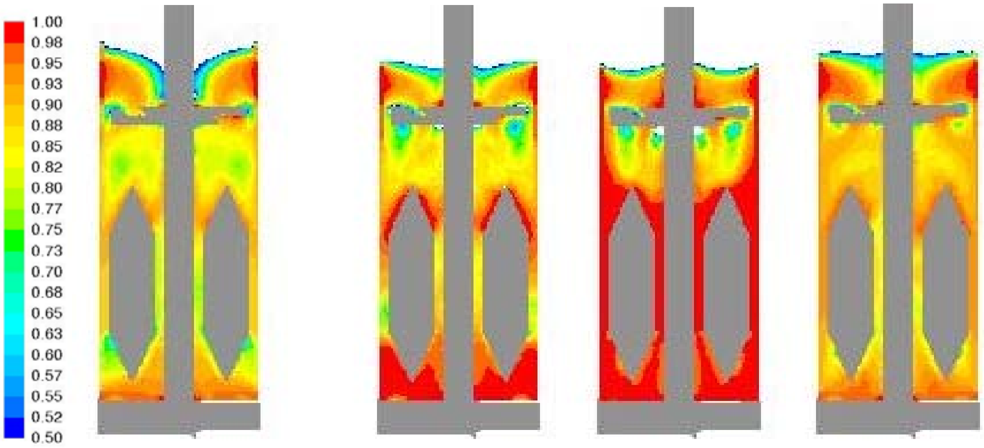
Figure 5: Power consumption vs impeller speed.

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).

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 depended on the bubble size assumption. Overall, a satisfactory gross behaviour of the reactor operating mode was obtained. 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.

As an example of the different level of gas entrainment predicted as a function of the bubble size, in Figure 6 the colour maps of the liquid volume fraction inside the draft tube are shown for either monodispese bubbles or bidispersed bubbles.



(a) d_b=0.50mm

(b) d_b=1.00mm

d_{b1}=0.25mm
d_{b2}=1.10mm

d_{b1}=0.3mm
d_{b2}=1.2 mm

Figure 6: 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 interphase 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 monosized bubbles of 0.50mm are not shown due to space constrains while those relevant to two bubble classes of 0.25mm and 1.1mm are shown in Figures 7.

The liquid flow field in the lower part of the vessel matches fairly well the experimental results (Figure 2) 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.

4. 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 dynamic 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.

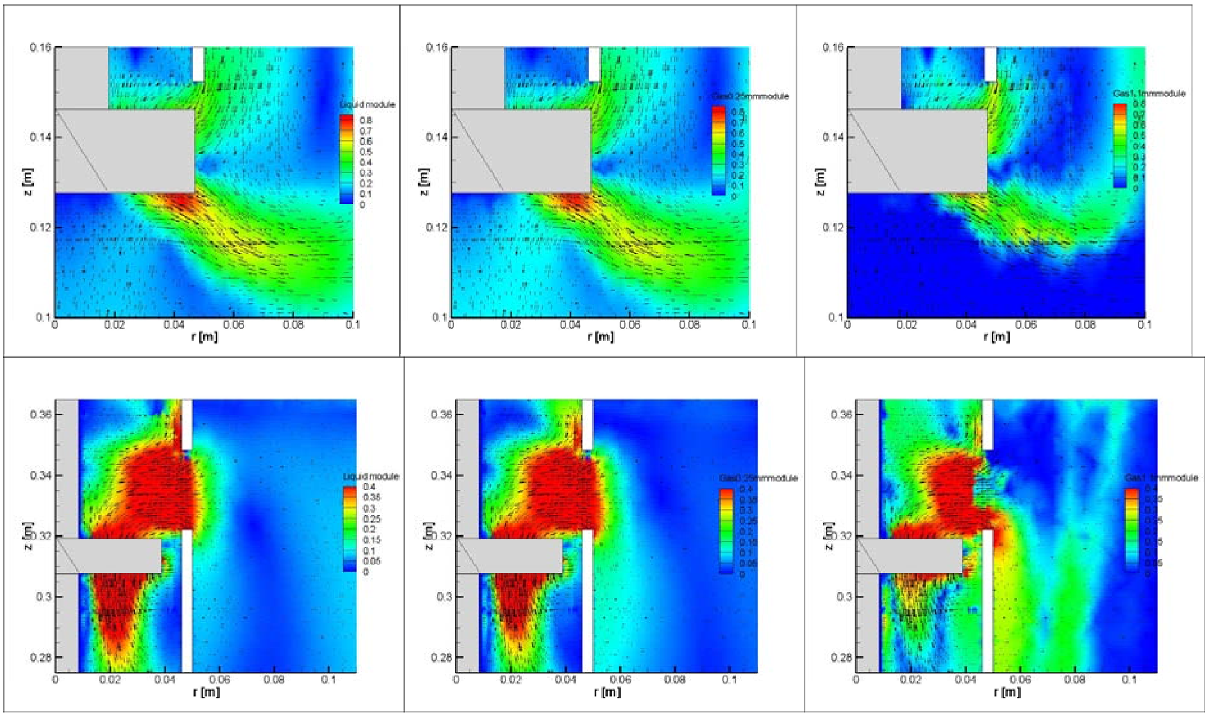


Figure 7: Liquid (left) and bubbles (center d_{b1}=0.25 mm, right d_{b2}=1.10 mm) flow field predictions under the assumption of bi-dispersed bubbles.

References

Cappelletti M., Bucchi G., De Sousa Mendes J., Alberini A., Fedi S., Bertin L., Frascari D., 2012, Biohydrogen production from glucose, molasses and cheese whey by suspended and attached cells of four hyperthermophilic Thermotoga strains, J. Chem. Technol. Biotechnol., 87, 1291-1301.

Cartland Glover G.M., Fitzpatrick J.J., 2007, Modelling vortex formation in an unbaffled stirred tank reactors, Chem. Eng. J., 127, 11-22.

Ding J., Wang X., Zhou X.-F., Ren N.-Q., Guo W.-Q., 2010, CFD optimization of continuous stirred-tank (CSTR) reactor for biohydrogen production, Bioresource Technology, 101, 7005-7013.

Levin D. B., Pitt L., Love M., 2004, Biohydrogen production: prospects and limitations to practical application, Int. J. Hydrogen Energy, 29, 173-185.

Massanet-Nicolau J., Guwy A., Dinsdale R., Premier G., 2010, Production of hydrogen from sewage biosolids in a continuously fed bioreactor: effect of hydraulic retention time and sparging, Int. J. Hydrogen Energy, 35, 469-478.

Motamedvaziri, S., Armenante, P.M., 2012, Flow regimes and surface air entrainment in partially filled stirred vessels for different fill ratios, Chem. Eng. Sci., 81, 231-250.

Nanqi R., Wanqian G., Bingfeng L., Guangli C., Jie D., 2011, Biological hydrogen production by dark fermentation: challenges and prospects toward scaled-up production, Current opinions in Biotechnology, 22, 365-370.

Ngo T. A., Kim M.-S., Sim S. J., 2011, Thermophilic hydrogen fermentation using Thermotoga Neapolitana DSM 4359 by fed-batch culture, Int. J. Hydrogen Energy, 36, 14014-14023.

Noebauer S., Schnitzhofer W. 2011, Efficient Hydrogen Fermentation for 2 - Stage Anaerobic Digestion Processes: Conversion of Sucrose Containing Substrates, Chemical Engineering Transaction, 25, 953-958. 953.

Torré J-P., Fletcher D.F., Lasuye T., Xuereb C., 2007, Single and multiphase CFD approaches for modelling partially baffled stirred vessels: Comparison of experimental data with numerical predictions, Chem. Eng. Sci., 62, 6246-6262.

Wang J., Wan W., 2009, Factors influencing fermentative hydrogen production: A review, Int. J. Hydrogen Energ., 34, 799-811.