CFD Optimization of a Submerged Membrane Reactor for Biohydrogen Production

Z. Trad, Ch. Vial, J.-P. Fontaine, and Ch. Larroche

***Abstract*— This paper deals with the modeling of an anaerobic submerged membrane bioreactor (AnMBR) devoted to biohydrogen ($BioH_2$) production by dark fermentation process. The AnMBR consists of a stirred tank reactor equipped with a two-stage radial impeller and coupled with an external hollow fibre membrane module in a forced circulation loop. The AnMBR is simulated using 1D and 3D modelling methodology, respectively. For 3D modelling, a commercial Computational Fluid Dynamics (CFD) software package has been used. The objective is to optimize the abiotic environmental parameters. Several modelling approaches have been used to investigate mixing in the stirred tank, as it is usually operated in the transition region between laminar and turbulent flow conditions. Consequently, a special focus has been put on the influence of numerical issues (grid size, discretization schemes) on the prediction of the hydrodynamics and the mixing time. The comparison between simulations and experiments was carried out by comparing the predicted results with the experimental data from mixing time and Residence Time Distribution measurements using a passive tracer. The details of the flow field deduced from the computations and their analysis are discussed and are shown to be useful to improve the abiotic culture conditions in anaerobic bioreactors that combine mixing and mass transfer limitations.**

***Index Terms*— AnMBR, stirred tank design, CFD, hydrodynamics, mixing**

I. Introduction

In recent years, an increasing interest can be observed on the *anaerobic dark fermentation* process devoted to biohydrogen ($BioH_2$) production from any organic substrate and biomass material [1]. When $BioH_2$ derives agro- and food waste or wastewater, it is considered as a 2nd generation biofuel. As a result, $BioH_2$ is a promising biofuel and is regarded as an attractive future clean energy carrier which can, therefore, have a direct positive effect on greenhouse gas reduction. $BioH_2$ constitutes a key step of any sustainable development strategy and has a great potential to become one of the most attractive alternative to fossil fuels, especially for transportation that depends on oil for 95% at the moment. The production of $BioH_2$ is, indeed, a necessary step for the development of fuel cell vehicles. Fuel cells present, actually, higher energy efficiency than conventional heat engines, but their development is still limited because fuel cell electric vehicles are currently too expensive to compete with hybrid and conventional gasoline or diesel cars. But another issue is the availability of hydrogen from renewable resources, as hydrogen is currently produced from natural gas. Among the sustainable alternatives, mainly the thermochemical routes, namely photofermentation and dark fermentation, the latter presents the advantage to be driven under mixed cultures which exhibit usually a lower $BioH_2$ yield, but do not require sterile conditions and do not involve obligate anaerobe microorganisms. In this case, dark fermentation proceeds as a conventional liquid-phase anaerobic digestion process in which the methanogenic step has been removed. The degradation products correspond to a biogas phase that should contain only $BioH_2$ and CO_2 with a typical yield of 1-2 mol H_2/mol glucose, while most of the carbon is converted into volatile fatty acids (VFA) in the liquid phase, mainly acetate and butyrate. Recent research has focused preliminary on the biological and chemical features of dark fermentation that is usually described as a three-step biochemical process, involving successively biomass hydrolysis, acidogenesis and acetogenesis [1-3]. Numerous works have investigated the chemical and biological parameters of dark fermentation to better understand $BioH_2$ production, especially the optimization of the biotic factors by identifying the most appropriate microbial strains that combine high yield, high productivity and low production cost [2]. However, $BioH_2$ production by dark fermentation is a rather complex process [1-3], in which many physical processes have to be accounted for and involve a multiphase phase flow with suspended solid waste and biogas bubbles in the liquid phase. This implies that liquid-solid mass transfer and gas-liquid mass transfer with gas desorption kinetics may compete with those of biological process. Mixing plays, therefore, a key role because it determines the spatial maldistribution of the suspended solid phase and the inhomogeneity of the concentrations in the liquid phase, which affects the rates of biochemical reactions. Similarly, these are highly sensitive to pH and may be inhibited by VFA, but also soluble hydrogen and

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hydrogen partial pressure P_{H2} in the gas phase. While mixing, concentration homogeneity and mass transfer are enhanced by highly turbulent flow conditions, the biological processes of anaerobic fermentation usually require gentle mixing. Similarly, biomass hydrolysis is a slow reaction that requires high Solid Retention Time (SRT) in the bioreactor, while a low Hydraulic Retention Time (HRT) is needed to prevent inhibition by VFA. This is the reason why experimental works on $bioH_2$ production by dark fermentation have been conducted in various bioreactors, such as anaerobic sequencing batch (AnSBR), fluidized bed or continuously stirred bioreactors. However, these works have almost never tried to quantify or to optimize the influence of the hydrodynamic features at the local scale, such as the velocity field, the local turbulence intensity, and the spatial distribution of concentrations, microorganism population and solid particles, or the inhomogeneity of mass transfer efficiency. To enhance the design and the performance of bioreactors for $BioH_2$ production, it is therefore necessary to introduce hydrodynamics in the abiotic environmental parameters that are accounted for and to develop a new methodology for the design of bioreactors devoted to dark fermentation. In this work, the following strategy has been retained to circumvent the above-mentioned issues:

- An anaerobic membrane bioreactor (AnMBR) has been used: this has theoretically an infinite SRT (in practice from several weeks to several months), while the HRT is controlled by membrane filtration;
- The AnMBR is formed by a mechanically stirred tank equipped with a two-stage impeller, while the membrane is placed on a forced circulation loop.

Mechanically stirred tanks present the advantages to be employed for a wide range of industrial applications in addition to $bioH_2$ production, in particular the suspension of solids. They have been extensively studied in the literature, in particular their macromixing and micromixing properties. Macromixing is induced by the largest scales of motion in the flow, mainly driven by the impeller, while micromixing acts at smaller scales in which momentum diffusion due to turbulent velocity fluctuations superimposed on the main flow motion provides the final blending [5]. Methods for characterizing macromixing and micromixing can be found in [4-6], but as biochemical reactions present slow kinetics, only macromixing will be studied in this work. While numerous papers have identified the hydrodynamic characteristics of flows induced by common impellers and the relationship between most design parameters for multistage impellers (*e.g.* impeller diameter, impeller to tank diameter ratio, impeller to bottom clearance, etc.) [7], the configuration proposed in this work is atypical: First, the stirred tank is operated under gentle mixing conditions that correspond to a large extent to the frontier between transitional and turbulent flows, which has been less studied. Also, the role of the bottom impeller is to achieve solid suspension, while that of the top impeller is to maintain flow homogeneity and enhance $BioH_2$ desorption at the same time. CFD cannot replace experimentation, but it has become a helpful tool, which complements and improves the experimental labor.

Finally, the objective of this paper is to develop the above-mentioned strategy for the AnMBR devoted to $BioH_2$ production by dark fermentation, which combines 1D and 3D modelling methodology. These approaches will be validated using mixing time and Residence Time Distribution (RTD) experiments. Only non-reacting flow conditions will be considered in this paper, but a special focus will be put on the numerical issues (grid size and discretization schemes) that become more and more significant when one approaches transitional flow conditions. However, as dark fermentation remains a rather slow process that must be studied over more than one month, the validation of the proposed design and of the operating parameters cannot be conducted only experimentally. As a result, a combination of 1D methodology from biochemical engineering and of Computational Fluid Dynamics (CFD) has been used in this work. CFD is a powerful numerical tool that can be used to simulate the 3D flow in the AnMBR and is not only handy for predicting the hydrodynamic features of the reactor [8], but also to give access to the mixing properties through concentration fields, circulation patterns and turbulent intensities by solving a set of differential mathematical equations based on the Navier-Stokes equations describing the mass, the momentum, and energy balance. Its main drawback is that it implies CPU- and memory-intensive computations for 3D flows, especially for rotating impellers for which many strategies have been applied (rotating fluid, rotating domain…). However, it offers an invaluable contribution to the design of process for wastewater treatments and in the chemical process industries [9] for the prediction of single, multiphase and rheologically complex flows, coupled for example with heat and mass transfer, or with chemical reactions.

II. Materials and Methods

A. Reactor configuration and operating conditions

The experimental set-up used in this work is an anaerobic membrane bioreactor (AnMBR). The AnMBR is constituted of a 5-liter mechanically-stirred tank in which the bioreactions are conducted. This is associated with an external hollow fibre microfiltration (MF) membrane module that operates in the tangential “outside-in” mode. This is placed on an external recirculation loop in which the flow rate is imposed using a peristaltic circulation pump. The minimum residence time in the tank is 12.5 min. when the flow rate of the circulation pump is maximized. The permeate is recovered using a permeate peristaltic pump that sucks the liquid phase, causing a negative gauge pressure inside the fibres. As a result, the tank and the circulation loop can be operated under atmospheric pressure, which avoids inhibition by P_{H2}. The variable-flow permeate pump has a maximum flow rate 20 times lower than the circulation pump and is reversible so as to enable backwashing of the membrane module. This is equipped with 142 free polymeric fibers in PVDF with a 0.2 μm cut-off diameter placed in 32.5 cm length housing. The housing is cylindrical and the module packing configuration corresponds to a fiber bundle in which CO_2 gas injection at the bottom can also be used to prevent membrane fouling. In the MF module, the driving

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force of tangential filtration is the transmembrane pressure that is continuously deduced from the measurements of three piezoresistive pressure sensors. The objective is to operate continuously in the fed-batch mode (cyclic removal of permeate compensated by addition of an equivalent volume of culture medium). As a result, the membrane will maintain the solid substrate and the microorganisms in the AnMBR, while soluble molecular compounds, in particular VFA, will be recovered with the permeate. The stirred tank consists of a round-bottomed vessel mechanically agitated using a two-stage impeller placed in the center of the tank. The internal diameter of the vessel is T=19.5 cm for a liquid height of H=32 cm. The bottom impeller is a four-blade disk Rushton turbine of D_T=5.6 cm diameter, which is a radial impeller. The dimensionless clearance C/T is 0.23 to enhance the suspension of the solid substrate. The second impeller is a three-bladed 45° pitch turbine of D_A=8.8 cm diameter placed at a distance equal to T from the bottom of the vessel. Contrary to the Rushton turbine, this promotes a flow discharge both axially and radially, nearly in equal proportion due to the 45° angle. To avoid the inhibition of $BioH_2$ production, the rotation speed of the impeller lies usually between 100 and 150 rpm, as this value ensures that the solid phase is fully suspended, which is not the case, *e.g.* at 75 rpm. In terms of biokinetics, anaerobic cultures have been conducted using a mesophilic microbial consortium at 35°C and under controlled pH conditions (pH 6) using the addition of a NaOH alkaline solution that prevents pH decrease due to the production of VFA. The gas flow rate and the gas composition (especially H_2 and CO_2 species) are monitored using a digital gas flow meter and an on-line gas chromatography device, respectively. In the liquid phase, the composition was analysed using HPLC (high pressure liquid chromatography) after sampling twice per day. Cultures were conducted using either glucose or straw as the substrate. As straw is present in the form of large tabular particles of about 2 mm length, these do not really modify the viscosity of the fluid that is only affected by soluble proteins and polysaccharides. As a result, the fluid remained Newtonian, with a viscosity between 1.3 and 0.2 mPa.s at 20°C. Due to their irregular shape, straw particles orient along to the direction of the velocity vector. Actually, there is a region in the middle of the tank in which particles are nearly horizontal, which corresponds to the region in which the flow discharges of the two impellers interact and, therefore, poor mixing conditions occur. However, tracer experiments are necessary to capture the details of the mixing properties of the AnMBR.

B. Mixing properties using passive tracer dispersion

Mixing time and RTD can be obtained using experiments involving the dispersion of a passive tracer that does not modify the hydrodynamics. In practice, conductivity and colorimetric tracer techniques are the most common in chemical and biochemical reactors, mainly using pulse experiments in which a small volume of tracer is injected very rapidly in comparison to the duration of the experiment, so that it approaches a Dirac δ function. In closed systems, the *bulk mixing time* (often denoted t_m) is the time necessary to achieve the fluctuations of the tracer property (color, conductivity…) measured locally lower than 5% around the final average value which corresponds to homogeneity. Usually, the tracer property oscillates in a stirred tank before reaching the final value and the mean circulation time (t_c) is defined as the time between two consecutive peaks on the response curve. In open systems, the injection is usually placed at the inlet and the tracer is detected at the exit using either a pulse or a step injection. The RTD is the probability density function that describes the amount of time a fluid element could spend inside the reactor. In this work, the conductivity tracer technique has been applied. The pulse injection of a very small volume (10 mL) of a salt solution (usually 1.0 M NaCl) has been used. A conductivity meter with a separate probe was used and the linearized signal of the meter was recorded using an ADLINK usb-1901 data device at a frequency of 1 Hz. Mixing was analyzed using experiments in the different sections of the AnMBR, *i.e.* both on the stirred tank and the membrane module. Due to their difference in volume 5 L for the stirred tank and 0.5 L for the membrane module, respectively, the residence time in the latter was 10 times lower than in the tank. As a result, only mixing and circulation times could be measured in the stirred tank that was treated as a batch system, which means that the residence time was expected to be far higher than t_m. Conversely, RTD was measured on the membrane module with and without permeate extraction. Three configurations were tested. The experimental setup and the different set of experiments are schematically described in Fig. 1.

In the present paper, mixing experiments will be used to assess CFD simulations, as the conventional experimental techniques of fluid mechanics (such as laser Doppler, particle image or hot-film velocimetry) are unable to deal with the solid suspensions encountered in anaerobic bioreactors. However, it is also worthy of note that mixing properties not only describe the suspension of organic waste and the degree of homogeneity of local concentrations, but also enhance hydrogen desorption or may disturb the biological processes. In addition, they may provide useful information to set the position of the inlet of the membrane module in the tank, first for preventing the aspiration of suspended solids in the loop, but also if possible, where VFA concentrations are maximal to avoid local inhibition of biological processes.

C. Methodology of 1D and 3D hydrodynamic modeling

The computational strategy consists of the combination of 1D and 3D CFD methodologies [8], using a comparison between experimental data on RTD and mixing time based on a conductivity tracer technique with the simulations. For 1D modeling, the RTD® free software package from *CISP St Petersburg Ltd.* (Russia) was used. This is able to describe the RTD response curves for the membrane module. For 3D modeling, a commercial CFD software package was used [8, 10], Phoenics®, from *CHAM Ltd.* (UK). This solves the continuity, the Navier-Stokes and the turbulence model equations by a finite-volume approach.

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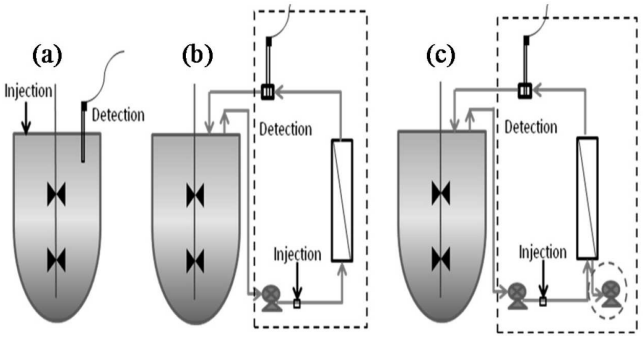

Fig 1. Experimental setup for mixing time analysis in the stirred tank (a), for RTD analysis in the membrane module without permeate extraction (b), and for RTD analysis in the membrane module permeate extraction (c).

Species transport equations can also be added, so that the transport of non-reacting species can easily be simulated. Multiphase modeling, such as the VOF (volume of fluid) approach which is able to describe segregated gas-liquid flows, is also implemented in order to capture the topology of the liquid-gas free-surface in the unbaffled stirred tank. In this work, the VOF model was used first, but vortex formation was limited in the range of rotation speed investigated in this work. This agreed with experimental observation, and further simulations were conducted with the assumption of non-deformable free-slip planar surface as the boundary condition.

As already mentioned, several CFD strategies have been developed for modeling rotating flows driven by impellers. The most common way is the Multiple Reference Frame (MRF) approach, which is a steady approximation of rotating flows. In this case, one must define stationary zones far from the impellers from moving zones in which a rotating velocity is imposed and which encompass the impellers. In fact, neither the grid nor the impeller moves in the MRF model, but a relative velocity formulation is superimposed to the rotating speed. The first alternative consists in using a sliding mesh in the moving zones that move together with the impeller. This implies transient simulations that are far more CPU-intensive than MRF steady simulations. However, both MRF and moving mesh approaches usually require unstructured grids in the moving zones due to the complex geometry of the impeller. Unlike these two common methods, Phoenics® proposes a third way, denoted MOFOR (Moving Frame of Reference) defined as follows:

- a structured Cartesian grid is defined using the cut-cell technique in which the cells crossed by solid wall cross receive a special numerical treatment;
- The impeller moves in the stationary structured grid without affecting the grid, which requires transient simulations.

This approach has been used in this work. It presents the advantage to avoid complex unstructured grids, but need transient simulations that are more computer-intensive than with the MRF model. The tank geometry and a typical example of Cartesian grids used in the simulations (between 300,000 and 600,000 cells to investigate the effect of grid size) are presented in Fig. 2. Other features of the simulations are similar to those usually encountered in the CFD modeling of stirred tanks: low- and high-Reynolds k-ε models have been compared, including k-ε variants (RNG, Chen-Kim…). The influence of the discretization scheme has also been investigated, as it may play a more important role on the simulations in the cut-cell technique (from the first-order upwind to the second/third-order MUSCL scheme). The simulations of mixing time and RTD response curves required to solve the transport equation of an additional scalar, the species concentration, assuming a value of 0.7 for the turbulent Schmidt number. The time step was varied between 0.01 s and 0.001 s, depending on the rotation speed; residuals lower than 10^{-3} were required at each time step. The calculations were carried out in parallel on a PC computer equipped with a 6-core 12-thread CPU.

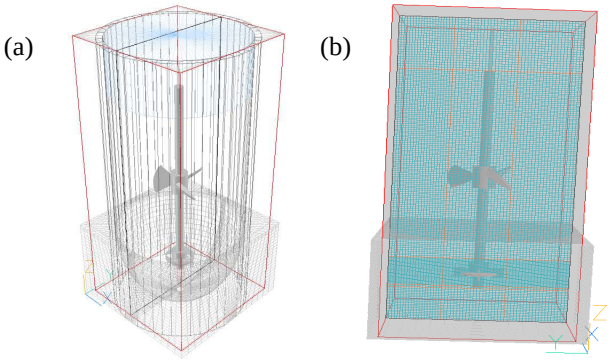

Fig 2. (a) Bioreactor geometry; (b) 2D view of the mesh.

III. Results

D. Experimental study of mixing in the AnMBR

In the experiments, rotation speed in the tank was varied between 20 and 150 rpm. Fig. 3a illustrates the evolution of the salt concentration normalized by the value obtained when homogeneity is achieved near the impeller for a saline injection close to the free surface and a rotation speed of 30 rpm using the configuration of Fig. 1a. Mixing time is about 110 s, which is far lower than the minimum residence time of the fluid in the AnMBR when the recirculation pump operates at its maximum flow rate. Experiments also confirmed that t_m was unaffected by the circulation pump. Fig. 3a shows also that the salt rapidly reaches the sensor with a circulation time measured between two peaks lower than 20 seconds; this result can be extended to higher agitation speed. However, above 100 rpm, the circulation time became so small that it could not be measured any more, as t_m seems to be inversely proportional to rotation speed and t_c is about $t_m/5$. Reynolds number varied between 1,000 and 20,000 for both impellers, considered separately, which covers a region from the transitional flow to fully-developed turbulent flow conditions. However, all the response curves presented a similar shape, which is in agreement with the gradual transition between the flow regimes usually observed in stirred tanks. As a conclusion, the stirred tank appears to be perfectly mixed in less than 110 s at the lowest rotation speed and in less than 20 s at the highest one. This is far lower than the residence time in the tank and also than the residence time of the fluid in the MF module at the corresponding flow rate. Conversely, the RTD curves E(θ) vs. normalized time θ obtained with the

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membrane module without the extraction of permeate (Fig. 1b) exhibit an atypical shape, with a peak that emerges at the half of the residence time in the module, θ=0.5, followed by a long tail (Fig. 3b). This reveals that laminar flow conditions always prevailed in the housing, which is confirmed by the fact that Reynolds number defined as in a pipe was lower than 1000 at the highest flow rate. The curves always presented the same shape that nearly fits the theoretical curve for an empty pipe in Fig. 3b, which corresponds to a decrease proportional to $1/t^2$. Experimental data also highlights that the effect of rotation speed in the stirred tank is negligible on the response curves in the membrane module. When the permeate was sucked at maximum low rate of the permeate pump (Fig. 1c), the E(θ) curves were never significantly affected, which can be explained by the fact that the extraction rate is low in comparison to the recirculation flow rate. Finally, this confirms that the MF module can be described as a simple pipe under laminar flow conditions.

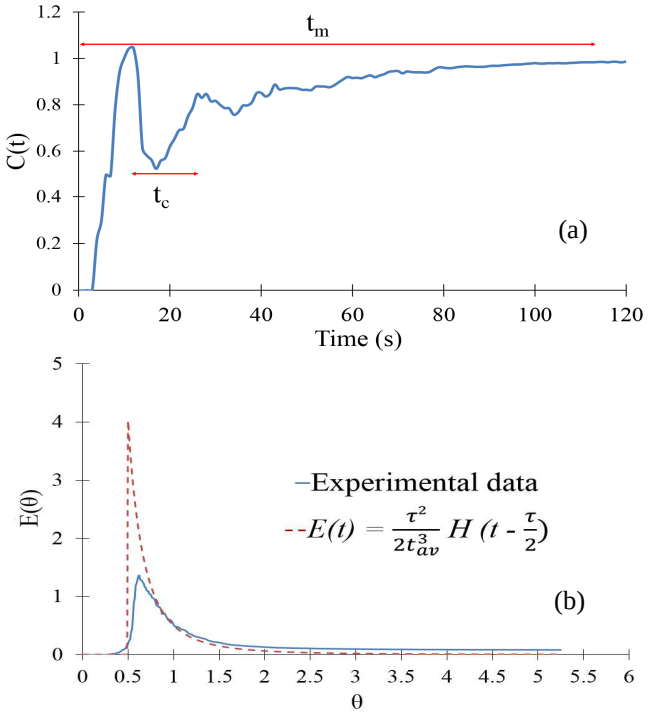

Fig 3. (a) Normalized concentration vs. time in the batch stirred tank (30 rpm); (b) Normalized RTD (E) function vs. normalized time at a circulation flow rate of 300 mL/min.

As a conclusion, RTD experiments show that it is possible to establish a simple mixing model for the AnMBR, which consists of a perfectly mixed tank coupled to a recirculation loop that can be assimilated to a tubular laminar flow region (Fig. 4a). In practice, this result may be biased, as it was not possible to place the probe close to the bottom turbine in the tank. This may explain why the observed trends do not correspond to the segregation of straw particles that emerges from video captures. This is the reason why an alternative model, shown in Fig. 4b, may also be proposed: this assumes that the stirred tank is divided into two perfectly mixed zones that are mixed independently by the top and the bottom impeller, respectively, and between which the circulation is limited. CFD modeling will be used to assess this assumption.

E. 3D CFD modeling

Even though biological reactions are inherently slow, they are highly sensitive to inhibition that can result from soluble H_2 or VFA concentrations, while dark fermentation is known to be impaired by excessively high stirring speeds. As already mentioned, the free surface was shown to remain nearly undisturbed using the VOF approach and only single-phase simulations will be discussed.

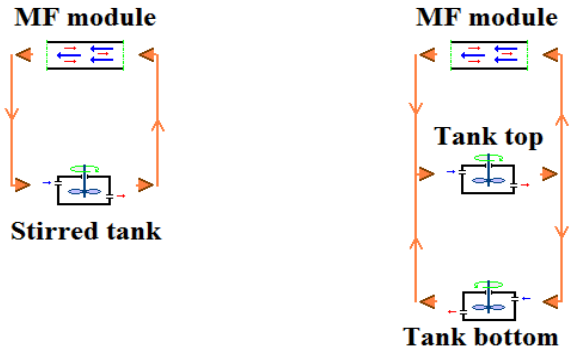

Fig 4. (a) RTD model from mixing experiments; (b) Suspected RTD model with two zones in the stirred tank.

First, the influence of mesh size was studied. The advantage of the MOFOR approach is that a structured mesh is used. The drawback is that the estimation of the boundary in the cut cells is computer-intensive and finally requires grid refinement in the regions of the two impellers. This emerges clearly in Fig. 5a: using 300,000 cells (coarse grid), unphysical trends were observed with high velocity in the wall region. Conversely, with 600,000 cells, the radial discharge of the Rushton turbine clearly appears and the same stands for the axial-radial discharge of the pitch blade turbine (Fig. 5a). In particular, the radial discharge of the Rushton turbine is shown to impinge on the vessel wall, which may favor solid suspension at the bottom of the stirred tank. However, the need for fine grid when moving boundaries are involved constitutes a key limitation of the cut-cell technique. Fig. 5a shows also that both impellers interact only slightly, which was expected due to the high axial gap between the two turbines (literature assumes no interaction when the gap the higher than 1.5 times the impeller diameter). A similar result could be observed in the whole range of rotation speed studied in this work. Then, the comparison of turbulence models lead to a surprising result: the discharge of the two turbines did not significantly differ between the various models tested, except for the k-ε RNG model. Using 600,000 cells, convergence could always be achieved for the prediction of flow properties over 100 s. As velocity was rather low except in the region of the impellers, only low-Re turbulence models should be selected, which is in agreement with the low turbulent viscosity values that were estimated in the tank. However, the k-ε Chen-Kim model was selected because it provided flow fields very close to the other k-ε models, especially the low-Re k-ε models, but with far smaller computation time. The analysis of the influence of the discretization scheme using this turbulence model showed that small differences in the flow profiles appeared between the first-order upwind scheme and higher-order schemes for the convective terms in the

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transport equations. Conversely, the MinMod and the MUSCL high-resolution non-linear schemes provided similar results, but the MinMod scheme presented the advantage to reduce computation time by 7% with the k-ε Chen-Kim model and by a factor 2 for the standard and the RNG k-ε turbulence models. This result was strongly linked to the interplay between the turbulence model and the discretization scheme, as the computational time was identical for simulations with the MUSCL and MinMod schemes when laminar flow conditions were assumed. Another important finding is that the flow pattern remained nearly unchanged in the whole range of rotation speed. This appears clearly in Fig. 5b and shows that in most of regions of the reactor, flow properties varied proportionally to rotation speed, even with the assumption of turbulent flow, although this is typical of laminar flow conditions. As already mentioned, this is probably due to the low turbulence intensity that is observed in the tank, except in the regions close to the impellers. Also, the streamlines, for an injection close to the pitch blade turbine, show that the fluid remains trapped for a long time in the region of this turbine before reaching the region of the Rushton turbine, which confirms that the stirred tank behaves at least as a two-zone reactor. This has to be confirmed by simulations involving the mixing of a passive tracer.

For the prediction of mixing time experiments using CFD, it was necessary to achieve, first, established flow conditions. For example, for a rotation speed of 100 rpm, the evolution of local velocity vs. time showed that a reproducible cyclic behavior was achieved after computations corresponding to 35 s. Using established flow as the initial condition of mixing time simulations, calculations were conducted to simulate about twice the experimental mixing time. They showed a good agreement with experimental data, as they predicted for example 40 s mixing time for an experimental value of 23 s. As a conclusion, coupled hydrodynamic and mixing simulations using the MOFOR approach and the k-ε Chen-Kim model are able to predict correctly the mixing time in the stirred tank at the expense of high computation time because transient modeling is imposed.

III. Conclusions and Perspectives

As a conclusion, a simple 1D model has been established to describe mixing in the AnMBR, using the conventional mixing and RTD experimental methodology of Chemical Engineering. This shows that the MF module can be described using the assumption of laminar flow, following nearly the features observed in a simple pipe. Conversely, if the top of the mixer seems to be perfectly mixed, CFD simulations highlight that the tank seems divided into two regions, as the top and the bottom impellers weakly interact. The simulations demonstrate that the bottom impeller, designed to promote the suspension of the solid substrate, will probably have to be modified. CFD simulations have also shown that the MOFOR approach can be used to simulate the local features of the flow and predict mixing time, but is computationally intensive. A good compromise in terms of computation time and accuracy has been found, using the k-ε Chen-Kim turbulence model coupled to the MinMod discretization scheme for the convective terms. The perspectives of this work are, now, to validate the Eulerian simulations using Particle Image Velocimetry and to implement a simplified biokinetic model of $BioH_2$ production by dark fermentation in the CFD code using the transport equations of additional scalar variables, first with a simple substrate such as glucose for which the metabolic pathways have been already described in the literature.

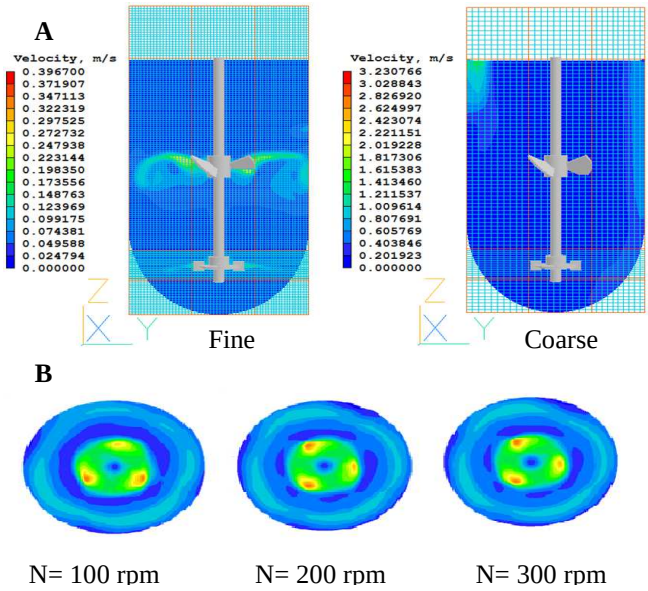

Fig 5. (A) Influence of mesh size on the predictions (100 rpm); (B) Influence of rotation speed on flow pattern.

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