Identifying dominant spatial and time characteristics of flow dynamics within free-surface baffled stirred-tanks from CFD simulations

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Abstract

In many chemical and biochemical processes, it is fundamental to accurately predict flow dynamics within reactors of different sizes and its influence on reactions and their kinetics. Computational Fluid Dynamics can provide detailed modeling about hydrodynamics. The objective of the present work is to assess the abilities of CFD to simulate free-surface turbulent flow within baffled stirred-tanks reactors. Transient simulations are carried out using a homogeneous Euler-Euler multiphase approach, the Volume-of-Fluid (VOF) method, with a Realizable $k-\varepsilon$ turbulence model. Two methods are considered to account for the impeller motion, namely the Multiple Reference Frame (MRF) and Sliding Mesh (SM) approaches. Global and local results obtained by CFD are presented by means of statistical analysis, including the estimation of characteristic turbulent length scales. Instantaneous numerical data fields obtained with the SM model are then interpreted using modal decompositions methods, *i.e.* the Proper Orthogonal Decomposition (POD) and the Dynamic Mode Decomposition (DMD) in order to extract their dominant spatial structures with their time behavior. All simulations are discussed based on comparison with experimental data.

Keywords: Stirred-tank, Hydrodynamics, CFD, PIV, POD, DMD

1. Introduction

Stirred-tank reactors are commonly used in various chemical and biological processes because of their flexibility and relatively good performance due to the wide range of available conditions. In this kind of reactor configuration, hydrodynamics governs bulk fluid mixing and gas-liquid mass transfer. Many large-scale processes give a lower yield than could be expected from lab-scale experiments. A possible explanation is that, with few exceptions, small-scale stirred-tank reactors are generally used with a high specific power input, resulting in a rapid mixing of the liquid bulk and a high mass transfer rate. At a production-scale, the power input is restricted for economical and mechanical reasons, potentially causing mixing issues, as well as mass and heat transfer problems. Problems linked to scale-up are thus qualitatively explained and seem unavoidable (Sweere et al., 1987). However, at the present time, their impact on process performance cannot be quantitatively predicted because they are not completely assessed. Indeed, even if it is obvious that they are related to hydrodynamics, the interactions of the latter with other mechanisms, *e.g.* mixing, mass and heat transport, within industrial reactors are not fully understood and quantified as a function of reactor size (Wernersson and Trägårdh (1999b), Wernersson and Trägårdh (1999a)). Advanced experimental optical techniques, in particular Par-

ticle Image Velocimetry (PIV), are extensively used at lab-scale for hydrodynamic characterization (*e.g.* Escudié and Liné (2003), Khan et al. (2004), Micheletti et al. (2004), Gabriele et al. (2009)). However, they cannot be applied to most industrial stirred-tank reactors for describing the spatio-temporal evolution of local quantities within the vessels for several reasons, *e.g.* equipment size, opaque walls and media. This is the reason why computational models have been used to study various aspects of the stirred-tank reactor design, as well as to predict product formation during fast chemical reaction (*e.g.* Jaworski and Nienow (2003), Rudniak et al. (2004), Cheng and Fox (2010)) or culture processes within these systems (*e.g.* Reuss et al. (2000), Morchain et al. (2014), Haringa et al. (2017)). Most numerical models that have been presented in that context are based on Computational Fluid Dynamics (CFD) to quantify the impact of factors that play a key role in the optimization of stirred-tank reactor design, such as geometry, fluid mechanics as well as heat and mass transport (*e.g.* Sahu et al. (1999), Brucato et al. (2000), Ranganathan and Sivaraman (2011), Zakrzewska and Jaworski (2004), Lane (2017)). Even if, over the past two decades, development of numerical solvers and of computers have allowed the calculation of 3D unsteady flow fields in complex geometries, a complete numerical evaluation of all phenomena at all scales often remains quite difficult, due to the intricacy of turbulence modeling in multiphase fluid dynamics (*e.g.* Alopaeus et al. (1999), Petitti et al. (2010), Buffo et al. (2012), Tamburini et al. (2013), Blais and Bertrand (2017)).

Experimental and computational techniques have been developed in parallel and in a strongly coupled manner to investi-

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gate flow, temperature and concentration fields, as well as heat and mass fluxes. Despite some major differences between these two approaches, their integration into a common methodology can leverage their complementarity and provide a deeper insight into complex flow dynamics (*i.e.* Sheng et al. (1998), Montante et al. (2001b), Hartmann et al. (2004), Coroneo et al. (2011), Trad et al. (2017)). On the one hand, modeling tools are growing in importance and many studies have already demonstrated their strength in many situations. Simulations provide the value of each quantity at every point in the field with the possibility of a total control on the flow conditions and configurations. However, constraints due to computational cost often impose the use of simplified models to describe the physics of phenomena, such as Reynolds-Averaged Navier-Stokes (RANS) turbulence models in CFD simulations. On the other hand, experimental techniques are fundamental for the engineering and research community. They give access to the actual physics, but they are always affected by experimental noise. Due to current limitations of experimental systems in terms of resolution and sample size (measurement volume, recording time), measurements are necessarily restricted to the ranges of spatial and time scales that they could capture. Even if there is a trend towards replacing pilot-scale experimental studies by simulation work for time and cost constraints, experiments may not be eliminated because of the complexity of the investigated phenomena. To fully benefit from an integrated experimental and computational approach, quantitative comparisons between the respective results are required, so that numerical results could be validated by experimental data and in return experimental results can be enriched by numerical data. Although this methodology is relatively trivial for global quantities, such as specific dissipated power P/V , accurately comparing unsteady velocity fields is much more challenging.

The aim of the present work is the assessment, by comparison with experimental data, of the capability of CFD simulations to predict free-surface turbulent flow inside a pilot-scale mechanically-agitated vessel within the frame of an integrated approach.

The CFD data are first globally and locally characterized by means of statistical analyses, including the estimation of characteristic turbulent length scales. Then, these numerical outputs are reduced to the most relevant dynamics, thus allowing the comparison between different approaches and the identification of key physical phenomena. To this end, two decomposition techniques are applied to the present case: Proper Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD). Both methods are complementary and highlight different physical features (Schmid et al. (2012), Semeraro et al. (2012), Sakowitz et al. (2014), de Lamotte et al. (2018), Weheliye et al. (2018)): POD evidences the most energetic structures while DMD evidences structures characterized by a single frequency and their associated expansion rate. All numerical outcomes are presented and compared with experimental results which were analyzed in previous works (de Lamotte et al. (2017), de Lamotte et al. (2018)).

2. Material and Methods

2.1. Stirred-tank configuration

The stirred tank considered for the CFD approach and its comparison with experiments corresponds to a standard configuration of bioreactor used for fermentation experiments and already described in previous works (Delafosse et al. (2014), de Lamotte et al. (2017)). The system, depicted in Fig.1, consists of a flat-bottomed cylindrical tank of diameter $T = 0.22$ m, with four equally-spaced baffles and agitated by two four-blade Rushton turbines of diameter $D \approx 0.5T = 0.1$ m. The vessel is filled with water up to $2T = 0.44$ m at room temperature (20°C: density $\rho_L = 998 \text{ kg}\cdot\text{m}^{-3}$, kinematic viscosity $\nu_L = 1.002\cdot 10^{-6} \text{ m}^2\cdot\text{s}^{-1}$) and atmospheric pressure, which corresponds to a working volume $V = 16.5$ L. All simulations and experiments are performed at a rotational speed, $N = 300 \text{ rpm} = 5 \text{ s}^{-1}$, corresponding to a Reynolds number, $Re = 47\,125$.

Figure 1: Front and top views of the computational domain

2.2. Computational Methods

To represent the stirred-tank configuration, a finite-volume mesh is generated using ANSYS DesignModeler and ANSYS Meshing, explicitly including the baffles and Rushton turbine geometries.

The computational domain is divided into two zones, as illustrated in Fig.2. The first one, the "moving" zone, consists of two inner cylindrical regions enclosing the impellers, with a height of 0.1 m and a diameter of 0.12 m. The second one, the "fixed" zone, represents the remaining part of the tank.

In theory, the density of cells in a mesh must be fine enough to capture all flow details, but, in practice, the overall number of cells in the domain has to be limited to keep computational time in a reasonable range. A non-uniform structured mesh is used. It is refined in the impellers regions and around the gas-liquid interface location. The grid in the "moving" zone contains over 470 000 hexahedrons with a minimum edge size between 0.0125 and 0.6 mm with an average of 0.33 mm to better resolve this highly turbulent region. The rest of the tank contains approximately 870 000 hexahedrons with a coarser grid

size, between 0.01 mm and 1.2 mm with an average of 0.55 mm. The total number of grid elements is larger than $1.4 \cdot 10^6$ with average orthogonal quality and aspect ratio of 0.99 and 3.5, respectively.

The grid analysis has not been performed but, on the basis of published works (Aubin et al. (2004), Deglon and Meyer (2006), Coroneo et al. (2011)), the mesh may be assumed as fine enough.

Figure 2: Front and top views of the computational grid

The numerical simulation of the free-surface turbulent flow within the baffled stirred-tank is based on an Euler-Euler multiphase approach, the Volume of Fluid (VOF) model. It is a surface-tracking technique applied to a fixed Eulerian mesh and designed to determine the position of the interface between two immiscible fluids. The two fluids, air and water (surface tension coefficient $\sigma = 0.0735 \text{ N}\cdot\text{m}^{-1}$), share a single set of momentum equations, and the volume fraction of each fluid is tracked throughout the computational domain. The resulting velocity field is shared by both phases. Based on local values of the volume fractions of the liquid α_L and gas α_G phases, the appropriate properties and variables are assigned to each control volume within the domain.

The incompressible flow inside the tank is then computed by solving the Reynolds-Averaged Navier-Stokes (RANS) continuity and momentum conservation equations for the two-fluid mixture in conjunction with a turbulence closure model using the ANSYS Fluent software (v.18, ANSYS (2017)):

$$\frac{\partial}{\partial t} \rho_m + \nabla \cdot (\rho_m \bar{\mathbf{U}}) = 0 \quad (1)$$

$$\frac{\partial}{\partial t} (\rho_m \bar{\mathbf{U}}) + \nabla \cdot (\rho_m \bar{\mathbf{U}} \bar{\mathbf{U}}) = -\nabla \bar{p} + \nabla \cdot (\mu_m \nabla \bar{\mathbf{U}} - \boldsymbol{\tau}_t) + \rho_m \mathbf{g} + \mathbf{F} \quad (2)$$

where $\bar{\mathbf{U}}$ is the Reynolds-averaged (mean) component from the Reynolds decomposition of the instantaneous velocity $\mathbf{U}$, $\bar{p}$ is the mean pressure, $\mathbf{g}$ is the gravitational acceleration, $\mathbf{F}$ is the body force due to the surface tension acting on the gas-liquid interface; and ρ_m and μ_m are the volume-averaged mixture den-

sity and viscosity:

$$\begin{aligned} \rho_m &= \alpha_L \rho_L + \alpha_G \rho_G \\ \mu_m &= \alpha_L \mu_L + \alpha_G \mu_G \end{aligned} \quad (3)$$

The Reynolds stress $\boldsymbol{\tau}_t$ is obtained using the Realizable $k - \varepsilon$ (Rke) model with the enhanced wall treatment. It is worth noting that other turbulence closure models have been tested: the Shear-Stress Transport $k - \omega$ (SST- $k\omega$) model and the non-linear Reynolds Stress Model (SSG-RSM). Both have presented important convergence and stability issues even when modifying simulation parameters (mesh, pressure-velocity coupling algorithm, discretization schemes ...). Moreover, the SSG-RSM model required a significantly more expensive computational effort.

The VOF model formulation (ANSYS, 2017) assumes that the two fluids are not interpenetrating, *i.e.* in most computational cells, α_L and α_G are either 1 or 0. The tracking of the moving interface between the gas and liquid phases, characterized by $0 < \alpha_L < 1$ and $0 < \alpha_G < 1$, is carried out by solving the following advection equation for the volume fraction of the secondary phase, *i.e.* the gas phase α_G :

$$\frac{\partial}{\partial t} \alpha_G + \nabla \cdot (\alpha_G \bar{\mathbf{U}}) = 0 \quad (4)$$

The volume fraction of the liquid phase (the primary phase), is calculated with the constraint on the phase volume fractions:

$$\alpha_L + \alpha_G = 1 \quad (5)$$

The interface is then represented by means of the geometric reconstruction (Geo-Reconstruc) scheme which uses a piecewise linear approach (ANSYS, 2017).

To account for impeller rotation, two approaches are adopted (Jaworski et al. (2000), Bujalski et al. (2002), Aubin et al. (2004), Lane (2017)). The first one is the Moving Reference Model (MRF), where the "moving" zone remains in a single fixed position but is placed in a rotating frame of reference, such that the Rushton turbines appear steady. The second approach is the Sliding Mesh (SM) model in which the "moving" zone physically moves during the equation resolution with small angular steps. The SM model is the most realistic solution method for stirred-tank simulations as it accounts for transient impeller-baffle interactions. However, it is more computationally demanding.

The stirring system is initially set at rest. The bottom part of the computational domain was filled with water up to $2T = 0.44 \text{ m}$. The remaining region was patched with air.

The no-slip wall boundary condition is applied at all walls, while the top boundary of the domain is considered as a pressure outlet zone with a backflow volume fraction of air fixed to 1.

The PISO algorithm (ANSYS, 2017) is adopted to couple the continuity and momentum equations. The momentum, turbulence and volume fraction equations are discretized with the second-order upwind scheme, and the pressure term with the PRESTO! scheme (ANSYS, 2017). The first-order implicit time-stepping formulation (ANSYS, 2017) is used for time discretization. The simulations are thus performed in transient mode,

with a time step of 0.000625 s which corresponds to a 1.125° impeller rotation per time step.

The completion of each simulation occurs based on two main criteria. Firstly, a steady (MRF) or cyclically repeating (SM) pattern is obtained and becomes constant (MRF) or steady (SM) with further time steps for local velocity magnitude, volume-averaged turbulent dissipation rate in the "moving" zone and moment coefficients from the impeller shaft. Secondly, the scaled residuals of all conservation equations have to be reduced to less than 10^{-5} at the end of each time step.

2.3. Experimental Methods

All experiments are performed in a transparent Plexiglas vessel, installed in a rectangular transparent Plexiglas container filled with tap water thermoregulated at 20°C. This surrounding container also minimizes optical distortions due to the curvature of the cylindrical wall during PIV measurements. This stirred-tank reactor has already been experimentally characterized in previous studies (Delafosse et al. (2014), de Lamotte et al. (2017)). All these experimental results are used in the present paper to assess the capabilities of the CFD modeling approach. The corresponding measurement technique is briefly described below.

The experimental set-up for PIV measurements consists of an optical equipment designed for vessel illumination and image detection detailed in an earlier work (de Lamotte et al., 2017). Measurements are performed on a vertical plane passing through the impeller axis and located at an angle of 12.5° behind one of the baffles. To visualize the flow over the entire height of the tank while maintaining a spatial resolution small enough to correctly characterize the turbulent flow, PIV measurements are performed simultaneously with two cameras with their optical axis perpendicular to the laser sheet: one for the bottom of the tank and the other one for the top.

The liquid instantaneous radial and axial velocity fields, $U_r(r, z, t)$ and $U_z(r, z, t)$, are determined using the PIV technique. The fluid is seeded with inert polyamide particles (density $\rho_p = 1030 \text{ kg}\cdot\text{m}^{-3}$, mean diameter $d_p = 5 \text{ }\mu\text{m}$). Their positions are recorded at $f_{\text{acq}} = 16 \text{ Hz}$ ($\Delta t = 0.0625 \text{ s}$) on 3 sets of 725 image pairs. An instantaneous velocity field is extracted from each image pair. The spatial resolution of the velocity fields equals 0.6 mm.

Due to current limitations of PIV system in terms of time resolution, measurements are necessarily limited to the details they are able to capture. In stirred vessels, in the impeller region, the flow field is characterized by two kinds of fluctuations: a periodic component due to the impeller blades passage, and the real turbulent fluctuations of the overall flow field. For $N = 300 \text{ rpm}$, the organized periodic flow motion is consequently associated with the blade passage frequency $f_{\text{BPF}} = N_{\text{blades}} \cdot N = 4 \cdot 5 = 20 \text{ Hz}$. Therefore, in the frame of signal analysis, data acquisition is not properly sampled. Indeed, the Nyquist sampling criterion requires that the data should be sampled at a rate that is at least twice the highest frequency to avoid aliasing effects (actual modification of frequencies). However, it should not be interpreted too pessimistically. In some cases, a signal can be sampled more slowly than the

Nyquist frequency, especially when the nature of the signal is known as shown in a previous work (de Lamotte et al., 2018). The potential alias frequency f_{alias} of the periodic signal related to the blade passage at the given sampling rate f_{acq} is predicted by:

$$f_{\text{alias}} = |f_{\text{BPF}} - (n \cdot f_{\text{acq}})| \quad (6)$$

where $(n \cdot f_{\text{acq}})$ is the integer multiple of the sampling rate closest to the input signal frequency. The 20 Hz signal, sampled at $f_{\text{acq}} = 16 \text{ Hz}$, is expected to pose as a 4 Hz signal.

2.4. Processing Methods

The modal decomposition techniques, POD and DMD, are briefly introduced in this section. More details may be found in a previous paper (de Lamotte et al., 2018) and in the literature, *e.g.* POD by Sirovich (1987), Berkooz et al. (1993), Chatterjee (2000), Liné et al. (2013) and Liné (2016), and DMD by Rowley et al. (2009), Schmid (2010), Schmid (2011), Schmid et al. (2011) and Tissot et al. (2014).

The main goal is to analyze, in parallel, the spatial structures and their time evolution in a given data set to identify their dominant behaviors. The dataset of velocity fields $\mathbf{U}(r, z, t)$, obtained experimentally or numerically at a given frequency f_{acq} , are represented as a sequence of snapshots, *i.e.* N snapshots $\mathbf{U}_k(r, z)$ where k is the index of the instantaneous event ($k \in [1, N]$). POD and DMD techniques decompose this data ensemble into time amplitudes $\theta(t)$ and spatial modes $\phi(r, z)$:

$$\mathbf{U}(r, z, t) = \sum_{i=1}^N \theta_i(t) \phi_i(r, z) \quad (7)$$

To do so, the snapshot sequence needs to be properly written out. The N snapshots $U_{rk}(r, z)$ and N snapshots $U_{zk}(r, z)$ are assembled column-wise in a $2RC \times N$ snapshot matrix, where R and C are, respectively, the numbers of rows and columns in the investigated (r, z) -plane.

2.4.1. Proper Orthogonal Decomposition

The POD technique can be considered as a purely statistical method based on the identification of the orthogonal modes that best reconstructs the whole dataset, to capture the energy contained as much as possible. The goal of this technique is the extraction of energetic information, *i.e.* the identification of the most energetic spatial structures from a given snapshot sequence.

A spatial correlation matrix is formed from the snapshot matrix. The main objective is to solve the eigenvalue problem of such a covariance matrix to capture a maximal energy content in each identified spatial structure while simultaneously maintaining a zero correlation between all of them. The results of POD analysis comprise eigenvalues λ^{POD} and eigenvectors ϕ^{POD} . The eigenvectors represent the transport spatial structures whose energies are given by the corresponding eigenvalues. The POD algorithm and associated procedural steps are given in a previous work (de Lamotte et al., 2018).

2.4.2. Dynamic Mode Decomposition

The DMD technique is based on the eigendecomposition of a best-fit linear operator that approximates the dynamics present in the data. The snapshots are assumed to be generated by a linear dynamic system, which implies that the extracted basis is characterised by growth rate and frequency content of the snapshots.

A linear time operator is assumed between the successive concentration fields. The main objective is to solve the eigenvalue problem of such an operator to establish the time stability, *i.e.* time growth or decay, of various spatial transport structures. The results of DMD analysis comprise complex eigenvalues and eigenvectors. The eigenvector ϕ^{DMD} corresponding to each eigenvalue indicates the spatial structure. The real part of the eigenvalues ($\Re\{\lambda^{\text{DMD}}\}$) shows the growth rate g and the imaginary part ($\Im\{\lambda^{\text{DMD}}\}$) indicates the frequency f . The DMD algorithm and associated procedural steps are detailed in an earlier study (de Lamotte et al., 2018).

3. Results and Discussion

3.1. Description of the flow fields

The CFD simulations of the multiphase turbulent flow in the tank are validated by comparing the mean and r.m.s. turbulent velocity components on a vertical plane and on a vertical profile ($r = 0.055$ m) with 2D-PIV results. These experimental and numerical results have been determined through an ensemble-averaged treatment corresponding to complete rotations of the impellers.

Fig. 3 presents the magnitude of the velocity vectors $\sqrt{\overline{u_r^2} + \overline{u_z^2}}$, computed from CFD/MRF (a) and CFD/SM (b) simulations, and from 2D-PIV measurements (c). All three velocity fields, normalized by ND , reveal the typical flow pattern observed for the dual impeller Rushton turbine configuration: a stream is radially discharged from each turbine with a maximum velocity magnitude of *ca.* $1.8 \cdot ND$. These flow streams are then swept up and down because of the presence of the baffles to form two large circulation loops in the vessel. The CFD/MRF contour plot (Fig.3(a)) clearly shows the dependence of such modeling approach on the fixed position of the Rushton turbines. The CFD/SM simulation (Fig.3(b)) reproduces satisfactorily the mean velocity field and the circulation loops generated by both impellers are very well predicted. These observations are confirmed by the comparison of the dimensionless vertical profiles of the radial and axial mean velocity vectors, $\overline{u_r}/ND$ and $\overline{u_z}/ND$, reported in Fig. 5(a) and (b) from both experiments and simulations. The numerical results predict the mean radial velocity component very well. However, they estimate a bit more poorly the vertical evolution of the axial velocity component, especially for CFD/MRF modeling approach due to impeller steadiness (Fig. 5(b)).

Fig. 4(a) and 4(b) present the r.m.s. turbulent velocity field computed from the turbulent kinetic energy k solved by the CFD/MRF and CFD/SM simulations respectively, while Fig. 4(c) and 4(d) display the radial $\sqrt{\overline{u_r^2}}$ and axial $\sqrt{\overline{u_z^2}}$ r.m.s. turbulent velocity components calculated from 2D-PIV measure-

ments. All the fields shown are normalized by ND . The regions of highest r.m.s. fluctuating velocity fields are in the impellers discharge. In most parts of the tank, the rms turbulent velocity, in both experiments and simulations, exhibits similar trends. The determination of the r.m.s. turbulent velocity from CFD results is based on the hypothesis of isotropic turbulence, which is probably not entirely valid in all the reactor volume. Indeed, the two experimental r.m.s. components differ in certain zones, indicating that turbulence is not locally isotropic. For instance, turbulence seems isotropic in the region of the liquid jet axis but anisotropic in several regions really close to the impeller (close to the disc and the impeller tip) or the axis. These observations agree with results from experimental studies of anisotropy of the flow field inside tanks stirred by a Rushton turbine (Derksen et al. (1999), Galletti et al. (2004), Escudié and Liné (2006)). It is worth noting that PIV results may undergo some local inaccuracies because of the laser reflections on the free-surface and on the baffle located just behind the measurement plane. These observations are confirmed by the comparison of the dimensionless vertical profiles of r.m.s. turbulent velocity computed from the 2D-PIV data and the CFD simulations reported in Fig. 5(c). CFD simulations correctly predict the total kinetic energy away from the impeller, but slightly over-predict its value close to the blades. This is due to the well-known defect of $k - \varepsilon$ models that results in an over-prediction of the turbulent kinetic energy at stagnation points (Delafosse et al., 2014).

Hydrodynamics consists of turbulent flow structures of various length and time scales whose relative contributions to the interfacial transfer rate and to the mixing of scalar quantities such as dissolved gas concentration depend on the equipment-scale. The continuous range of length-scales extends from the tank diameter T over at least three orders of magnitude down to the Kolmogorov scale η .

On the basis of Kolmogorov's hypotheses, it is possible to estimate the spatial distributions of three characteristic turbulent length scales from the CFD prediction of turbulent kinetic energy k and its rate of dissipation rate ε : the Taylor macro-scale (or integral scale) Λ (Eq.(8)) and micro-scale λ (Eq.(9)), and the Kolmogorov scale η (Eq.(10)). The Taylor macro-scale corresponds to the size of the most energetic structures. These large scales are generally not statistically isotropic, since they are determined by the particular geometrical features of the flow and its boundaries. The Taylor micro-scale is an intermediate one between the largest and smallest turbulent scales, and corresponds to the minimum size of eddies that significantly contributes to the turbulent kinetic energy. These small eddies are less dependent on the agitation system and tend to be more isotropic. The Kolmogorov scale η is the scale at which the turbulent kinetic energy is dissipated as heat. Although they rest on the theory of homogeneous isotropic turbulence, Equations 8, 9 and 10 provide practically-useful length scale estimates for characterising the turbulent eddies (Baldi and Yianneskis, 2004).

$$\Lambda = A \frac{k^{\frac{3}{2}}}{\varepsilon} \text{ with } A = \text{adjustable constant} \sim 1 \quad (8)$$

Figure 3: Comparison of CFD with PIV for the dimensionless magnitude of the mean velocity components $\sqrt{u_r^2 + u_z^2}$ on a vertical plane: CFD/MRF (a), CFD/SM (b), PIV (c)

Figure 4: Comparison of CFD with PIV for the dimensionless r.m.s. velocity components on a vertical plane: CFD/MRF $\sqrt{u_r^2} = \sqrt{2k/3}$ (a), CFD/SM $\sqrt{u_r^2} = \sqrt{2k/3}$ (b), PIV - radial $\sqrt{u_r^2}$ (c) and PIV - axial $\sqrt{u_z^2}$ (d)

Figure 5: Comparison of CFD with PIV for the dimensionless mean and r.m.s. velocity components on a vertical profile ($r = 0.055$ m): radial mean component $\overline{U}_r/ND$ (a), axial mean component $\overline{U}_z/ND$ (b), r.m.s. component $\sqrt{u_i^2}/ND$ (c)

$$\lambda = \sqrt{\frac{10\nu_L k}{\varepsilon}} \quad (9)$$

$$\eta = \left(\frac{\nu_L^3}{\varepsilon}\right)^{\frac{1}{4}} \quad (10)$$

As proposed by Taylor (Taylor, 1935) and detailed in literature (Bugay (1998), Escudié and Liné (2003), Khan et al. (2004), Micheletti et al. (2004), Gabriele et al. (2009)), spatial autocorrelation functions of the experimental velocity fields were used to estimate the distributions of two characteristic length scales (de Lamotte et al., 2017): the longitudinal integral length-scales Λ_{rr} and Λ_{zz} , and the longitudinal Taylor micro length-scales λ_{rr} and λ_{zz} . On the basis of their definitions, these longitudinal length scales have a direct physical significance (Hinze (1959), Jakobsen (2008)). To accurately deduce the spatial distribution of η , the PIV spatial resolution should be equal to or smaller than η . The mean Kolmogorov scale over the whole vessel $\bar{\eta}$ can be estimated from the global dissipation rate $\bar{\varepsilon}_V$ using Equation (10). The latter quantity is deduced from measured values of the mechanical torque M exerted on the impeller shaft (Eq.11) and is equivalent to $0.45 \text{ m}^2\cdot\text{s}^{-3}$. The corresponding Kolmogorov scale is found to be *ca.* $40 \mu\text{m}$.

$$\bar{\varepsilon}_V = \frac{P}{\rho_L V} = \frac{2\pi N M}{\rho_L V} \quad (11)$$

The smallest scales of turbulence cannot be thus determined from the present PIV data as the spatial resolution ($\Delta x = 0.6 \text{ mm}$) corresponds to *ca.* 15 times the mean Kolmogorov scale. Fig. 6 shows the integral length-scale Λ maps within a vertical plane. The first two spatial fields correspond to those predicted from CFD/MRF (a) and CFD/SM (b) simulations by means of Equation 8. They have been estimated with a scaling constant $A = 2/3$, which has been fixed to best fit 2D-PIV data. This value for A is consistent with those in the literature which have been set to 0.5 (Trad et al., 2017) or 1 (Escudié and Liné, 2003). The CFD macro-scales account for the three components, including the tangential one which is not available from the present 2D-PIV measurements. In this regard, the experimental average macro-length scale (c) has been evaluated from available information, *i.e.* the longitudinal integral length-scales Λ_{rr} and Λ_{zz} (de Lamotte et al., 2017), as follows:

$$\Lambda = \sqrt{\frac{3}{2} (\Lambda_{rr}^2 + \Lambda_{zz}^2)} \quad (12)$$

The experimental and computational data present comparable trends for their spatial patterns and distributions, with maximal values located near the liquid free-surface. These results are coherent with the hydrodynamics associated with the agitation configuration, *i.e.* the (axial) influence of the baffles on the (radial) flow generated by the Rushton turbines. The numerical mean size of large eddies are equal to $\bar{\Lambda} = 0.0201 \text{ m}$ and are nearly equivalent to the experimental value $\bar{\Lambda} = 0.0212 \text{ m}$. The discrepancies observed between PIV and CFD results are explained by their calculation methods. Moreover, numerical predictions rely on the local values of k and ε and are consequently subject to some uncertainties. Indeed, both turbulent quantities,

in particular ε , are not accurately approximated in the impeller-swept volume and discharge by RANS $k - \varepsilon$ models.

Fig. 7 shows the Taylor micro length-scale λ maps within a vertical plane. The first two spatial fields correspond to those predicted from CFD/MRF (a) and CFD/SM (b) simulations by means of Equation 9. As for the integral scale Λ , the experimental average micro-length scale λ (c) has been evaluated from available information, *i.e.* the longitudinal Taylor micro length-scales λ_{rr} and λ_{zz} (de Lamotte et al., 2017). Spatial patterns of experimental and computational micro-scales present higher values in the vicinity of the liquid free-surface although both differ from each other in the zones of the impeller stream. Numerical Taylor micro-scales roughly lie between 0.5 mm and 2.5 mm within the vertical plane with $\bar{\lambda} = 1.6 \text{ mm}$. It is worth noting that the experimental values are between 0.5 mm and 5 mm , with $\bar{\lambda} = 2.5 \text{ mm}$; which is coherent with the spatial resolution of the PIV technique ($\Delta x = 0.6 \text{ mm}$). The differences noticed between PIV and CFD results are explained by their definitions and the dependence of CFD results on the local values of k and ε .

Information on energy consumption can be obtained from CFD simulations. Indeed, the power number P_0 associated with the agitation configuration can be estimated either from the calculation of the mechanical torque M exerted on the impeller shaft as performed experimentally, or by integrating the dissipation rate over the computational domain to estimate the specific energy dissipation rate $\bar{\varepsilon}_V$. The power number P_0 associated with the agitation configuration can thus be obtained as it is related to these two global parameters:

$$P_0 = \frac{P}{\rho_L N^3 D^5} \text{ with } P = 2\pi N M = \bar{\varepsilon}_V \rho_L V \quad (13)$$

The CFD predictions and experimental measurements are presented in Table 1. The calculations based on the torque give better results, *i.e.* values close to the experimental ones. The ε integration method leads to an under-prediction of the dissipation rate and consequently of the power number. This can be attributed to the limitations of the $k - \varepsilon$ models. Indeed, while the turbulent kinetic energy k is relatively well predicted (except for the over-prediction at stagnation points), it is known that the spatial distribution of the turbulence dissipation rate ε is not correctly approximated (Delafosse et al., 2008).

Table 1: Comparison of CFD with global measurements for the prediction of the power number P_0 of the agitation configuration

	Power number P_0 [-]	
	from M	from $\bar{\varepsilon}_V$
CFD - MRF	6.5 ($M = 0.260 \text{ Nm}$)	3.6 ($\bar{\varepsilon}_V = 0.273 \text{ m}^2\text{s}^{-3}$)
CFD - SM	6.7 ($M = 0.267 \text{ Nm}$)	3.6 ($\bar{\varepsilon}_V = 0.276 \text{ m}^2\text{s}^{-3}$)
Experiments	5.9 ($M = 0.235 \text{ Nm}$)	-

From this description of the flow fields, simulations seem to satisfactorily report the complex physics of the flow within a

Figure 6: Comparison of CFD with PIV for the integral length scale maps in a vertical plane: longitudinal macro length-scales Λ predicted by CFD/MRF (a) and CFD/SM (b) simulations, and Λ (c) estimated from PIV measurements

Figure 7: Comparison of CFD with PIV for the Taylor micro length-scale maps in a vertical plane: longitudinal Taylor micro length-scales λ predicted by CFD/MRF (a) and CFD/SM (b) simulations, and λ (c) estimated from PIV measurements

baffled stirred-tank. The RANS approach can predict mean values ($\overline{U}$, $\overline{u'^2}$ and M) quite well, but fails to accurately estimate values of turbulent quantities, in particular the energy dissipation rate ε , and derived quantities ($\overline{\varepsilon_v}$, Λ and λ). Even so, the spatial distributions of all local quantities ($\overline{U}$, $\overline{u'^2}$, Λ and λ) computed from CFD simulations agree relatively well with those observed with 2D-PIV experiments.

These comparisons based on statistical considerations do not relate the discrepancies to the CFD capabilities to identify the most relevant dynamic features. Indeed, the hydrodynamic fields obtained with both modeling techniques for impeller rotation (MRF and SM), are found to be almost the same, while the MRF method only provides a snapshot of the flow with the impeller fixed in a single position. Previous works also using $k - \varepsilon$ models (*e.g.* Montante et al. (2001a), Aubin et al. (2004), Lane (2017)), have already observed that the difference between the ensemble-averaged flow fields and values calculated with the stationary (MRF) and the time-dependent (SM) approaches may be negligible. Nevertheless, the SM approach better represents the local evolution of hydrodynamic quantities. Indeed, although the velocity fields appear very similar (Fig.3 and 4), the associated profiles (Fig.5) evidence major differences.

3.2. Analysis of the flow dynamics

This section aims at giving a deeper comparison, relative to the dynamic behavior, between numerical and experimental results on the basis of the properties of their POD and DMD analyses. The two modal decomposition methods are applied without subtracting the mean flow from the data. It is worth noting that POD and DMD analyses of PIV velocity fields have been carried out and extensively discussed in a previous work (de Lamotte et al., 2018).

One has to keep in mind that the structures evidenced by POD analysis are those characterized by a given energy level, while structures associated with DMD modes are characterized by a given frequency. In general, DMD and POD analyses should thus lead to different, but complementary, information about the flow. However, the modes obtained with the two methodologies tend to be similar when the flow behaves as a periodic oscillator (Schmid et al. (2012), Semeraro et al. (2012)), which is the case in the present study. Indeed, the flow field inside the stirred-tank is unsteady not only due to turbulence, but also to impeller rotation, including the periodic passage of the impeller blades in front of the baffles. POD and DMD analyses are consequently performed only for the SM modeling approach as the MRF one does not account for transient impeller-baffle interactions.

Concerning the CFD simulations, any acquisition frequencies can be used, but the time step needs to be kept to a minimum to accurately capture the smallest time scales. It is clear that the time interval between two consecutive snapshots can be very important for modal decomposition methods, but the aim of the present work is to assess the capabilities of CFD data to account for the flow behavior on the basis of comparison with experimental datasets. For that reason, POD and DMD

have been performed on the radial and axial velocity fields extracted with different time intervals from CFD/SM simulation: 0.0625 s ($f_{\text{acq}} = 16$ Hz) as it was the time resolution for PIV, and 0.00125 s ($f_{\text{acq}} = 800$ Hz). The latter time interval corresponds to twice the CFD time step used to perform the transient simulations.

Due to current limitations of computing resources and the present state of development of turbulence models, simulations are necessarily limited in the detail they could capture. Work has been done to investigate RANS turbulence models for unsteady flows. Menter and Egorov (2010) have shown that when used in transient mode the $k - \varepsilon$ produces single-frequency unsteady features (Howard et al., 2017). Indeed, unsteady classical RANS models average out all turbulent fluctuations and resolve only frequencies far lower than those of turbulent fluctuations. It is expected that the $k - \varepsilon$ model mainly reproduces the single frequency of the vortex shedding (and its overtones), *i.e.* the blade passage frequency $f_{\text{BPF}} = N_{\text{blades}} \cdot N = 4 \cdot 5 = 20$ Hz. As detailed in Section 2.3, due to the Nyquist criterion, the 20 Hz signal corresponding to the blade passage frequency f_{BPF} , sampled at 16 Hz either by PIV or CFD, is expected to be masquerading as a 4 Hz signal. The time step $\Delta t = 0.00125$ s is forty times smaller than a typical shedding cycle and is assumed to be fine enough to accurately apprehend the smallest time scales of the flow.

3.2.1. POD

The POD eigenvalues correspond to the contribution of each mode to the total kinetic energy in the observed vertical plane. The energy content of the modes is expressed as a percentage of the total energy contained in all modes together from data acquired at $N = 300$ rpm for both experimental and numerical datasets. Fig. 8(a) zooms in on the percentage of the total energy contained in the first five hundred most energetic POD modes, and Fig. 8(b) on the first six ones. As the mean has not been removed from the velocity fields, this first mode mainly corresponds to the mean flow. Most of the energy is consequently contained in the first mode ϕ_1^{POD} : about 90% for CFD and 70% for PIV. Modes ϕ_2^{POD} and ϕ_3^{POD} contain around 90% and 98% of the remaining energy for modes for CFD/SM - 16 Hz and CFD/SM - 800 Hz results respectively, and about 6.5% for PIV results.

Both CFD datasets differ not only due to their time intervals ($f_{\text{acq}} = 16$ Hz *vs.* $f_{\text{acq}} = 800$ Hz) but also to the number of snapshots ($N = 385$ *vs.* $N = 19\,200$). The energy content is expected to be better assessed, and is distributed over a larger number of POD modes with the CFD/SM - 800 Hz set. As detailed in Section 2.4 (Eq.(7)), the number of modes is indeed equal to the number of snapshots. It is worth noting that the number of snapshots has been limited because of limitations due to computing memory and CFD simulation time.

Only the first three CFD modes have a significant contribution to the total energy. The lower energetic content of the higher-order computational POD modes is mainly due to the fact that RANS simulations do not feature turbulent fluctuations or noise. It can be seen that the higher-order experimental modes tend to follow a $(-11/9)$ power scaling (black line, Fig.

Figure 8: Comparison of CFD with PIV for POD eigenvalues spectrum of velocity fields with different acquisition frequencies: percentage of the total energy in the first 500 modes (a) and in the first six modes (b)

8(a)), which is a characteristic of inertial range of turbulence (Sirovich (1987)). In the experiments, periodicity is affected by disturbance or turbulence in the impellers stream and more modes are required to express the flow fields with accuracy. In other words, energy is shared over a larger number of modes.

The time behavior of a mode is described by the POD time coefficients $\theta_i^{\text{POD}}(t)$. Fig. 9 shows the frequency content of seven POD modes ($i = 1 \mapsto 6$ and 50) for CFD and PIV results. The frequency analysis is performed using the Lomb-Scargle method as it is able to detect a periodic signal in noisy data and to accurately determine the single and multiple frequencies that may be expected or not (Roussinova et al., 2004). It is worth noting that, as a consequence of its optimization principle, POD does not necessarily separate the flow into its frequency content. Therefore, one mode often encompasses several frequencies and several physical phenomena.

For experimental and numerical cases, the first POD mode contains not only the mean field, but also pulsations at f_{BPF} , *i.e.* at $f = 4$ Hz for CFD/SM - 16 Hz and PIV, and at $f = 20$ Hz for CFD/SM - 800 Hz. The spectral content of all other CFD POD modes is also characterized, as expected, by these frequencies. Although a first inspection of the spectrum shows no obvious coupling between some of the first modes, their time evolution contains more information and reveals interesting features. POD coefficients θ_2^{POD} and θ_3^{POD} , from numerical data as well as from experimental ones, present the highest amplitudes at f_{BPF} and its upper partials. Higher POD modes from CFD display a less and less time behavior pronounced, while the modes θ_5^{POD} and θ_6^{POD} from PIV have a peak at $f = 5$ Hz, not observed on CFD POD modes.

The sharp peaks detected in CFD periodograms are thus produced by the coherent, periodic vortex shedding induced by the blade motion. The unsteady RANS computation contains energy at this frequency and its overtones. This contribution to the unsteady energy is computed explicitly along with the mean flow. Although CFD/SM - 16 Hz results correspond to a quite large time step, they seem adequate to capture the flow behavior. Indeed, the CFD/SM - 800 Hz dataset does not evidence any additional information.

Nonetheless, the periodic behavior of the flow generated by the impellers is more complex (not a single frequency) and small-scale structures are present within the tank. PIV experiments capture much more physical behavior than RANS simulations. They give more detail while identifying another frequency besides f_{BPF} as the time coefficients $\theta_5^{\text{POD}}(t)$ and $\theta_6^{\text{POD}}(t)$ have clear peaks at the rotating speed $f = 5$ Hz = N (de Lamotte et al., 2018).

The spatial characteristics of the first four POD modes are illustrated in Fig. 10 for CFD/SM - 16 Hz (a), CFD/SM - 800 Hz (b) and PIV (c) results.

The first POD mode (POD mode 1) is characteristic of the mean flow contribution. The velocity fields associated with this first mode can be reconstructed for both experimental and numerical data, and are presented in Fig. 10 (first column) as the magnitude of the mean velocity vectors normalized by ND . The results are rather identical; the velocity field associated with the first POD mode fully corresponds to the mean flow.

The remaining modes are related to the fluctuating part of the flow field. Previous studies (*e.g.* Ducci et al. (2008), Liné et al. (2013), Liné (2016)) have shown that POD makes it possible to decompose the fluctuating term into an organized periodic component associated with the impeller rotation and a random turbulent component. The magnitudes of the first three other POD modes, $|\phi_i^{\text{POD}}| = \sqrt{(\phi_{r,i}^{\text{POD}})^2 + (\phi_{z,i}^{\text{POD}})^2}$ ($i = 2 \mapsto 4$), are shown in Fig. 10 for both experimental and numerical data.

Concerning CFD data (Fig.10 (a,b)), the analysis of the spatial distribution of the modes gives further insights on the abilities of unsteady RANS simulations to describe the main dynamic flow features within the baffled stirred-tank. Comparison between the CFD datasets extracted with different time intervals shows that any acquisition is dominated by the first four modes ϕ_i^{POD} ($i = 1 \mapsto 4$), which hardly differ from each other regardless of the acquisition frequency f_{acq} . The contour plots of the norm of POD mode 2 suggest that this mode corresponds to the interaction between the two Rushton turbines and the organized periodic motions within the vessel. POD modes 3 and 4 exhibit symmetrically-organized structures with respect to each Rushton turbine plane and correspond to the pair of trailing vortices

Figure 9: Comparison of CFD with PIV for the first POD coefficients θ_i of velocity fields based on their Lomb-Scargle periodogram ($i = 1 \mapsto 6$ and 50): CFD/SM - 16 Hz and PIV (a), and CFD/SM - 800 Hz (b)

induced by the impeller blades. Indeed, because of the presence of a disk, two vortices are generated behind a Rushton turbine: above and below the disk. The second CFD mode seems related to the fourth PIV mode, while the third and fourth CFD modes appear very similar to the second and third PIV modes.

The analysis of the POD time coefficients has revealed that the experimental POD modes 5 and 6, not displayed here, do not have equivalent modes resulting from the decomposition of the numerical results. As detailed in an earlier study (de Lamotte et al., 2018), both modes are associated with the rotating speed and present vortical structures in the zone of the impeller discharge flow.

POD analysis of CFD velocity fields effectively captures the most energetic features of the agitation system, *i.e.* the mean and periodic components of the flow field. By retaining only these dominant modes, the dimensionality of the data can be reduced in order to only represent the main characteristics of the flow. An overall good agreement between experiments and simulations is found for the identification of the main energetic modes, *i.e.* the mean flow and the trailing vortices. CFD is not able to predict the energy-containing higher-order modes ($\phi_{i>4}^{\text{POD}}$). Their assessment is indeed difficult because of the limitations of $k - \varepsilon$ model and the lack of bijective relationship between single frequencies and POD modes.

3.2.2. DMD

The POD method is useful to compare modes among themselves but the physical insight of the flow dynamics provided by the method is limited. DMD is thus used to further investigate the spatio-temporal variation of the velocity fields.

As explained in Section 2.4.2, the DMD procedure leads to a decomposition into modes oscillating at single frequencies. The eigenvalues λ^{DMD} contain information about the dynamical behavior of their corresponding modes ϕ^{DMD} . To reveal these time data, the eigenvalues are transformed into frequencies f and associated expansion rate g . The Euclidean norm $\|\phi^{\text{DMD}}\|$

of the dynamic modes can be used to sort them along with their associated frequencies, which gives a basis for ordering them with respect to their relevance as the amplitude spectrum helps identify the modes associated with the most physically relevant phenomena. In order to identify the most relevant ones, the modes are consequently selected based on their expansion rate and their amplitude in order to discard strongly damped modes. This procedure is proven to determine the modes related to the mean ($f = 0$ Hz) and the blade passage (shedding) frequency ($f = f_{\text{BPF}}$), as the most relevant DMD modes (de Lamotte et al., 2018). Indeed, since the flow is originally periodical, the most important DMD modes should be characterized by a very small expansion rate, and their corresponding frequency should be the vortex shedding frequency and its higher harmonics.

Results of CFD/SM - 16 Hz (a), CFD/SM - 800 Hz (b) and PIV (c) datasets are shown in Fig. 11. In the $f - g$ spectra, the size and the color (from yellow = low to blue = high) of the symbol (circle marker) associated with each eigenvalue indicate the amplitude of the respective structure in the dataset. The results show a strong alignment along the zero-growth limit, *i.e.* $g = 0$ which represents the dynamically stable or stationary processes. On these spectra, one can observe an eigenvalue at the origin, which reveals the existence of a corresponding structure that is steady in time. It is the only one which is represented by a pure real function. The associated dynamic mode corresponds to the structure of the mean flow. All the other modes are complex, indicating that they are travelling wave-like structures. None of them lies exactly on the horizontal neutral line. However, some modes are characterized by small but non-zero expansion rate. The Euclidean norms $\|\phi^{\text{DMD}}\|$ are shown with the same coloring as for the $f - g$ spectra. Each mode is displayed with a vertical line scaled with the logarithm of its amplitude at its corresponding frequency. Specific dynamic modes are extracted by focusing on small damping rates and spatial coherence. This selection is based on the assumption that within the sampling period the corresponding structures are persistent and

Figure 10: Comparison of CFD with PIV for the magnitude of the POD modes on the observed vertical plane $\sqrt{(\phi_{r,i}^{\text{POD}})^2 + (\phi_{z,i}^{\text{POD}})^2}$ ($i = 1 \mapsto 4$): CFD/SM - 16 Hz (a) and CFD/SM - 800 Hz (b) and PIV (c)

Figure 11: Comparison of CFD with PIV for the dynamic mode spectra growth rate (g vs. frequency f spectra (upper row), and amplitude $\|\phi^{\text{DMD}}\|$ vs. frequency f spectra (lower row)): CFD/SM - 16 Hz (a), CFD/SM - 800 Hz (b) and PIV (c)

representative of the largest features of the flow. Both experimental and numerical datasets are in agreement with the POD findings. The highest peaks in the magnitude spectra, the DMD modes at $f = 0$ Hz laid aside, are seen near the passage blade frequency, or its alias, and its higher harmonics, *i.e.* at $f = 4$ Hz for CFD/SM - 16 Hz and PIV, and at $f = 20$ Hz for CFD/SM - 800 Hz. Moreover, the amplitude distribution of CFD - 800 Hz, like the PIV one, points out structures at $f = N = 5$ Hz and its overtones. One might think that the CFD/SM - 16 Hz set brings out other particular frequencies, multiples of 0.5 Hz. They seem to form a significant peak on the spectrum, centered on $f = 0$ Hz; which might imply that they are related to the mean flow field. Nonetheless, the corresponding spatial modes exhibit no clear patterns and are consequently not shown.

Two modes are at least required to accurately represent the physics: the mean mode $\phi_{f=0\text{Hz}}^{\text{DMD}}$ and the mode $\phi_{f=f_{\text{BPF}}}^{\text{DMD}}$. The dynamic mode associated with $f = 0$ Hz represents the structure of the mean flow and its time coefficient $\theta_{f=0\text{Hz}}$ is thus approximately constant. As for POD, the velocity fields associated with this mode can be reconstructed for both experimental and numerical data, and are presented in Fig. 12 (first column) as the magnitude of the mean velocity vectors normalized by ND . The results are identical; the velocity field associated with this DMD mode fully corresponds to the mean flow. The magnitude of the real and imaginary parts of DMD mode $\phi_{f=f_{\text{BPF}}}^{\text{DMD}}$, $|\phi_{f=i}^{\text{DMD}}| = \sqrt{(\phi_{r,f=i})^2 + (\phi_{z,f=i})^2}$, are shown in Fig. 12 for both numerical (a, b) and experimental (c) data. These fields based on DMD mode $\phi_{f=f_{\text{BPF}}}^{\text{DMD}}$ show symmetrically organized structures with respect to each Rushton turbine plane, which exhibit similar patterns for all datasets. The real part of this mode is characterized by large structures spanning the mean impeller jet flow;

the imaginary part is staggered due to the phase difference of 90° between them. Both parts, when combined with the time behavior of the mode, represent the pair of trailing vortices developed from the tips of each blade.

Because of the periodicity of the flow, the modal structures capturing fluctuations (POD) and the dynamically important features are similar. This mode $\phi_{f=f_{\text{BPF}}}^{\text{DMD}}$ closely resembles the POD modes (Fig.10) that are also characterized by this well-defined frequency: ϕ_3^{POD} and ϕ_4^{POD} for CFD, and ϕ_2^{POD} and ϕ_3^{POD} for PIV. The agreement between POD and DMD results is confirmed.

The CFD - 800 Hz and PIV datasets have both identified a spatial structure at $f = 5$ Hz = N . The other CFD results fail to evidence such a DMD mode due to the relatively low sampling rate. The $\phi_{f=N}^{\text{DMD}}$ patterns are presented in Fig. 12 (second and third rows), where the magnitude of the real and imaginary parts of these DMD modes are displayed.

The fields based on the DMD mode $\phi_{f=N}^{\text{DMD}}$ show vortical structures in the zone of the impeller discharge flow, which are quite similar not only between CFD and PIV, but also to the ones detected for PIV POD modes 5 and 6 (not shown here). However, the CFD DMD modes exhibit clear disturbances in the surroundings of the impeller walls. Two computational specificities can be the reasons for this numerical artifact. On the one hand, in these zones close to the Rushton turbines, the meshing is really fine and the time step used for the simulations was perhaps not small enough. On the other hand, one main limitation of $k-\varepsilon$ models is the modeling of the near-wall region. Indeed, it predicts a wrong behavior for k and ε near the solid walls.

These results show that DMD is a powerful tool for isolating structures when distinct frequencies are present in the flow field. With this method, it is possible to extract information on

Figure 12: Comparison of CFD with PIV for the magnitude of the DMD modes (real and imaginary parts) associated with f_{BPF} : CFD - 16 Hz (a), CFD - 800 Hz (b) and PIV (c)

the flow that is otherwise hard to visualize due to the interaction and to the superposition of different phenomena characterized by different dynamic behaviors. The direct comparison of the DMD results shows dominant modes at similar frequencies for the experimental and computational datasets, *i.e.* $f = 0$ Hz and $f = f_{\text{BPF}}$. The DMD mode shapes are in a good overall agreement although some discrepancies are found in the trailing vortices predictions. Time filtering has an impact on the CFD datasets: spatial structures detected at $f = 5$ Hz = N by PIV are identified only by the CFD dataset with the smallest time interval (CFD - 800 Hz).

4. Conclusion

To fully benefit from an integrated experimental and computational approach, quantitative comparisons between the respective results are required, so that numerical results could be validated by experimental data and in return experimental results can be enriched by numerical data. Although this is in most cases relatively trivial for global quantities, accurately comparing unsteady fields is much more challenging. Therefore, the objective of the present work was to assess the abilities of CFD to simulate free-surface turbulent flow within baffled stirred-tanks reactors, in particular to predict the spatial and time evolutions of its representative local quantities.

Transient simulations are carried out using a homogeneous Euler-Euler multiphase flow model with the Realizable $k - \varepsilon$ turbulence model. Two methods are considered to include impeller geometry and account for its motion, namely the Multiple Reference Frame (MRF) and Sliding Mesh (SM) approaches. All simulations are discussed based on comparison with detailed data relative to a large volume fraction of the stirred tank obtained by PIV.

Global and local CFD results are first introduced by means of statistical analysis. From this traditional description of the flow fields, simulations seem to partially report the complex physics of the processes within a baffled stirred-tank. Overall, apart from slight differences, simulations adequately predict the spatial distributions of the local characteristic hydrodynamics (velocity and Taylor length-scales) quantities. However, this kind of comparison between experimental and computational results do not relate the discrepancies to the CFD capabilities to identify the most relevant dynamic features.

Spatio-temporal numerical data obtained with the SM model are thus interpreted using modal decompositions methods, POD and DMD, in order to extract their dominant spatial structures along with their time behavior. DMD and POD analyses lead to different, but complementary, information about the three investigated physical phenomena. The spatial patterns evidenced by POD are characterized by a given energy level, while those associated with DMD modes are characterized by a given frequency.

POD analysis captures, on the whole, the dominant features of hydrodynamics inside the agitation system. Besides, by retaining only the dominant modes, the dimensionality of the data can be reduced in order to only represent the main characteristics of the flow. An overall good agreement between experiments and

simulations is found for the identification of the main energetic modes, *i.e.* the mean flow and the trailing vortices. CFD is not able to predict the energy-containing higher modes. Their assessment is indeed difficult because of the limitations of $k - \varepsilon$ models and the lack of bijective relationship between single frequencies and POD modes.

DMD is an efficient technique for isolating structures when distinct frequencies are present in the data fields. With this method, it is possible to extract information on the processes that is otherwise hard to visualize due to the interaction and to the superposition of different phenomena characterized by different dynamic behaviors. The direct comparison of the DMD results shows dominant modes at similar frequencies for the experimental and computational datasets, *i.e.* $f = 0$ Hz (mean field) and/or $f = f_{\text{BPF}}$ (blade passage frequency and its overtones) and/or $f = N$ (rotating speed).

Additionally, in the CFD simulations, the time step needs to be kept to a minimum to accurately capture the smallest time scales. It is clear that the time interval between two consecutive snapshots can be very important for modal decomposition methods. Given the aim of the present work, POD and DMD have been performed on data fields extracted with different time intervals from CFD simulations, in particular those matching the one used for PIV measurements. Experimental results are less sensitive to this time filtering. PIV effectively indicates the presence of coherent patterns that are only identified by the CFD dataset associated with the finest time resolution.

CFD is a powerful tool that can properly simulate the overall features of hydrodynamics in free-surface baffled stirred-tanks reactors. However, this modeling approach is very time consuming despite the progress in computing performance. Time-dependent simulations of scalar transport and transfer phenomena could take hours or even days depending on the grid size and the computer performance. Moreover, as it has been shown in this work and others, all these numerical results strongly depend on the limitations of the models used for turbulence and impeller rotation (Brucato et al. (2000), Jaworski et al. (2000), Bujalski et al. (2002), Yeoh et al. (2005), Hartmann et al. (2006)).

In many (bio)chemical processes, the interaction between physical and (bio)chemical phenomena is weak. If interest is only shown on macroscopic gradients, another suitable modeling approach can be therefore considered, *i.e.* a coarse-grained description of the fluid dynamics by means of a compartmental model in order to reduce the computational costs of the CFD simulation (Delafosse et al. (2014), Delafosse et al. (2015)). With this approach, CFD is only employed to obtain hydrodynamic information, such as the mean and turbulent flow fields and physical properties for each defined compartment. Physical processes, such as mixing and gas-liquid transfer, can be solved, from the definition of the compartments and the flow rates between them, by means of ordinary differential equations, without being affected by local turbulent flow field inaccuracies.

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