Chemical Engineering Science 192 (2018) 128–142

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

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

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HIGHLIGHTS

- CFD simulations of free-surface turbulent flow within baffled stirred-tanks reactors.
- Global and local description of the flow fields by means of statistical analysis.
- Identification of the most relevant flow features by means of POD and DMD.
- Comparison with detailed experimental data obtained from 2D-PIV measurements.

ARTICLE INFO

Article history:
Received 10 April 2018
Received in revised form 6 July 2018
Accepted 12 July 2018

Keywords:
Stirred-tank
Hydrodynamics
CFD
PIV
POD
DMD

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.

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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, 1999a,b).

Advanced experimental optical techniques, in particular Particle 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

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https://doi.org/10.1016/j.ces.2018.07.024
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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 multiphasic 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 investigate 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, 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 $\nu_L = 1.002\cdot10^{-6}\ \text{m}^2\cdot\text{s}^{-1}$) and atmospheric pressure, which corresponds to a working volume $V = 16.5$ L. All simulations and experiments are performed at a rotational speed, $N = 300$ rpm $= 5\ \text{s}^{-1}$, corresponding to a Reynolds number, $Re = 47\,125$.

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

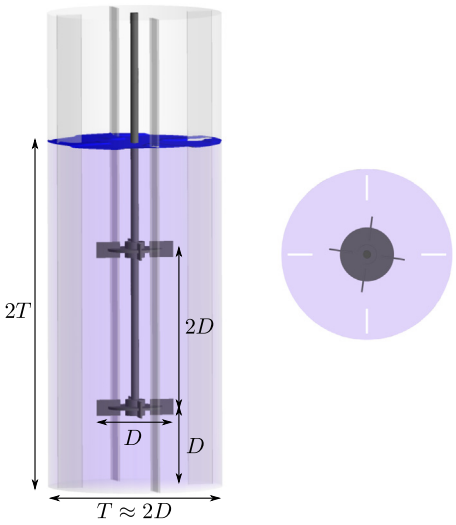

Fig. 1. Front and top views of the computational domain.

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