Chemical Engineering Science 65 (2010) 4307–4322

Contents lists available at ScienceDirect

Chemical Engineering Science

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

Large-eddy simulation of the turbulent free-surface flow in an unbaffled stirred tank reactor

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ARTICLE INFO

Article history:
Received 27 November 2009
Received in revised form
8 March 2010
Accepted 10 March 2010
Available online 13 April 2010

Keywords:
Unbaffled tank
Chemical reactors
Multi-phase flow
Large-eddy simulation (LES)
Turbulence
Mixing

ABSTRACT

This article deals with the large-eddy simulation (LES) of a complex turbulent free-surface flow in an unbaffled mixing tank reactor. The free-surface vortex generated in such a configuration is captured using a front-tracking method, while the stirrer is modelled with an immersed boundary condition technique. Comparisons of mean and fluctuating velocities show good agreement with both theory and experimental laser Doppler velocimetry measurements. The study of mean and instantaneous hydrodynamics points out several interesting features, especially coherent structures, which may have a strong impact on mixing in the reactor. Finally, Reynolds stresses analysis confirms the high anisotropy of turbulence throughout the tank.

1. Introduction

Mixing tanks are very common in chemical process engineering and used in a wide range of industrial applications, such as biology, metallurgy, nuclear engineering, mining, water treatment, paper, petroleum or food industries (Xuereb et al., 2006). Most often, reactors are baffled so as to break the circular motion generated by the stirrer and increase the axial flow rate. Therefore, baffles enhance turbulent macro-mixing, hence process efficiency. Moreover, by cancelling the tangential movement, baffles avoid free-surface vortex formation. However, they also create some zones in the fluid, where any sort of accumulation and attrition can occur, which may either reduce the process efficiency, block the impeller, or even be dangerous for the system (Xuereb et al., 2006). For instance, the device studied here (Auchapt and Ferlay, 1981) belongs to the nuclear fuel reprocessing industry, where accumulation zones have to be limited as much as possible. In this case, this is one of the reasons why an unbaffled tank is preferred.

A lot of experimental or computational studies have been carried out during the last two decades to better understand the complexity of the turbulent flow inside stirred vessels (Ciofalo et al., 1996; Brucato et al., 1998, 2000; Escudié and Liné, 2003; Xuereb et al., 2006; Delafosse et al., 2008; Murthy and Joshi, 2008). With the increase of computational power, computational fluid dynamics (CFD) has allowed to get some local and/or global data that were difficult to collect experimentally. Therefore, it has also become a powerful tool for engineers to design, optimize and scale up mixing tanks. Often, computations are mostly devoted to the mean flow characteristics, which are solved using Reynolds-averaged Navier–Stokes (RANS) equations. This methodology provides precious information about mean velocity or scalar (e.g. concentration) fields and some turbulent quantities (kinetic energy, dissipation). Nevertheless, any unsteady characteristic of the flow is lost. Moreover, many limitations of RANS methods have already been pointed out, especially when solving complex flows with strongly anisotropic turbulence: the popular $k-\varepsilon$ model is, for instance, unable to solve for secondary flow and often leads to unsatisfactory results (Ciofalo et al., 1996; Armenante et al., 1997). Besides, it should be stressed that, due to the rotation of the stirrer, it may be more relevant to consider phase averaged quantities, instead of classical mean RANS values, leading to the use of unsteady RANS methodologies (Hartmann et al., 2004a; Montante et al., 2006; Delafosse et al., 2008). Even though some sophisticated models are available, it remains very

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0009-2509/$ - see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ces.2010.03.014

difficult to produce high-quality predictions with RANS methods (Hartmann et al., 2004a; Delafosse et al., 2008).

Recently, however, several large-eddy simulations (LES) of flows in stirred vessels have been described in the literature (Revstedt et al., 1998, 2000; Derksen and Van den Akker, 1999; Baker and Oshinowo, 2004; Hartmann et al., 2004a, b; Zhang et al., 2006; Fan et al., 2007; Delafosse et al., 2008; Murthy and Joshi, 2008). LES is a very promising alternative to RANS techniques and direct numerical simulations (DNS—turbulent motions, from the bigger vortices to the smaller Kolmogorov scales, are all resolved by a sufficiently fine grid), the latter one still being much too expensive. LES consists in solving the larger scales of the flow, while only modelling the effects of the smaller. Then, it is both accurate and affordable. Comparisons have clearly proved the superiority of LES for predicting flows in mixing tanks (Hartmann et al., 2004a; Murthy and Joshi, 2008; Delafosse et al., 2008), even as far as the mean flow is concerned. Furthermore, LES enables to capture macro-instabilities (Hartmann et al., 2004b; Alcamo et al., 2005) that can have a strong influence on mixing or particle segregation.

As underlined by Alcamo et al. (2005), most studies deal with baffled tanks since they are much more used in industrial applications. This is all the truer as far as CFD and particularly LES is concerned. Murthy and Joshi (2008) have reviewed the main studies of stirred tanks using LES. It can be seen that the impeller is generally a disc turbine (Rushton turbine). Even though CFD surveys are primarily focused on baffled tanks, there exists some work on partially baffled and unbaffled ones. Ciofalo et al. (1996) describe the mean flow, inside a cylindrical vessel with no baffle, generated by two different impellers. Equations are solved using RANS models, highlighting the limitations of $k-\varepsilon$ model against Reynolds stress formulations. Armenante et al. (1997) provide comparisons between LDV and eddy viscosity and Reynolds stress models in a closed unbaffled tank, at two different agitation speeds. They underline the strength of the tangential motion in comparison with the other components. Besides, from a numerical point of view, their study confirms the superiority of Reynolds stress methods. More recently, Montante et al. (2006) studied the effect of shaft eccentricity in an unbaffled tank and Alcamo et al. (2005) have carried out a LES of unbaffled stirred tank agitated by a Rushton turbine, obtaining very good agreement with experiments. Nevertheless, in both cases, the vessel is provided with a flat lid that avoids the free-surface vortex formation. On the other hand, it must be noted that free-surface profiles are computed in some simulations, which is still rare and allows comparisons with experimental results or with Nagata's (1975) theory. As Ciofalo et al. (1996), Haque et al. (2006) have simulated the free-surface flow in an unbaffled tank. Liquid deformation is predicted using the volume-of-fluid (VOF) method. Moreover, a comparison between eddy viscosity and Reynolds stress models for turbulence is provided. Both retrieve correct free-surface vortex shape. Nevertheless, as in the other studies, the latter globally behaves better because of the complexity of turbulent stresses in the reactor. Torré et al. (2007a) have also studied the free-surface vortex formation in a non-standard, partially baffled tank, with the help of RANS and VOF methods. They show very good agreement with experiments. They also indicate the presence of macro-instabilities in their configuration (Torré et al., 2007b). Recently, Mahmud et al. (2009) have described their work on an unbaffled reactor agitated by a cylindrical rod. They show comparisons between experimental velocity measurements and CFD calculations using VOF technique and obtain good agreement. Moreover, they also provide a good prediction of the free-surface deformation.

The present paper deals with the study, by means of LES, of the turbulent flow in an unbaffled mixing tank, accounting for free-surface. In this work, as in Mahmud et al. (2009), the fluid is stirred by a magnetic rod, instead of a more classical mixing device, such as paddle or propeller impellers. Moreover, this mixer is located at the bottom of the vessel. Both phases are solved in the calculation, in order to be able to take into account the free-surface vortex formation as much realistically as possible. To our knowledge, this is one of the first LES of this kind.

Section 2 gives a brief description of the experimental setup used to make velocity measurements and comparisons by using LDV. The main features of the flow are also recalled while reviewing the analytical developments of Nagata (1975) and Le Lan and Angelino (1972). The computational tool and calculation parameters are then presented in Section 3. Comparisons with theory and experimental results are provided in Section 4 and confirm the reliability of LES. Moreover, the flow topology is described and the unsteady motion analysis points out a strong hydrodynamic activity in the tank. Finally, a study of turbulence anisotropy is realized in Section 5. It shows the complexity of the turbulence structure in such a configuration.

2. Configuration description

2.1. Geometry

The geometry of the unbaffled tank studied in this article consists of a cylindrical glass vessel (see Fig. 1) with a diameter T and a height H. Their ratio is $H/T=1.65$. The reactor is filled with water, initially at rest (height H_i) and then agitated by a cylindrical magnetic rod, lying at the bottom of the tank and which length is noted D. The ratio between the rod length and tank diameter is equal to $D/T=0.47$ and in this study, the impeller Reynolds number, defined by $Re_a=ND^2/\nu$, is about 70 000, where N is the impeller rotation speed and ν is the kinematic viscosity. As a consequence, the flow is turbulent (Perry and Chilton, 1973).

2.2. Hydrodynamics

The main mean flow features have been described by Nagata (1975) for several decades. According to his theory, the main motion in the tank is tangential and hydrodynamics is characterized by two different macro-mixing zones. Near the axial centre of the tank, the fluid almost rotates as a solid body with angular

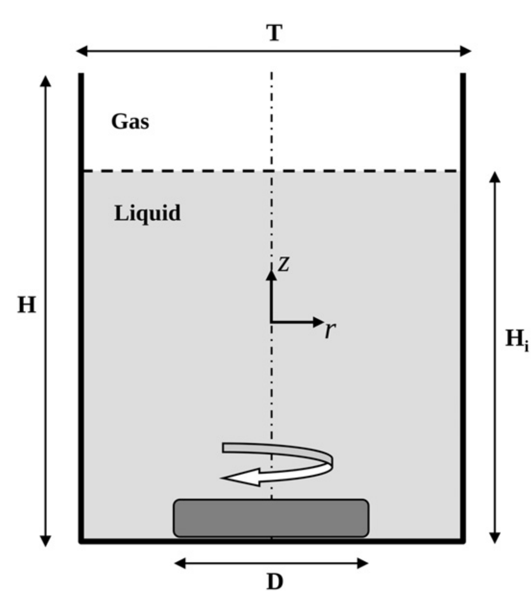

Fig. 1. Simplified geometry of the tank (free-surface is sketched at rest).