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Direct numerical simulations of creeping to early turbulent flow in unbaffled and baffled stirred tanks

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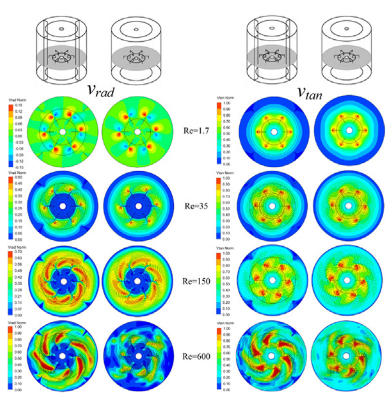
HIGHLIGHTS

- Direct Numerical Simulations were performed in baffled and unbaffled stirred tanks.
- Transition from creeping to early turbulent flow was studied in both systems.
- Bifurcation between baffled and unbaffled vessels was correctly predicted and explained.
- Bifurcation was found not to strictly coincide with the transition to turbulence.
- A travelling wave disturbance rotating with the impeller was found in the unbaffled tank.

GRAPHICAL ABSTRACT

Radial and tangential velocity components in a horizontal plane in baffled and unbaffled vessels at different Reynolds numbers.



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ABSTRACT

It has been known for a long time that the fluid flow and several global quantities, such as the power and pumping numbers, are about the same in baffled and unbaffled mechanically stirred vessels at low Reynolds numbers, but bifurcate at some intermediate Re and take drastically different values in fully turbulent flow. However, several details are not yet completely understood, notably concerning the relation of this bifurcation with the flow features and the transition to turbulence. In order to shed light on these issues, computational fluid dynamics was employed to predict the flow field in two vessels stirred by a six-bladed Rushton turbine at Reynolds numbers from 0.2 to 600 (covering the range from creeping flow to early turbulent flow). The two vessels differed only for the presence or absence of peripheral baffles. All simulations were conducted by a finite volume method in time-dependent mode, and a sliding-mesh technique was used in the baffled case to deal with the relative motion of baffles and impeller blades. A sensitivity analysis proved that a grid of about 5 million finite volumes was adequate to yield grid-independent results. The study proved that the bifurcation between quantities related to baffled and unbaffled tanks occurs when the inner (near-impeller) and outer (near-wall/baffles) flow fields interact significantly. It also elucidated the mechanisms of transition to turbulence in baffled and unbaffled tanks, notably showing in this latter case the existence (in the rotating reference frame of the impeller) of a periodic flow regime which involves a travelling wave instability.

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Nomenclature

Co	Courant number (–)
D	vessel diameter (m)
d	impeller diameter (m)
H	vessel height (m)
k	turbulent kinetic energy ($m^2\ s^{-2}$)
M	fluid mass (kg)
N	rotational impeller speed (s^{-1})
N_p	power number, $W/(\rho N^3 d^5)$ (–)
N_q	pumping number, $Q/(Nd^3)$ (–)
N_θ	number of azimuthal divisions in 2π (–)
Q	discharge flow rate issuing from the impeller ($m^3\ s^{-1}$)
T	impeller revolution period, $1/N$ (s)
t	time (s)
u_τ	friction velocity, $(\tau_w/\rho)^{1/2}$ ($m\ s^{-1}$)
v	velocity ($m\ s^{-1}$)
W	mechanical stirring power (W)
Greek letters	
Δt	computational time step (s)
ε	turbulence dissipation ($W\ kg^{-1}$)
Λ_K	Kolmogorov length scale (m)
μ	viscosity (Pa s)
ν	kinematic viscosity ($m^2\ s^{-1}$)
ρ	density ($kg\ m^{-3}$)
τ_w	wall shear stress (Pa)
Ω	angular velocity of the impeller, $2\pi N$ (rad/s)
ω	angular celerity of a travelling wave (rad/s)

1. Introduction

Cylindrical vessels, in which fluids are mechanically stirred by different types of impellers, are widely employed in the chemical process industry and have been the subject of a vast literature. Many studies have focused on the dependence of power consumption and mixing effectiveness upon impeller type and size, vessel geometry or impeller location, with special reference to off-bottom clearance (Alvarez et al., 2002a,b; Campolo et al., 2003; Montante et al., 2006; Cabaret et al., 2008; Hidalgo-Millàn et al., 2011, 2012; Takahashi et al., 2012; Bulnes-Abundis et al., 2013; Tamburini et al., 2016).

Baffles are usually present on the peripheral wall of the vessel with the purpose of converting radial and circumferential flow into axial flow, thus improving mixing (Oldshue, 1983; Ammar et al., 2011). Unbaffled vessels are regarded as less effective mixers and, traditionally, their use has been confined to those cases in which baffles may have undesired effects (Aloi and Cherry, 1996; Assirelli et al., 2008; Tamburini et al., 2013), e.g. scaling, and to low Reynolds number applications in which baffles may promote the formation of stagnant zones (Vakili and Nars Esfahany, 2009). However, recent studies have demonstrated that unbaffled vessels may represent a competitive alternative to baffled vessels also in conventional processes, in regard both to mixing time (Busciglio et al., 2014) and to solids suspension (Wu et al., 2012, Tamburini et al., 2012a, 2014). In particular, the minimum impeller speed for complete suspension and the relevant power requirements were found to be lower in laboratory-scale unbaffled tanks than in baffled ones (Tezura et al., 2007; Tamburini et al., 2011a). Potential advantages of unbaffled vessels have been demonstrated also at industrial scale (Wu et al., 2016).

Moreover, baffles are usually omitted in the case of very viscous fluids (Re < 20), where baffles can lead to the formation of dead zones, that badly affect mixing performances (Nagata, 1975; Busciglio et al., 2016). Unbaffled tanks are also advisable in crystallizers, where the presence of baffles may promote the particle attrition (Mazzarotta, 1993; Busciglio et al., 2014). Finally, in bioreactor applications, when shear-sensitive cells are involved, mechanical agitation and especially sparging aeration (and associated bubble bursting) can cause cell death (Chisti, 2000; Nienow et al., 1996). In unbaffled vessels, at low agitation speeds, the required oxygen mass transfer may well take place through the free surface deep vortex produced by agitation (Scargiali et al., 2014, 2015).

In recent years, several studies, both computational and experimental, have focused on laminar mixing. Despite its deficiencies, such as the formation of closed recirculation regions where the fluid remains trapped (Lamberto et al., 1996, 1999; Cabaret et al., 2008), laminar mixing may be an advantageous alternative to turbulent mixing in a number of applications. For example, these include processes in which turbulence and high shear rates would damage the products, e.g. cultures of shear-sensitive cells or micellar broths as well as manufacture of creams and detergents (Alvarez et al., 2002a,b).

Experimental results, notably regarding the power number N_p, show that – independently of impeller type – results obtained for baffled and unbaffled vessels are very similar at low Reynolds number, while a bifurcation occurs at Re ≈ 100, with baffled vessels always exhibiting larger N_p (Rushton et al., 1950; Furukawa et al., 2012; Driss et al., 2012). This is not surprising if one considers that, in baffled tanks at low Re, only a weak hydrodynamic interaction exists between the impeller and the baffles. At higher Re, the more intense radial jet issuing from the impeller reaches the peripheral wall region, i.e. the baffles, and interacts with them. Similar results, though less clear because experimental data are more scarce, hold for the pumping number N_q, mixing time, and other flow features. Several details of the above picture, however, are still fuzzy. Among the open issues:

i. Do different flow quantities, e.g. the power and pumping numbers, bifurcate at the same time, i.e. at the same values of Re?
ii. What changes in the flow field accompany the bifurcation between baffled and unbaffled vessels?
iii. Does the bifurcation coincide with the transition to turbulence? And, more generally, what is the scenario of transition to turbulence in stirred vessels, and how does it differ between baffled and unbaffled vessels?

The present study aims to answer these questions, at least at a coarse-grained scale, by means of CFD simulations (validated by experimental measurements) in two reactors differing only for the presence or the absence of baffles. Both vessels were stirred by a six-bladed Rushton turbine and were provided with a top-cover to avoid the complications associated with the central vortex (Tamburini et al., 2009).

Given the increasing interest towards unbaffled tanks and the great advantage that they may provide in some applications, properly understanding their fluid dynamics at different Reynolds numbers and recognizing their differences with baffled tanks is a matter of considerable importance. For the first time, the present work tries to elucidate the earlier appearance of the differentiation between the behaviour of baffled and unbaffled tanks. Hopefully,