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CFD Simulation of Radially Stirred Baffled and Unbaffled Tanks

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Stirred tanks typically employed in process industries are provided with baffles. Although the presence of baffles is known to guarantee good mixing rates, unbaffled vessels may be compulsory in some applications as crystallization, bioremediation, biotechnology and ore industry. A better understanding of unbaffled stirred vessels flow dynamics may allow (i) a proper design to be performed and (i) conditions/processes where baffle presence can be avoided to be recognized.
In the present study, the k-ω SST was used to simulate an unbaffled tank from early to fully turbulent regime (Re≈600-33,000). The unbaffled tank simulated has a diameter T=0.19m and is stirred by a standard six-bladed Rushton turbine with diameter D=T/2 and clearance C=T/3. A corresponding baffled tank was also simulated in order to compare the the two systems. A time dependent Sliding Grid approach was employed for the baffled tank to account for the impeller-to-baffle relative rotation. Conversely, for the case of the unbaffled vessel, a reference frame rotating with the impeller was adopted. Experimental literature data concerning the power and pumping numbers were employed for the simulation validation. RANS results were in good agreement with the experimental data for the baffled case at the largest Re, whereas predictions for the unbaffled vessel exhibited a less satisfactory agreement with experimental data. The latter finding may be due to the poor capability of the two-equations model to manage the anisotropic turbulence typical of high swirling flows.

1. Introduction

Mixing is a unit operation which can be easily encountered in many process industries (Pukkella et al., 2019). This unit operation is usually performed in tanks mechanically agitated by stirrers (Gong et al., 2018). Such tanks are traditionally provided with baffles (Oldshue, 1983): these are thin metal strips typically deployed along vessel walls with the purpose of suppressing the otherwise highly swirling fluid motion inside the tank. Their introduction quite dramatically changes tank fluid-dynamics, flattening liquid free surface and also prompting a number of other effects, among which a faster mixing rate. Due to the latter benefit, tanks unprovided with baffled, named unbaffled tanks, are rarely employed at industrial scale (Busciglio et al., 2017). More precisely, unbaffled stirred vessels are conventionally employed only when baffles presence may be an issue for the process (Tamburini et al., 2009). For instance, when baffles may lead to incrustation issues, dead zones formation, or undesired nucleation (crystallization), or cell damage (biotech processes), their presence is avoided (Ameur et al., 2017; Aloi and Cherry, 1996; Chisti, 2000; Wang et al., 2016). However, some recent publications are reporting good performances of the unbaffled vessels also in common applications like the suspension of solid particles into liquids (Tamburini et al., 2014; Tamburini et al., 2012; Wang et al., 2012; Wu et al., 2016). When unbaffled vessels are not equipped with a top-cover, a vortex is generated at the tank centre due to the high swirling flow. Although its presence is traditionally considered as a possible issue, some advantages have been shown in recent years (Tamburini et al., 2016). Just to give an example, the central vortex has been used as a source of oxygen to be used for biological applications (Scargiali et al., et al., 2015; Busciglio et al., 2010). In particular, oxygen transfer rates appear to be comparable with those of baffled

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vessels equipped with air-spargers (Labik et al.,2018; Petricek et al, 2018), with the additional advantage of tackling the clogging issues typical of slurry processes.

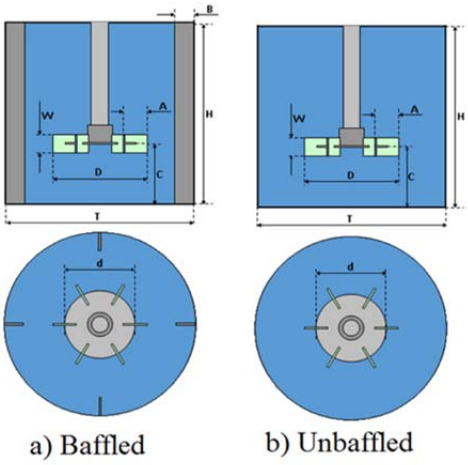
Due to the traditional use of baffled vessels, scientific literature is missing data and studies on unbaffled vessels. This represents another reason for which baffled tanks are preferred.

The present work aims at contributing to the increase of knowledge on unbaffled vessels. More precisely, literature lacks sufficient information on the fluid-dynamics of such kind of systems. A fully understanding of the different fluid-dynamics features of baffled and unbaffled vessels would be beneficial for guiding the choice and the design of the best reactor. In this regard, in a previous work (Tamburini et al., 2018), Direct Numerical Simulations (DNS) were carried out to predict the flow field of both a baffled and an unbaffled stirred tank in a broad range of Reynolds numbers encompassing creeping to early turbulent flow conditions (Re≈1.7-600).

In the present work, the k-ω Shear Stress Transport turbulence model is tested to simulate the two reactors at larger Reynolds numbers, that is from early to fully turbulent regime (Re≈600-33,000). This model was chosen as it has been recently proven to be more effective than the k-ε and RNG k-ε in simulating uncovered unbaffled stirred tanks (i.e. with a central air vortex) (Zamiri and Chung 2017) at high Reynolds numbers.

2. Tanks under study and cases investigated

Both an unbaffled and a baffled tank were investigated. These are sketched in Figure 1. Each tank has a diameter T=0.19 H, a liquid height H=T. Both tanks are radially stirred by a standard six-bladed Rushton turbine with a diameter D=T/2 and a clearance C=T/3. A top-cover is employed in the vessels in order to avoid the central vortex formation, thus allowing an easier comparison of the fluid dynamics of both systems. Other geometrical details are reported in Figure 1.



T=0.19m	$\frac{d}{D}=\frac{3}{4} \Rightarrow d=0.07\text{m}$
$\frac{D}{T}=\frac{1}{2} \Rightarrow D=0.095\text{m}$	$\frac{W}{D}=\frac{1}{5} \Rightarrow W=0.019\text{m}$
$\frac{H}{T}=1 \Rightarrow H=0.19\text{m}$	$\frac{A}{D}=\frac{1}{4} \Rightarrow A=0.0237\text{m}$
$\frac{C}{T}=\frac{1}{3} \Rightarrow C=0.063\text{m}$	$\frac{B}{T}=\frac{1}{10} \Rightarrow T=0.063\text{m}$

Figure 1: Sketch and relevant geometrical features of the tanks investigated

Different cases were investigated, each one corresponding to a different impeller speed N. Relevant Reynolds numbers, assessed as Re= $\rho ND^2/\mu$, are reported in Table 1. All these cases are representative of a non-stationary regime ranging from early to fully turbulent.

Table 1: Reynolds numbers simulated

Re	500	1000	2500	5000	10000	33000

3. Modelling and numerical details

All simulations were carried out by solving the continuity and momentum equations (not-reported here for the case of brevity). Since turbulent regimes are simulated and Reynolds numbers are quite high, Direct Numerical Simulations are inhibited by the prohibitive computational times and Reynolds Average Navier Stokes simulations were performed. In particular, the k-ω Shear Stress Transport (SST) turbulence model (Menter, 1993) is adopted to compute the Reynolds stresses arising in the momentum equations after Reynolds averaging. Basically, it is a two-equations eddy-viscosity model including a blending function switching from the standard k-ω formulation to predict the flow within boundary layers, to the k-ε model to compute the free-stream turbulence. k-ω SST is commonly considered as a low Reynolds k-ε model which has not been tested so far to predict the flow field of stirred tanks from early to fully turbulent regime.

Three different computational grids were tested: the coarsest one encompassed about 1 millions of computational volumes, the middle-one about 4 millions, the finest one about 9 millions. Preliminary simulations showed that the 4 million grid is more than sufficient to obtain results unaffected by any grid-dependence: both global and local quantities provided by this grid were found only a few percent different than the corresponding ones obtained with the finest grid.

All RANS simulations were performed under stationary conditions typical of RANS simulations. A number of iterations sufficient to obtain residuals to settle below 10^{-6} was adopted.

4. Results and Discussion

The CFD simulations performed were used to provide global performance parameters as the power number N_p and the pumping number N_Q: $N_p=P/(\rho N^3D^5)$ where P is the torque power consumed by the impeller, $N_Q=Q/ND^3$ where Q is the flow rate discharged by the impeller. The power number values predicted are reported in Figure 2 along with corresponding experimental literature data (Rushton et al. 1950, Scargiali et al., 2017) for comparison purposes. DNS simulation results relevant to creeping-to-early Re numbers flow obtained in a previous work (Tamburini et al., 2018) are shown for the sake of completeness. As it can be seen in Figure 2, the k-ω SST exhibit different performances for the baffled and unbaffled systems. For the case of baffled tank, a good agreement is observable at large Re, while an overestimation was encountered at low Re where early turbulent conditions are present. This appears somehow in contradiction with the k-ω SST model features which is commonly considered as a turbulence model able to deal with low Re cases where turbulence is not fully developed yet.

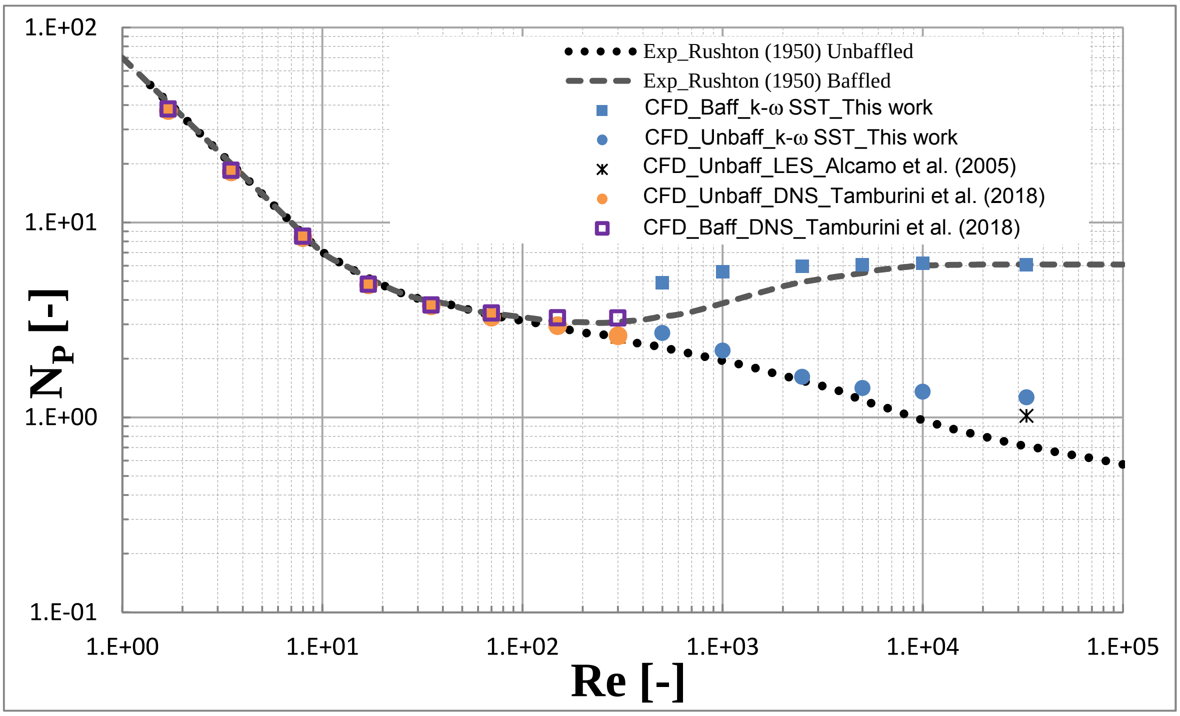


Figure 2: Power Number as a function of the Reynolds number

Interestingly, the opposite occurs for the case of the unbaffled stirred tank. At the low Re investigated in the present work the Np values predicted by the simulations match quite well the corresponding experimental data, while the two trends start diverging when turbulence is fully developed. In stirred tanks Re = 10000 is the commonly adopted cut off value beyond which fully turbulence conditions are achieved. The overestimation of experimental data is difficult to be explained properly. According to the collected data and to literature considerations for other eddy-viscosity based turbulence models (Ng et al., 1998; Yeoh et al., 2004; Murthy and Joshi, 2008), k-ω SST model fails in providing good predictions at high Re because, at these agitation velocities, the swirling flow is significant and turbulence is highly inhomogeneous. The higher the Re, the

higher the difference between the tangential velocity and the other two velocity components, thus allegedly leading to a higher anisotropy in turbulence patterns. k-ω SST model is a turbulence model based on Boussinesq's hypothesis and computes all Reynolds stresses as a function of the turbulence viscosity only. Thus, it is expected to be more suitable for homogenous turbulence cases and less prone than Reynolds stresses models to properly deal with high anisotropic turbulence. Clearly, other simulations to be carried out with Reynolds stresses models are needed to compare data and properly validate the above hypothesis at these Re values.
In Figure 3, the pumping number is reported as a function of Reynolds number. N_Q experimental data at different Re are not available in the literature for this geometry. The only experimental datum reported concerns the asymptotic N_Q values at the highest Re and comparison should be regarded as fully qualitative. The baffled tanks asymptotic datum is from Costes and Couderc (1988) who reported N_Q = ~0.73, while for unbaffled tanks the datum of N_Q = ~0.34 is from Nagata (1975).
For the case of the baffled tank the model is somehow able to follow the qualitative sigmoidal trend reported by Dickey and Fenic (1976) for the right end of the Re range. More precisely, the model is capable of predicting the increasing of N_Q up to the achievement of an asymptotic value, although the latter is slightly higher than the literature one.
As it concerns the unbaffled tank, a decreasing trend is predicted by the CFD simulations. The higher Re, the lower the slope of the points thus indicating the achievement of some asymptotic value which seems really similar to the one reported by Nagata (1975).
Summarizing, the two trends of N_Q vs Re are reasonable, but it is hard to give a quantitative indication of the model performance without a comparison with other model data.

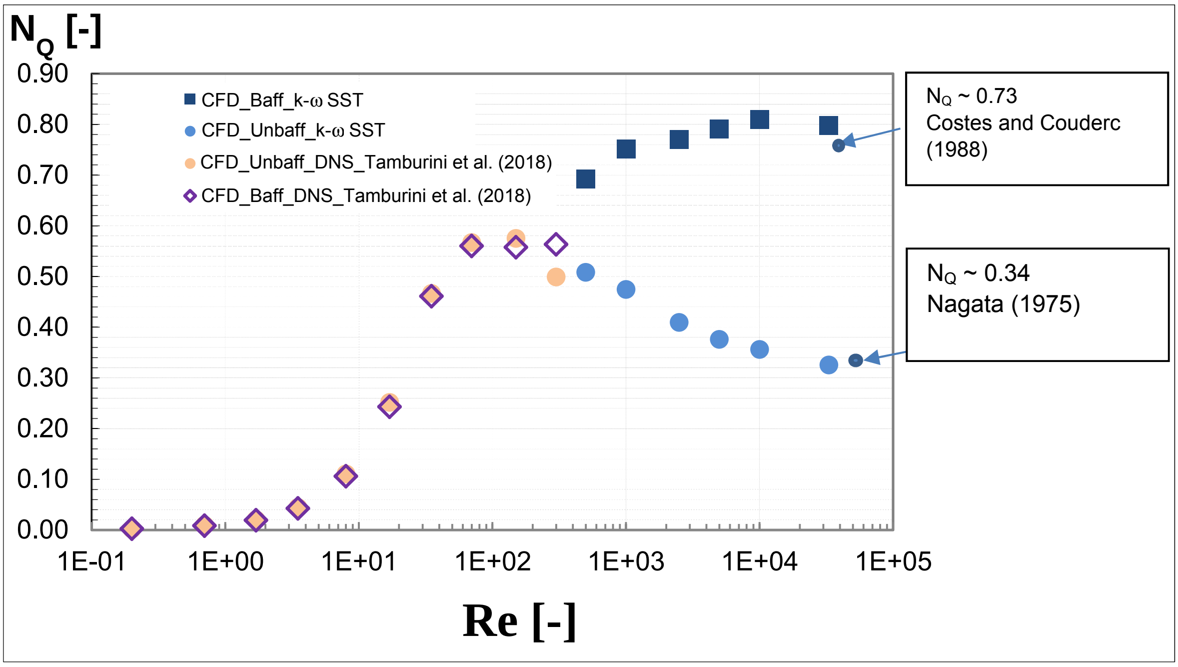


Figure 3: Pumping Number as a function of the Reynolds number

Azimuthally averaged radial profiles of axial and tangential velocity component were also calculated and are not reported for the sake of brevity. At the highest Re investigated (i.e. Re=33000), the k-ω SST predicted that axial velocities are higher in the baffled tank, while tangential velocity are higher in the unbaffled tank, as expected.
On overall, the comparison of the two systems suggest that in accordance with literature findings the higher flowrate discharged by the impeller (higher N_Q) is somehow paid by higher power requirements (higher N_p) in the baffled tanks at any Re larger than the bifurcation one. Thus, the flow patterns occurring within the so-called transitional regime conditions (i.e. from bifurcation to fully turbulent conditions) should be regarded as the main responsible for the differentiation of the two systems.

5. Conclusions

The k-ω SST was found able to catch the different behaviour of the two systems. At Re larger than the bifurcation one, the model was able to predict the increasing trend of N_p with Reynolds up to the achievement of a plateau at fully turbulent conditions at which a very good match with experimental data was found. Similarly, the decreasing trend of N_p with Re typical of unbaffled tanks was correctly predicted by the model, although the agreement with experiments was poor at large Re probably because of the high turbulence anisotropy typical of these Re.

Concerning the N_Q predictions, a reasonable trend of N_Q vs Re for both the baffled and unbaffled tank and the corresponding asymptotic values were fairly well predicted.

Additional simulations to be performed with different turbulence models are needed to compare results and properly assess k-ω SST performance within the investigated range of Re ranging from early to fully turbulent conditions.

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