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Bioreactor Mixing: a Comparison of Computational Fluid Dynamics and Experimental Approaches in the Pursuit of Sustainable Bioprocessing for the Bioeconomy

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This paper highlights the importance of bioreactors in the bioeconomy, focusing on the role of mechanical mixing in promoting optimal conditions for microorganism growth and productivity. Computational fluid dynamics (CFD) simulations are increasingly used in bioreactor design to predict fluid dynamics and mixing characteristics. This study utilizes CFD simulations with OpenFOAM® to predict the power number of various stirring devices in a lab-scale reactor. The torque and power number results of three different stirrers were compared through experimental and simulation methods. The pitched blade and cage impeller showed an increase in experimental torque and power number with rotational speed, while the paddle impeller had much higher experimental values than the simulated values at all speeds. The study demonstrates the value of CFD models for predicting bioreactor performance, despite some inaccuracies in simulations. These findings are important for industries seeking to optimize bioreactor design and increase productivity through better mixing processes.

1. Introduction

The European Union has made the bioeconomy a top priority, seeking sustainable economic growth, reduced dependence on fossil fuels, and solutions to environmental challenges. Bioreactors are a vital area of research within the bioeconomy, as they provide a means to create renewable and sustainable sources of energy, food, and materials from biological resources. Mechanical mixing is critical in bioreactors, influencing mass transfer, promoting homogeneous culture conditions, and affecting microorganism growth and productivity. Among these mechanical bioreactors, stirred-tank reactors are widely used. The proper function of the stirring equipment used is crucial for mixing, reaction, dissolution, and crystallization processes, making their design, optimization, and improvement a crucial research topic (Shen et al., 2021).

Impeller rotation creates complex flow in the stirred vessel, making it important to understand the fluid dynamics of impeller discharge flow for reliable design and scaling up of stirred reactors (Wang et al., 2006). Impellers can be categorized into two main groups: radial and axial flow, with radial impellers producing strong radial jets that create a high shear zone near the impeller (Basavarajappa and Miskovic, 2013). Axial impellers can create either up or down pumping flows depending on their rotation direction and blade shape, and produce less turbulence than radial impellers, which is why baffles are often used to reduce tangential flow and turbulence (Basavarajappa and Miskovic, 2013). The baffles play a significant role in converting tangential flow produced by agitation into three directional flows: axial, radial, and tangential; and prevent the formation of vortices on the level caused by centrifugal force (Foukrach et al., 2020). The most commonly used and studied baffles are the standard four vertical bafflesdue to their impact on fluid characteristics during stirring(Shen et al., 2021).

Several experiments in the literature have been dedicated to the effect of baffles on the hydrodynamics of stirred tank reactors. An examination of the impact of baffle number on mixing efficiency revealed that the optimal number of baffles can considerably enhance the degree of mixing, while an excessive number of baffles can increase mixing time (Lu et al., 1997).The experimental results of an unbaffled agitator and five baffled agitators

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with varying baffle lengths were compared by Sivashanmugam and Prabhakaran (2008), revealing that the length of the baffle has a significant impact on power consumption. Foukrach and Ameur (2019) studied with Computational Fluid Dynamics (CFD) the effects of the baffle shape on the fluid velocities, flow patterns, and power consumption in vessels agitated by a six-blade Rushton turbine. Shen et al. (2021) performed a CFD study, proposing a "V-shaped" horizontal baffle attached to the inner wall of the agitator at the height of the impeller to reduce energy consumption and improve mixing in liquid-liquid two-phase flow.
Many industries rely on mixing as a crucial process, hence insufficient comprehension of the process can lead to increased power consumption and longer process times, resulting in significant financial losses (Basavarajappa and Miskovic, 2013). The combination of experimental research and CFD has been widely used in studying agitators, and the advancement of CFD technology has facilitated the design and optimization of agitators (Shen et al., 2021). CFD has emerged as a valuable tool for predicting bioreactor performance and optimizing design. However, before relying on CFD models, it is essential to validate them against experimental data. Ding et al. (2010) performed a study with CFD simulations to investigate the impact of impeller type and speed on flow patterns in a gas-liquid two-phase flow CSTR for biohydrogen production. The authors (Ding et al., 2010) that an optimized impeller can generate better velocity distribution in the reactor with lower impeller speed, leading to higher average hydrogen yield and less startup time. Blanco-Aguilera et al. (2020) constructed and validated a CFD model of a new anaerobic-anoxic reactor using OpenFOAM®, and found that CFD simulations provide a deeper understanding of the hydraulic behavior of the fluid within the reactor. The analysis revealed the location and quantification of preferential flow channeling and dead volumes (Blanco-Aguilera et al., 2020). Maier et al. (2010) utilized CFD to investigate the mixing behavior and agitation system performance in biogas plants to support the scale-up process. Zhang et al. (2013) performed a CFD study on a CSTR and found that baffles significantly improve fluid exchange, prevent vortex formation, and exhibit cyclical variations in velocity direction and magnitude in the CSTR region.
Wang et al. (2006) employed CFD and digital particle image velocimetry (PIV) to investigate the flow patterns of a viscous fluid in a stirred tank that was agitated using a four-blade Rushton turbine. The CFD simulations yielded outcomes that were consistent with experimental results in terms of the flow field and velocity components (Wang et al., 2006).
In this study, CFD simulations were performed using the open-source OpenFOAM® software to predict the power number of three different stirring devices. Experimental data was collected on a lab-scale reactor, and the comparison of results will provide insights into the accuracy and reliability of CFD models for predicting power numbers in bioreactors.

2. Materials and methods

2.1. Experimental setup

Experiments were performed on a 45-liter lab reactor of 65 cm height and 15 cm radius, equipped with four baffles 24 cm height, 4.5 cm width, and 0.6 cm thick. The baffles are connected on the bottom with a ring baffle of 8.4 cm of inner radius, a height of 3.3 cm, and a thickness of 1.2 cm. The setup was equipped with a high-precision laboratory stirrer (IKA EUROSTAR 200 Control), which was utilized as a motor to precisely control the mechanical agitation and also as a torque measurement device. Liquid height was set to 42 cm, which equals to 30 liters. For the height of the reactor on the computational domain (shown in Figure 1), the height was set to the liquid's height. The experimental setup and the CFD domain are shown in Figure 1. Three stirrer types were utilized for this study (pitched blade, cage, and paddle), their dimensions are shown in Table 1 and the stirrers are shown in Figure 2.

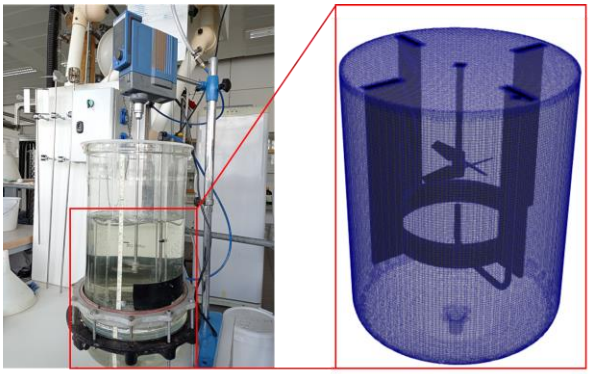

Figure 1: Experimental setup and CFD domain

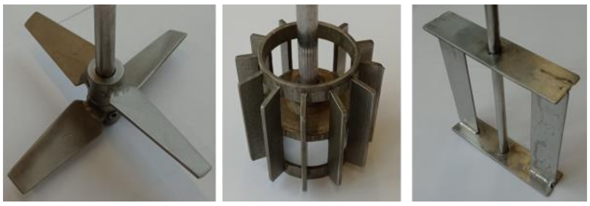

Figure 2: Stirrers utilized for experiments

Table 1: Stirrer dimensions

	Stirrer 1	Stirrer 2	Stirrer 3
Name	Pitched blade	Cage	Paddle
Type	Axial	Radial	Tangential
Stirrer diameter (cm)	11.5	6	11.5
Stirrer height (cm)	3.7	6	11.5
Quantity of blades	4	12	2
Shaft Length (m)	0.74	1	0.755
Blade length (cm)	4.6	5, 5.4	11.5
Blade width (cm)	1.1, 1.95	1	2.7
Blade thickness (mm)	2	2	2
Weight of single blade (g)	8.03	8.16	48.75
Total weight of stirrer (kg)	0.365	0.612	0.491

For the experiments, the velocity was gradually increased from zero to when the unstable vibrations did not allow torque measurement. Torque was recorded for stirrer 1 from 550 to 1300 RPM, for stirrer 2 from 400 to 950 RPM, and for stirrer 3 from 130 to 325 RPM.

2.2. CFD method

OpenFOAM® version 8 was utilized in this study with the single-phase SimpleFOAM solver. SimpleFoam utilizes the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm to solve for steady-state, incompressible, turbulent flow (Jeong et al., 2023). The single-phase was water. The simulations reached residual convergence of around $1x10^{-6}$, with most simulations requiring approximately 520 iterations to achieve this convergence.

The Multiple Reference Frame (MRF) method is considered the most appropriate technique to simulate impeller rotation in mixing systems, and accurate determination of the stationary and moving areas within the MRF method can lead to precise results in terms of mixing performance (Foukrach et al., 2020). The MRF approach is widely used for the numerical modeling of stirred reactors, particularly for simulating flow and mixing created by impellers (Ding et al., 2010). This method offers the advantage of a relatively low computational time. The MRF involves dividing the computational domain into two sections: a rotating cylindrical volume inside that encloses the impeller and a stationary outer volume containing the rest of the tank (Foukrach et al., 2020).

2.2.1. Geometries

For the stirrers, the geometries of stirrers 1 and 3 were completely digitalized, while for stirrer 2 the number of blades was reduced by half (to 6). Figure 3 shows three reactors with the baffles and the internals of the experimental setup, each with one stirrer. Table 2 shows the number of cells of each geometry. Each mesh was created by the trial-and-error method (Segui et al., 2022) with the combination of the OpenFOAM® meshing utilities blockMesh and snappyHexMesh.

Table 2: Cell count for each geometry

Geometry	1	2	3
No. of cells	~2,840,000	~2,670,000	~1,775,000

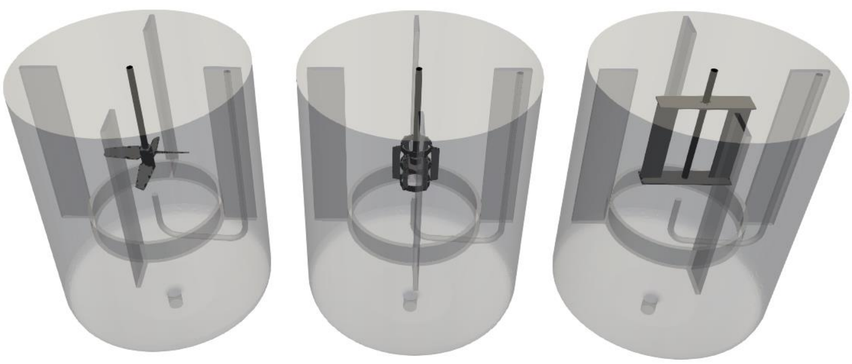

Figure 3: Geometries utilized in the CFD study

To have enough data to compare with the experiments a total of 26 cases were created for CFD simulation. For stirrer 1 velocities 550, 650, 750, 850, 950, 1050, 1150, and 1250 RPMs. For stirrer 2 velocities 400, 450, 500, 600, 700, 800, 850, 900, and 950 RPMs. For stirrer 3 velocities 130, 150, 175, 200, 225, 250, 275, 300, and 325 RPMs. For the torque and power number method, the moment is extracted from each blade.
In OpenFOAM®, the function object known as "forces" calculates the forces and moments acting on a specified list of patches by integrating pressure and viscous forces and moments, and can also include resistance forces and moments from porous zones as an option (OpenCFD Ltd, 2021). OpenFOAM® generates a data ".dat" file, containing 6 vectors per every time step. The first three vectors are pressure, viscous and porous forces, while the last three are the pressure, viscous and porous moments. To calculate the torque, the element of the shaft's axis of the fourth and fifth vectors (pressure and viscous moments) need to be added.
A Python 3.10 algorithm was developed to go into all the 104 ".dat" files generated by the patches on the blades and extract the pressure and viscous moment vectors of the converged iteration. Once these vectors have been extracted, the torque for each blade is calculated with Eq (1). The total torque of the stirrer is calculated by adding the torque of each blade. The power consumption and the power number are calculated with Eq (2) and Eq (3), respectively.

$$m\Gamma_{blade_n} = m_{py} + m_{\mu y} \tag{1}$$

$$P = 2\pi N m\Gamma \tag{2}$$

$$P_0 = \frac{P}{D^5 * \rho * N^3} \tag{3}$$

Where $m\Gamma_{bladen}$ is the torque of the blade, m_{py} and $m_{\mu y}$ are the vector components of the moment pressure and viscous moment, P is the power consumption, N is the stirring velocity, P0 is the power number, D is the impeller diameter and ρ is the density. The torque is determined by adding the moments due to viscosity and pressure across the surfaces of the impeller (Fernandes Del Pozo et al., 2019). The resulting torque needs to be multiplied by the density of the medium (~1000 kg/m^3 for water) since the pressure in OpenFOAM® is the kinematic pressure (static pressure divided by density).

3. Results

Table 3 presents the torque results obtained from the experimental study and simulation cases for three different stirrers. For Stirrer 1 and Stirrer 2, the experimental torque increases as the rotational speed rises. However, for Stirrer 3, the experimental torque consistently surpasses the simulated torque across all cases. The largest difference between experimental and simulated torque values is observed for Stirrer 3 at higher rotational speeds. One potential explanation for these discrepancies is that the equipment used for the experiments is primarily intended for teaching purposes and has not undergone calibration since its installation.

Table 3: Comparison of experimentally measured vs. simulated torque

Stirrer 1			Stirrer 2			Stirrer 3		
Case	Experimental ($x10^{-2}$ Nm)	Simulated ($x10^{-2}$ Nm)	Case	Experimental ($x10^{-2}$ Nm)	Simulated ($x10^{-2}$ Nm)	Case	Experimental ($x10^{-2}$ Nm)	Simulated ($x10^{-3}$ Nm)
550	1	5.59	400	2	2.11	130	2	3.03
650	6	7.84	500	11	3.30	150	11	4.06
750	11	10.45	600	17	4.75	175	17	5.55
850	15	13.37	700	24	6.42	200	23	7.24
950	19	16.70	800	31	8.42	250	39	11.23
1050	26	20.33	850	35	9.57	275	47	13.50
1150	30	24.36	900	40	10.76	300	57	16.06
1250	36	28.83	950	44	11.92	325	67	18.85

Table 4 presents a comparison between the experimentally measured and simulated power numbers for three different stirrers. For Stirrer 1, the experimental power number gradually increases as the rotational speed (case) increases. In contrast, the simulated power number remains relatively constant around 5.26 for all cases. Stirrer 2 exhibits a noticeable discrepancy between the experimental and simulated power numbers. At lower rotational speeds (cases 400-500), the experimental power number is significantly higher than the simulated power number. Stirrer 3 exhibited much higher experimental power numbers than simulated power numbers, particularly at higher rotational speeds, suggesting inaccuracies in CFD simulation predictions or discrepancies due to the fact that the laboratory stirrer controller IKA EUROSTAR 200 has never been calibrated.

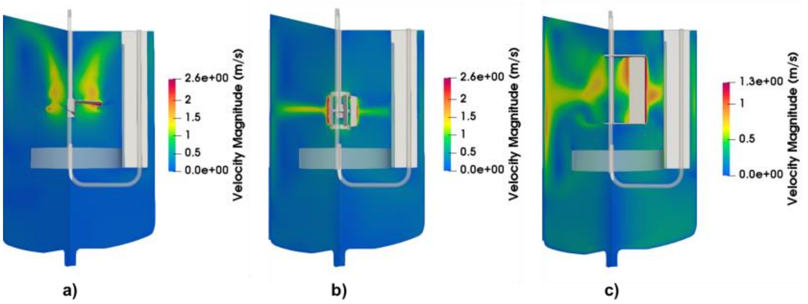

Figure 6: Velocity profiles of three stirrer types a) pitched blade a 600 RPMs, b) 6-cage impeller at 600 RPMs, and c) paddle impeller.

Table 4: Comparison of experimentally measured vs. simulated power number

Stirrer 1			Stirrer 2			Stirrer 3		
Case	Experimental	Simulated	Case	Experimental	Simulated	Case	Experimental	Simulated
550	0.94	5.26	400	66.74	70.24	130	33.73	5.12
650	4.05	5.29	500	234.92	70.44	150	139.34	5.15
750	5.57	5.30	600	252.12	70.51	175	158.22	5.17
850	5.92	5.28	700	261.51	69.96	200	163.89	5.16
950	6.00	5.27	800	258.61	70.22	250	177.85	5.12
1050	6.72	5.26	850	258.64	70.70	275	177.13	5.09
1150	6.47	5.25	900	263.66	70.89	300	180.51	5.09
1250	6.57	5.26	950	260.30	70.49	325	180.80	5.09

In the following section, 8 cases of each geometry are shown, coloring the velocity magnitude. Figure 7 shows the velocity profiles of stirrer 1 coloring the maximum velocity magnitude at 2.6 m/s. Figure 8 shows the velocity profiles of stirrer 1 coloring the maximum velocity magnitude at 1.2 m/s. Figure 9 shows the velocity profiles of stirrer 1 colouring the maximum velocity magnitude at 0.75 m/s.

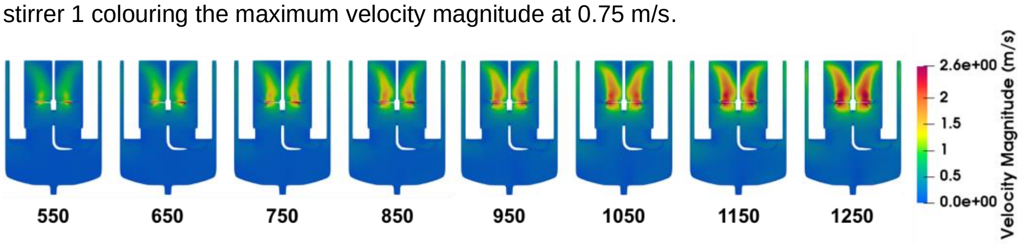

Figure 7: Velocity profiles stirrer 1 at 550, 650, 750, 850, 950, 1050, 1150, and 1250 RPMs

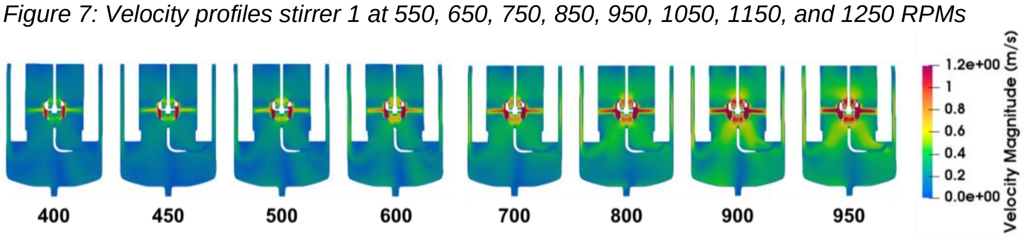

Figure 8: Velocity profiles stirrer 2 at 400, 450, 500, 600, 700, 800, 900, and 950 RPMs

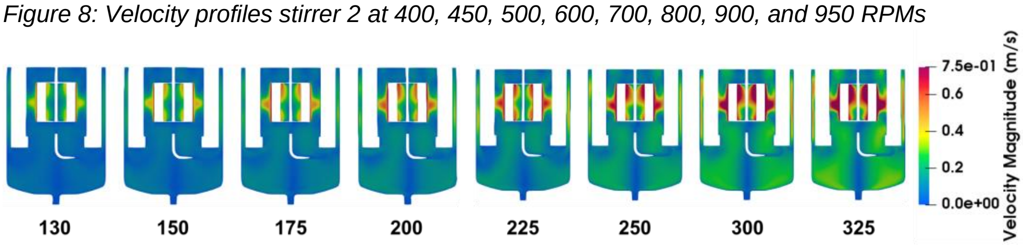

Figure 9: Velocity profiles stirrer 3 at 130, 150, 175, 200, 225, 250, 300, and 325 RPMs

4. Conclusions

This study aimed to evaluate the capability of a single-phase, steady-state solver in predicting the power consumption of lab-stirred tank reactors. Experiments were conducted to obtain torque in water of three stirring devices, and simulations using the OpenFOAM® solver SimpleFOAM were performed for comparison. While the simulations did not fully match the experimental results, the study validates the usefulness of CFD models in optimizing bioreactor design and predicting performance. Understanding CFD models is crucial for enhancing bioreactor design and performance prediction. Further research is necessary to reconcile the measured experimental values from the rotor with the simulated values from the blades. The observed discrepancies may be attributed to uncalibrated equipment.

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References

Basavarajappa, M., & Miskovic, S. (2013). Numerical study of single phase liquid mixing in stirred tanks fitted with Rushton turbine and flotation impeller. *ASME International Mechanical Engineering Congress and Exposition*, *56314*, V07AT08A047.

Blanco-Aguilera, R., Lara, J. L., Barajas, G., Tejero, I., & Diez-Montero, R. (2020). CFD simulation of a novel anaerobic-anoxic reactor for biological nutrient removal: Model construction, validation and hydrodynamic analysis based on OpenFOAM®. *Chemical Engineering Science*, *215*, 115390.

Ding, J., Wang, X., Zhou, X. F., Ren, N. Q., & Guo, W. Q. (2010). CFD optimization of continuous stirred-tank (CSTR) reactor for biohydrogen production. *Bioresource Technology*, *101*(18), 7005–7013. https://doi.org/10.1016/J.BIORTECH.2010.03.146

Fernandes Del Pozo, D., Liné, A., Dedeyne, J., Van Geem, K. M., & Nopens, I. (2019). Computational Fluid Dynamics validation study of an axial flow impeller often used in Anaerobic Digesters. *Watermatex 2019, the 10th IWA Symposium on Modelling and Integrated Assessment.*

Foukrach, M., & Ameur, H. (2019). Effect of baffles shape on the flow patterns and power consumption in stirred vessels. *SN Applied Sciences*, *1*, 1–11.

Foukrach, M., Bouzit, M., Ameur, H., & Kamla, Y. (2020). Effect of agitator's types on the hydrodynamic flow in an agitated tank. *Chinese Journal of Mechanical Engineering*, *33*, 1–18.

Jeong, K.-L., Park, S., & Jeong, S.-M. (2023). Enhancement of the Robustness on Advancing Layer Method with Trimmed Hexahedral Volume Mesh for the Generation of the Boundary Layer Grids. *Journal of Marine Science and Engineering*, *11*(2), 454.

Lu, W.-M., Wu, H.-Z., & Ju, M.-Y. (1997). Effects of baffle design on the liquid mixing in an aerated stirred tank with standard Rushton turbine impellers. *Chemical Engineering Science*, *52*(21–22), 3843–3851.

Maier, C., Weichselbaum, W., Schlerka, M., & Harasek, M. (2010). *Development of agitation systems in biogas plants: Investigation of mixing characteristics, improvement of energy efficiency and scale-up using CFD*. Citeseer.

OpenCFD Ltd. (2021). *OpenFOAM: API Guide: forces Class Reference*. https://www.openfoam.com/documentation/guides/latest/api/classFoam_1_1functionObjects_1_1forces.html#details

Segui, M., Abel, F. R., Botez, R. M., & Ceruti, A. (2022). High-fidelity aerodynamic modeling of an aircraft using OpenFoam – application on the CRJ700. *The Aeronautical Journal*, *126*(1298), 585–606. https://doi.org/10.1017/AER.2021.86

Shen, Y. Y., Qin, B., Li, X., Zhu, Z., Cui, P., Gao, J., & Wang, Y. (2021). Investigation of the flow characteristics of liquid–liquid two-phase mixing in an agitator equipped with a "V-shaped" horizontal baffle. *Environment, Development and Sustainability*, *23*(2), 2298–2313. https://doi.org/10.1007/S10668-020-00675-4/TABLES/6

Sivashanmugam, P., & Prabhakaran, S. (2008). Simulation of an effect of a baffle length on the power consumption in an agitated vessel. *International Journal of Food Engineering*, *4*(2).

Wang, Y., Rao, Q., Fan, J., & Fei, W. (2006). PIV measurements and CFD simulation of viscous fluid flow in a stirred tank agitated by a Rushton turbine. Proceedings of the 5th International Conference on CFD in the Process Industries.

Zhang, S., Müller, D., Arellano-Garcia, H., & Wozny, G. (2013). CFD simulation of the fluid hydrodynamics in a continuous stirred-tank reactor. Chemical Engineering, 32.