

Experimental and numerical investigation of free surface formation in an unbaffled stirred tank

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Abstract

The aim of this study was to conduct an experimental and numerical analysis of the hydrodynamics of two-phase flow in an unbaffled mixer equipped with a Rushton turbine. The analysis revealed clear limitations of RANS-based turbulence models under strong, axially symmetric swirling flow conditions. All analyzed models in this group (k - ϵ , SST k - ω , RSM) significantly overestimated the power number, with relative errors ranging from 95% to over 119%, which limits their utility as predictive tools in engineering practice. Furthermore, they failed to correctly represent velocity field structures, and predictions of vortex shape and depth showed poor correlation with experimental results. In contrast, the LES model demonstrated clear superiority: it predicted mixing power with a minimal error of 3.4% and velocity distributions with high precision. Additionally, it accurately reproduced the geometry of the vortex funnel, confirming its suitability for modeling flows with strong turbulence anisotropy and a dynamic free surface.

Keywords

CFD, stirred tank, LDA, turbulence modeling

1. INTRODUCTION

The advantage of unbaffled mixers over those with baffles is enhanced micromixing at a lower average specific power (Assirelli et al., 2008), alongside significant potential for power savings (Tamburini et al., 2015). This is of great importance in the pharmaceutical industry, in crystallization processes, or in certain chemical reactions involving catalysts, where the use of baffles is not recommended (Woźniowski, 2023). Furthermore, a strong vortex enables gas entrainment, a feature utilized in specialized vortex devices (Kourou et al., 2024). In (Stelmach et al., 2023), a method is proposed for approximate determination of the mixing power when a central vortex is present. In classic baffled mixers, where the liquid's vortex motion is effectively suppressed, the formation of a deep vortex at the free surface is not observed. Under such conditions, CFD modeling using Reynolds-Averaged Navier–Stokes (RANS) equations proves to be relatively effective in predicting global mixing parameters, such as power consumption or average velocity fields. For example, previous studies (Tamburini et al., 2019) demonstrated that for baffled mixers, RANS simulations (SST k - ω model) provided good agreement with experimental data regarding power characteristics and liquid discharge capacity in turbulent flow. The widespread use of RANS models stems from their relatively low computational requirements and the fact that flow in baffled mixers is less anisotropic and can be treated as steady under appropriate symmetry assumptions (Coroneo et al., 2011; Reid et al., 2025; Singh et al., 2011).

However, challenges arise in unbaffled configurations, where a vortex funnel forms at the liquid surface. Such systems are significantly more difficult to model because the flow is characterized by strong heterogeneity, anisotropic turbulence, and dynamic free-surface deformations. Studies indicate that classical RANS models lose accuracy under these conditions (Płusa and Duda, 2022; Yang and Zhou, 2015). Despite numerous studies, further research is needed to improve the accuracy of numerical models for designing unbaffled mixers. This study sought to develop, implement, and validate a numerical method capable of reliably and effectively predicting key operating parameters, such as velocity field distributions, turbulent kinetic energy, mixing power, free-surface shape, and aeration risk.

2. TEST BENCH AND MEASUREMENTS

Experimental measurements were conducted at the Chair of Thermal and Process Engineering, Faculty of Mechanical Engineering, Cracow University of Technology. The experimental apparatus consisted of an unbaffled stirred tank equipped with a centrally located Rushton turbine. The impeller featured six equally spaced blades attached to a central disc. The internal diameter of the tank was $D = 286$ mm, with the liquid level maintained at $H = D$. The impeller dimensions were as follows: diameter $d = D/3$, blade height $b = d/5$, blade width $w = d/4$, and a thickness of 4 mm. The central disc had a diameter of $d_d = d/3$ and a thickness of 4 mm (Fig. 1).



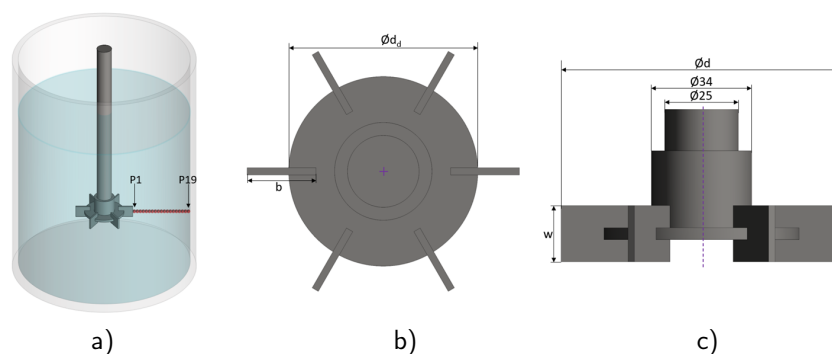


Figure 1. Object of research a) stirred tank, b) Rushton turbine – top view, c) Rushton turbine – side view.

To facilitate optical access, the tank walls were constructed from transparent DURAN glass. Dimethyl sulfoxide (DMSO) was selected as the working fluid to achieve refractive index matching with the laser light beam. The complete experimental setup is illustrated in Fig. 2, which shows the structural supports, the traversing system for the measurement device, and the tank coupled with the drive unit with a scheme of the test bench.

The measurements were performed at a rotational speed of $n = 225$ RPM in a clockwise direction. The operational impeller speed of $n = 225$ RPM ($Re = 16,186$) was chosen based on three key criteria: it ensures a fully turbulent regime ($Re > 10,000$) for model validation, captures the exact threshold for free-surface aeration inception, and satisfies Laser Doppler Anemometry (LDA) constraints. Although the DURAN glass and dimethyl sulfoxide (DMSO) were refractive-index-matched, higher speeds would generate excessive air entrainment. The resulting bubbles scattered laser light and caused severe data loss. Therefore, $n = 225$ RPM optimized free-surface deformation while maintaining continuous phase transparency. Throughout the experiments, the temperature of the fluid was maintained at $22.5\text{ }^{\circ}\text{C} \pm 0.2\text{ }^{\circ}\text{C}$. A Dantec two-channel Laser Doppler Anemometry (LDA) system was employed to determine velocity distributions, velocity fluctuations, turbulence intensity, and turbulent kinetic energy (TKE) within the mixer.

Shaft torque was measured using a VIBRO-METER TG-0.2 inductive torque transducer, featuring a manufacturer-specified accuracy of ± 0.01 Nm. The rotational speed was monitored via an ML-103 photoelectric rotation sensor. Additionally, the mixer's operation was recorded for several tens of seconds using a Canon EOS R10 digital camera, with a specific focus on the vortex funnel region. The recorded video footage was processed using MATLAB R2020a software (The MathWorks, Inc. 2020). The videos were decomposed into individual frames, which were then exported as image files for further digital image processing. Ultimately, this procedure allowed for the determination of the time-averaged profile of the free-surface vortex.

3. NUMERICAL MODEL

All numerical simulations were performed using the Simcenter STAR-CCM+ software package (version 2506) (Siemens Digital Industries Software, 2025). The computations were carried out on the Ares computing cluster, which is part of the Polish Grid Infrastructure (PLGrid). PLGrid provides a nationwide high-performance computing (HPC) infrastructure for the scientific community, offering access to supercomputers and advanced computational services for tasks such as CFD simulations, quantum calculations, and data science.

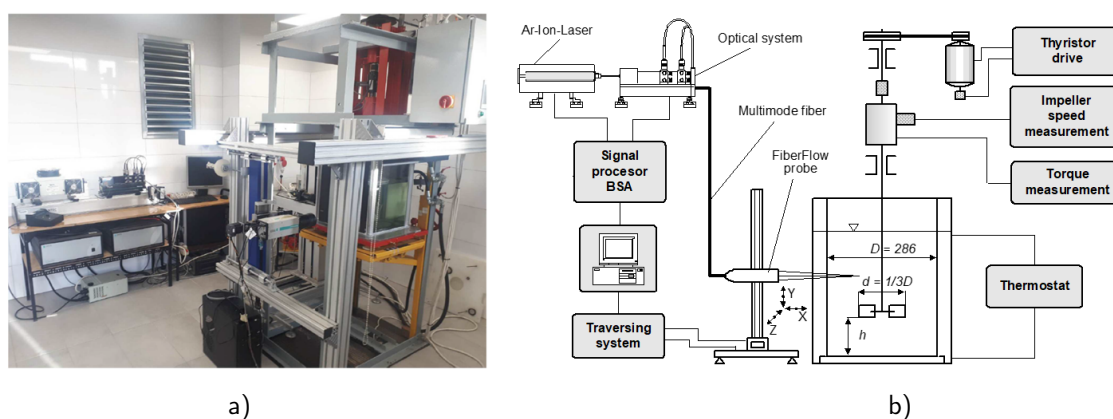


Figure 2. Test rig arrangement in the laboratory: a) photo, b) scheme.

The computational geometry included the mixer assembly and a 10 cm air headspace above the liquid surface. The tank walls, the shaft, and the impeller were assumed to be rigid bodies, as they were constructed from materials with a high Young's modulus. Consequently, it was assumed that no significant structural deformation occurred during operation that would lead to noticeable dimensional changes. This assumption allowed for the exclusion of solid domains from the simulation, focusing the analysis solely on the fluid volumes (liquid and air) within the mixer.

A sliding mesh approach was employed to model the impeller rotation. In this method, the computational domain is partitioned into stationary and rotating zones, each with its own independent mesh. These meshes move relative to one another, with the exchange of physical quantities across the non-conformal boundary facilitated by an interpolation interface (Siemens Digital Industries Software, 2025). This approach enabled an accurate representation of the actual rotational motion of the impeller and its associated hydrodynamic effects. The geometric model of the mixer is presented in Fig. 3.

The system was modeled as a transient, perfectly closed domain. A no-slip boundary condition was applied to all walls. For the cylindrical wall segment in contact with the rotating shaft, a tangential velocity was prescribed to match the peripheral speed generated by the shaft's rotation. The physical properties of dimethyl sulfoxide (DMSO) at the experimental temperature were set to a density of 1100 kg/m^3 and a dynamic viscosity of $0.0023 \text{ Pa} \cdot \text{s}$. Surface tension was $\sigma = 0.043 \text{ N/m}$. From the onset of the simulation ($t = 0 \text{ sec}$), the nominal rotational speeds of both the impeller and the shaft were applied. The initial liquid level in the tank was set according to the specifications provided in Section 2, as illustrated in Fig. 4.

A Cartesian-based mesh, referred to as a "trimmed cell mesh" in Simcenter STAR-CCM+ (and analogous to "cut-cell" or "Cartesian" meshes in other CFD packages), was utilized. This meshing approach is characterized by a regular structure

of hexahedral elements that are trimmed exclusively at the geometric boundaries of the computational domain to ensure an accurate representation of the surface. This approach ensures high cell quality throughout the volume, minimizing numerical errors and enhancing computational stability.

The near-wall boundary layer physics was captured using a hybrid y^+ wall treatment strategy ('All y^+ wall treatment'), which adaptively switches between direct low y^+ resolving and high y^+ wall-function modeling depending on the local cell refinement. In the dynamic rotating domain containing the impeller blades, the near-wall flow was fully resolved down to the viscous sublayer, achieving a highly accurate target grid resolution of $y^+ < 1$. In the stationary domain walls where the velocity gradients were substantially lower, the buffer and logarithmic boundary layers were modeled.

Furthermore, Cartesian meshes are particularly well-suited for Adaptive Mesh Refinement (AMR), which allows for efficient, local resolution enhancement in specific regions based on predefined criteria, without compromising the quality of the surrounding cells. This enables an accurate representation of complex geometries and key flow phenomena while maintaining high computational efficiency. To correctly resolve velocity gradients in the near-wall regions, prism layers (also referred to as inflation layers) were applied. These consisted of thin, high-aspect-ratio elements generated orthogonally to the wall surfaces, specifically designed to capture boundary layer effects. The computational grid was optimized to minimize the total cell count while selectively refining areas characterized by the highest velocity gradients. Particular attention was paid to the impeller region to effectively capture the developing vortical structures.

In this study, four turbulence models were evaluated ($k-\varepsilon$, SST $k-\omega$, RSM and LES). The $k-\varepsilon$ model was implemented in its Realizable formulation. Both the $k-\varepsilon$ and SST $k-\omega$ models were modified by incorporating the Curvature Correction term to account for rotational effects. For the high-fidelity LES approach, the subgrid-scale (SGS) turbulent fields were mod-

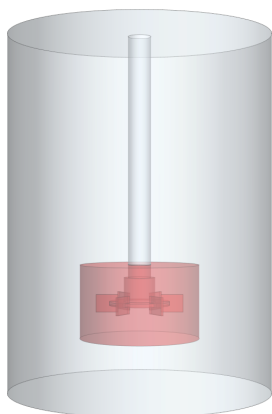


Figure 3. Visualization of stationary (gray) and rotating (red) domain.

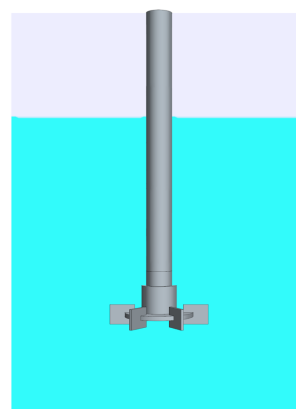


Figure 4. Initial height of the water.

eled using the algebraic Wall-Adapting Local-Eddy Viscosity (WALE) formulation. The implicit spatial filter width (Δ) within the finite volume discretization was defined as a function of the local cell volume according to the cubic relation:

$$\Delta \approx (|V_P|)^{1/3} \approx C_w(\Delta x \Delta y \Delta z)^{1/3} \quad (1)$$

where the filter coefficient was set to $C_w = 0.544$.

Since the simulations were performed in transient mode, the temporal domain also required discretization. A critical parameter in the simulation setup was the selection of an appropriate time step. To ensure numerical stability and adequate temporal accuracy of the solution, the time step selection was based on the Courant–Friedrichs–Lewy (CFL) criterion:

$$CFL = \left(\frac{u \Delta t}{\Delta x} \right) \quad (2)$$

An adaptive time-stepping strategy was employed, in which the time step size was determined based on the prescribed maximum and average CFL numbers at each time step, as presented in Equations (3) and (4).

$$\Delta t_{\max} = CFL_{\max}^{\text{target}} \cdot \min \left(\frac{\Delta x_i}{u_i} \right) \quad (3)$$

$$\Delta t_{\text{med}} = CFL_{\text{average}}^{\text{target}} \cdot \frac{\sum_{i=1}^N V_i}{\sum_{i=1}^N \left(\frac{u_i}{\Delta x_i} \cdot V_i \right)} \quad (4)$$

Subsequently, the time step corresponding to the lower value was selected. The values of $CFL_{\max}^{\text{target}}$ and $CFL_{\text{average}}^{\text{target}}$ were defined as follows, depending on the turbulence model:

- RANS model: for mesh cells containing the free surface, $CFL_{\max}^{\text{target}} = 2$; $CFL_{\text{average}}^{\text{target}} = 0.25$; for the remaining elements, $CFL_{\max}^{\text{target}} = 20$; $CFL_{\text{average}}^{\text{target}} = 0.5$
- LES model: for mesh cells containing the free surface, $CFL_{\max}^{\text{target}} = 2$; $CFL_{\text{average}}^{\text{target}} = 0.25$; for the remaining elements, $CFL_{\max}^{\text{target}} = 5$; $CFL_{\text{average}}^{\text{target}} = 0.2$

The number of inner iterations for the SIMPLEC algorithm (Van Doormaal and Raithby, 1984) was set to five. For the multiphase model, the High Resolution Interface Capturing (HRIC) scheme (Siemens Digital Industries Software, 2025) was employed for free-surface reconstruction. Spatial discretization was performed using second-order central differencing schemes, combined with an implicit temporal integration method.

To evaluate grid independence (mesh sensitivity), three distinct meshes – designated as M1, M2, and M3 were generated, as illustrated in Fig. 5.

For the LES model, the quality of the resolved turbulence was further evaluated using Pope's index (Pope, 2000), defined by the following equation:

$$M_{\text{Pope}} = \frac{k_{\text{SGS}}}{k_{\text{SGS}} + k_{\text{RES}}} \quad (5)$$

Pope (2000) recommends that the ratio of the sub-grid scale (SGS) kinetic energy to the total turbulent kinetic energy (resolved plus modeled) should not exceed 25%. In this study, the variable k_{SGS} was obtained directly from the Simcenter STAR-CCM+ solver, while the resolved turbulent kinetic energy k_{RES} was calculated based on the root-mean-square (RMS) velocity components as follows:

$$k_{\text{RES}} = 0.5 (u_{\text{RMS}}^2 + v_{\text{RMS}}^2 + w_{\text{RMS}}^2) \quad (6)$$

In Large Eddy Simulations, assessing the degree of resolved turbulence is of paramount importance. A higher fraction of resolved energy k_{RES} ensures a more high-fidelity representation of the flow dynamics and momentum transfer. Conversely, if the majority of the turbulent energy is modeled (k_{SGS}), the LES results may degenerate toward RANS-like behavior, potentially leading to an inaccurate representation of turbulent phenomena.

Table 1 summarizes the Power Number values obtained for both the SST $k-\omega$ and LES models across the M1, M2, and M3 meshes, along with the volume-averaged Pope's index for the LES cases. A mesh sensitivity study was conducted for the same system, but one equipped with baffles (Płusa,

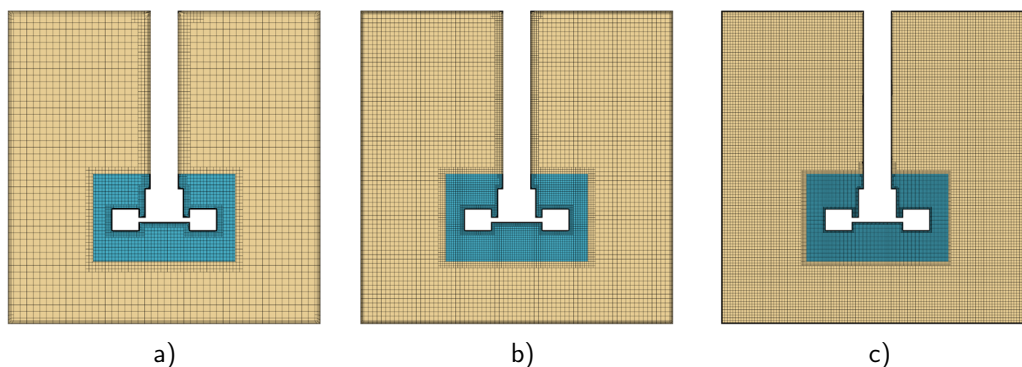


Figure 5. Mesh view in horizontal section for: a) M1, b) M2, c) M3.

2025). In the analyzed system without baffles, the findings from previous analyses were applied. This is a bit of an oversimplification, because the mesh independence of the baffled configuration does not automatically prove mesh independence for the unbaffled configuration. However, Płusa (2025) demonstrated that this approach is entirely sufficient and that the grid-generation strategy is universally applicable to various stirred tank configurations. A negligible impact of mesh density on the Power Number was observed for both turbulence models. Furthermore, the volume-averaged Pope's index indicates that both the M2 and M3 meshes satisfy the recommended $< 25\%$ criterion.

Table 1. Power number and Pope's index as a function of turbulence model and computational grid resolution for a baffled configuration.

Turbulence model	Mesh	Power number [–]	Pope criterion [–]
SST $k-\omega$	M1	4.77	—
SST $k-\omega$	M2	4.81	—
SST $k-\omega$	M3	4.82	—
LES	M1	5.05	0.284
LES	M2	5.09	0.153
LES	M3	5.12	0.0821

For the M1 mesh, local Pope index values exceeded 0.4, whereas for the M3 mesh, they remained below 0.25. The M2 mesh appears to be at the threshold of suitability for LES according to this criterion, despite its volume-averaged index being 0.153. Finally, the mesh M3 was selected for further calculations. Figure 6 shows the y^+ parameter distribution for mesh M3 and the LES model. The distribution meets the

requirements of the hybrid 'All y^+ wall treatment' model, meaning that the y^+ values in regions where the flow needs to be resolved within the viscous sublayer (the walls of the rotating domain) reach a maximum of approximately 1. In the remaining regions, the values range from 3 to 17. The average y^+ values for the rotating and stationary domains were 0.42 and 6.91, respectively. Since the M3 computational mesh was sufficient for the LES approach, it was assumed to be equally adequate for the RANS family of turbulence models.

4. RESULTS

A comparison between the numerical and experimental results for the stirred tank is presented. The axial, tangential, and radial velocity distributions, as well as the turbulent kinetic energy (TKE) were verified against LDA measurements. Furthermore, the power consumption obtained from the CFD simulations was compared with the values calculated using the experimental power number. The numerical results are provided for four turbulence models: $k-\varepsilon$, SST $k-\omega$, RSM, and LES. For all simulations, the total flow time was 45 seconds, with time-averaging of velocity, power, and free-surface profile initiated at the 35th second, after the velocity field had fully stabilized.

Figure 7 illustrates the instantaneous and time-averaged velocity fields in a horizontal cross-section at the impeller disk mid-plane. Significant differences between the various turbulence models are evident in the instantaneous velocity distributions.

As the complexity of the model increases, the hydrodynamic wakes (shadows) forming behind the rotating blades become both longer and narrower. The LES model accurately reflects the characteristic stochastic nature of the flow, whereas the instantaneous distributions for the RANS models ($k-\varepsilon$, SST $k-\omega$, RSM) exhibit a more regular, axisymmetric structure.

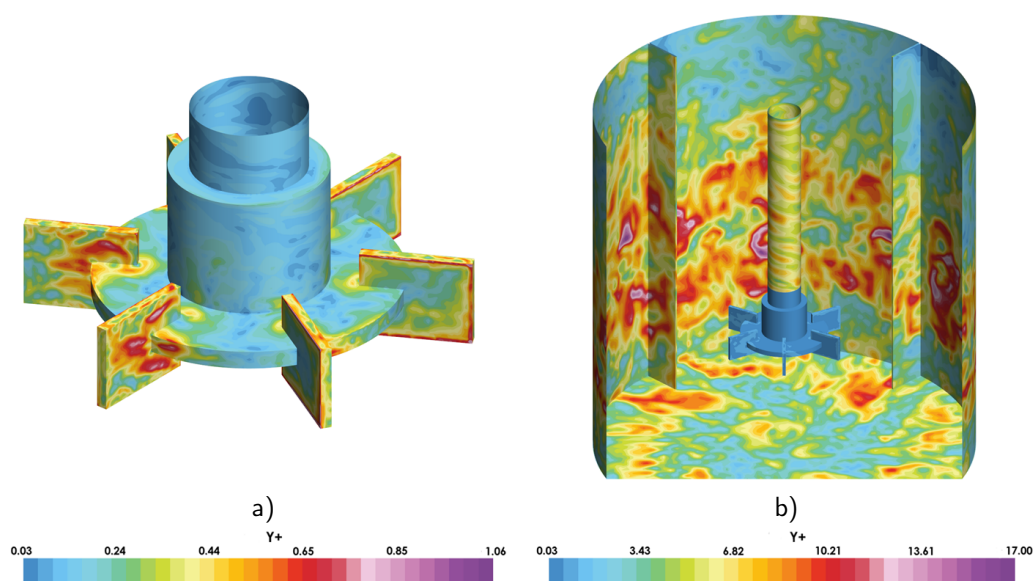


Figure 6. Distribution of the y^+ parameter: a) walls in the rotating domain, b) all walls except the top wall.

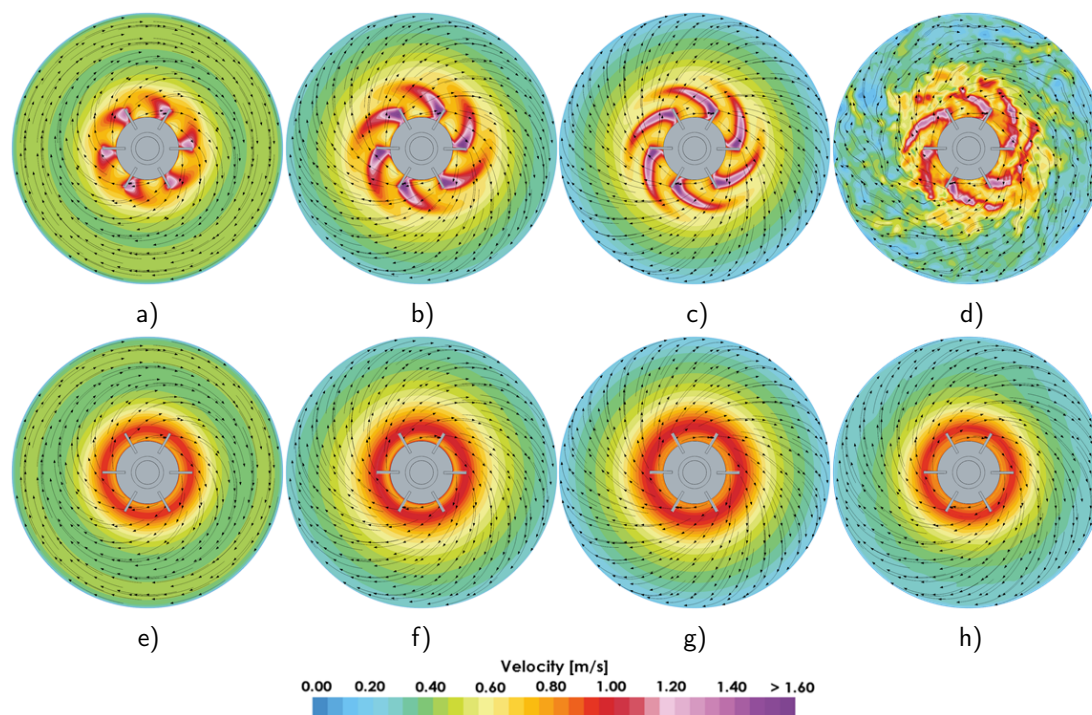


Figure 7. Velocity distributions in the horizontal plane: a) instantaneous $k-\epsilon$, b) instantaneous SST $k-\omega$, c) instantaneous RSM, d) instantaneous LES, e) average $k-\epsilon$, f) average SST $k-\omega$, g) average RSM, h) average LES.

Notable similarities were observed between the RSM and LES results, and between the $k-\epsilon$ and SST $k-\omega$ models. This is because RSM is a second-moment RANS closure, whereas the $k-\epsilon$ and SST $k-\omega$ models are eddy-viscosity closures. The former, therefore, allows for the anisotropy of turbulence. The SST $k-\omega$ model appears to serve as an intermediate approach between the $k-\epsilon$ and LES formulations. Specifically, the $k-\epsilon$ model exhibits lower velocity values near the impeller – approximately 0.3 m/s less than the other models. While the averaged velocity fields for the SST $k-\omega$, RSM, and LES models show similar characteristics regarding both the velocity values near the impeller and the gradients toward the walls, the $k-\epsilon$ model systematically underestimates the velocity in the impeller region while overestimating it at greater distances from the turbine. All profiles presented in Fig. 7 clearly demonstrate the strongly tangential nature of the flow.

Figure 8 presents the instantaneous and time-averaged velocity fields within a vertical cross-section passing through the axis of the stirred tank. Velocity vectors are displayed exclusively for the liquid phase. The vortex funnel is highlighted in orange; for the instantaneous fields, it represents the interface at a specific point in time, while for the time-averaged fields, the profile of the averaged free surface is shown.

Consistent with the horizontal plane analysis, significant differences are observed in the instantaneous velocity distributions depending on the turbulence model employed. Similarities in velocity magnitudes are evident between the RSM and LES models, as well as between the $k-\epsilon$ and SST $k-\omega$ models. The

$k-\epsilon$ and SST $k-\omega$ tend to overestimate the velocity in regions distant from the impeller. The LES model, as in the previous cases, reflects a strongly aperiodic flow nature. A characteristic feature of the LES results is the deviation from a purely radial discharge; specifically, an inclination of the stream exiting the turbine toward the bottom of the tank is observed.

Furthermore, the $k-\epsilon$ and SST $k-\omega$ models induce a bifurcation of the upper circulation loops into two smaller, counter-rotating vortices – a phenomenon not observed in the RSM and LES results. This discrepancy arises from the inherent limitations of the $k-\epsilon$ and SST $k-\omega$ models in accurately predicting velocity fields in flows characterized by strong turbulence anisotropy.

Using the SST $k-\omega$ model as an example, the contour map in Fig. 9 illustrates the spatial distribution of the turbulent viscosity ratio μ_t/μ . The highest values occur near the centers of the primary recirculation loops above and below the impeller plane, rather than within the high-shear discharge stream. It should be emphasized that a high μ_t/μ ratio in these recirculation centers does not represent high Reynolds shear stresses, as the local mean strain-rate tensor near the centers of the circulation loops is near zero. Instead of generating localized stresses, this elevated eddy viscosity acts as an unphysical momentum diffusion mechanism. It artificially damps the macro-scale circulation loops and over-diffuses bulk momentum transport across the unbaffled vessel, which contributes to the severe overprediction of global mixing power observed in RANS calculations.

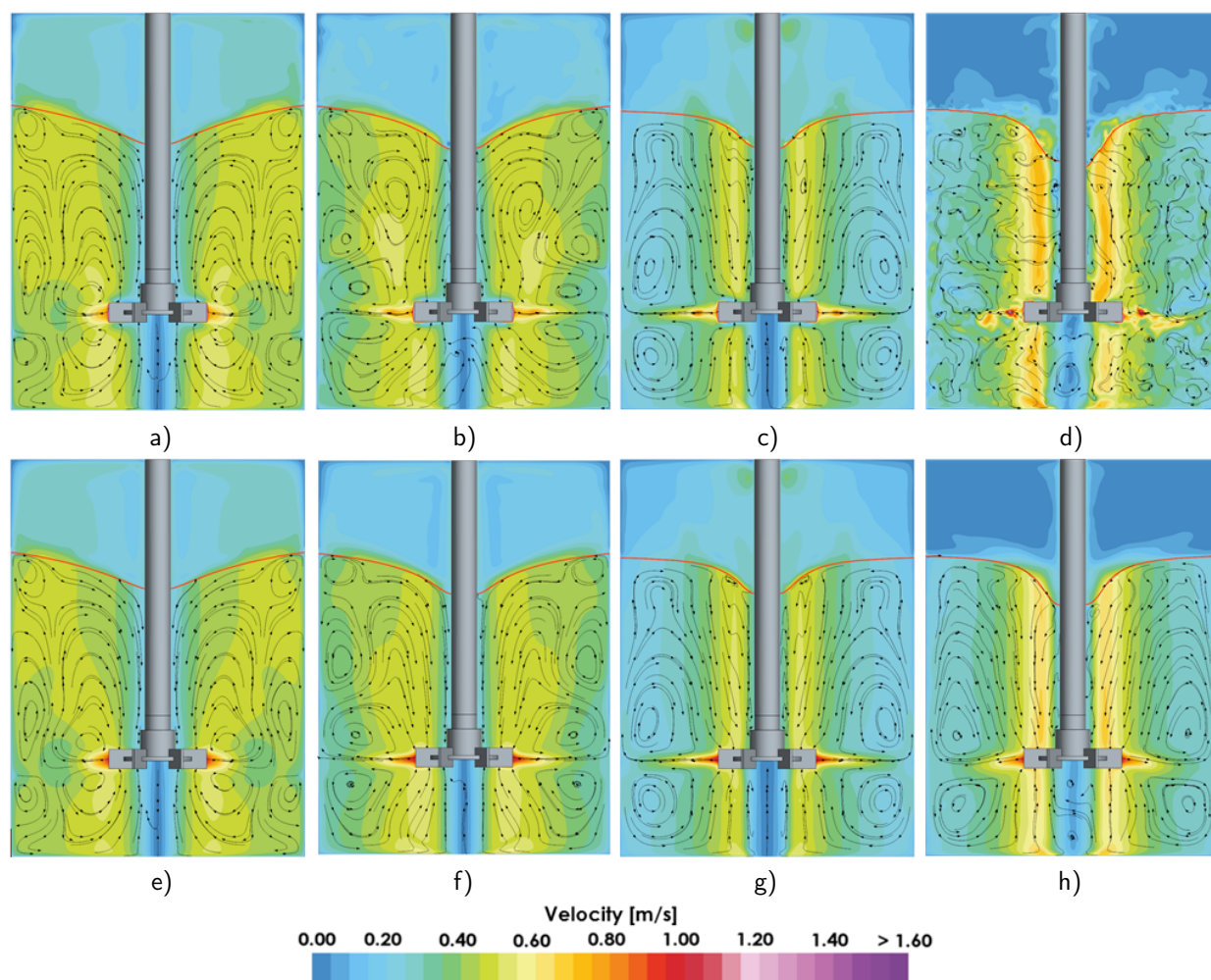


Figure 8. Velocity distributions in the vertical plane: a) instantaneous $k-\epsilon$, b) instantaneous SST $k-\omega$, c) instantaneous RSM, d) instantaneous LES, e) average $k-\epsilon$, f) average SST $k-\omega$, g) average RSM, h) average LES.

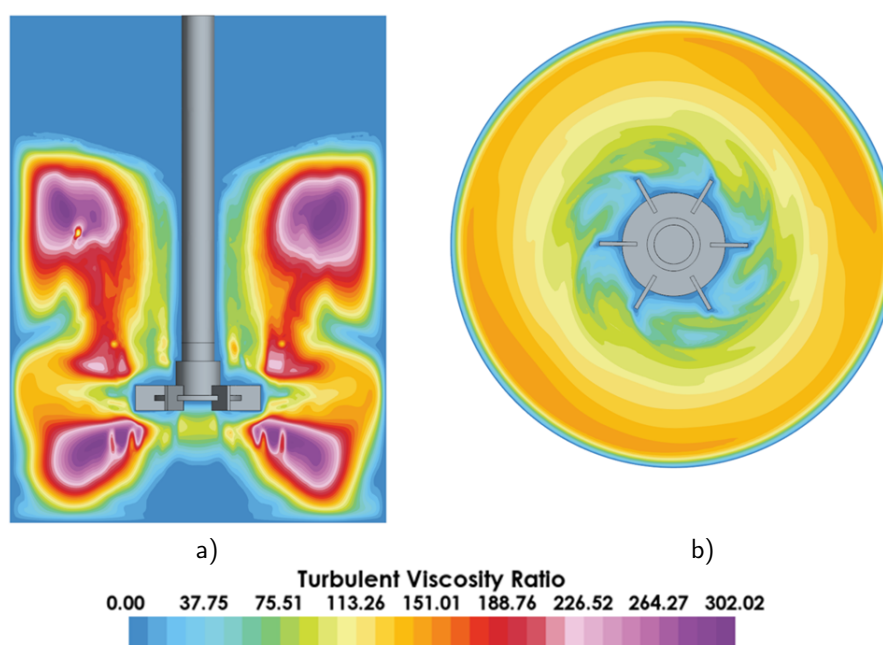


Figure 9. Turbulent viscosity ratio for SST $k-\omega$ turbulence model: a) vertical plane, b) horizontal plane.

Figure 10 illustrates the distributions of mean velocities and mean turbulent kinetic energy (TKE) between the outer radius of the agitator ($d/2 = 47.6$ mm) and the inner radius of the tank ($D/2 = 143$ mm). Regarding the axial velocity, the RSM and LES models show the closest agreement with the experimental data. The RSM model begins to underestimate the velocity at radial positions exceeding 105 mm, while exhibiting a nearly linear profile for smaller radii. The LES model slightly underestimates the velocity for radii below 90 mm, overestimates it in the range between 95 and 120 mm, and subsequently underestimates it again relative to the measured values beyond this range. Notably, the $k-\epsilon$ and SST $k-\omega$ models fail to accurately reproduce the experimental trend and, furthermore, predict an opposite flow direction.

The best correlation with the radial velocity distribution was achieved by the LES model, with deviations from the measured values not exceeding 0.08 m/s. Conversely, the RSM model exhibited the largest discrepancies, which is somewhat surprising given that it was specifically developed for flows characterized by strong swirl. While the SST $k-\omega$ model reproduced the radial velocity distribution relatively well, it showed larger deviations from the experimental data compared to LES. The $k-\epsilon$ model overestimated the velocity for radii smaller than 110 mm, particularly in the impeller region, though it predicted values with reasonable accuracy near the tank walls.

Regarding the overall radial velocity trend, the LES model again provided the highest fidelity, overestimating the velocity by only 0.1 m/s in the vicinity of the impeller blades. The $k-\epsilon$ model overestimated the velocity across nearly the entire radius while maintaining a qualitatively correct trend relative to the experimental data. A similar behavior was observed for the RSM model, which, nevertheless, underestimated the velocity for radii exceeding 90 mm. The SST $k-\omega$ model followed a distribution similar to LES but began to overestimate values compared to the experiment for radii beyond 90 mm.

The trend for turbulent kinetic energy (TKE) was once again best captured by the LES model, which showed the smallest deviations from experimental results, despite a slight overestimation in the impeller region. The RSM model exhibited the lowest agreement with the experimental trend, generating the largest discrepancies among all analyzed turbulence models. The SST $k-\omega$ model showed relatively good consistency with the experimental curve but significantly underestimated TKE values for radii smaller than 75 mm. The $k-\epsilon$ model yielded average agreement across the entire radial distribution.

The power consumption was time-averaged over the final 10 seconds of each simulation. After converting the mean power values into dimensionless power numbers they were compared with the experimental value in Fig. 11. The RANS-based

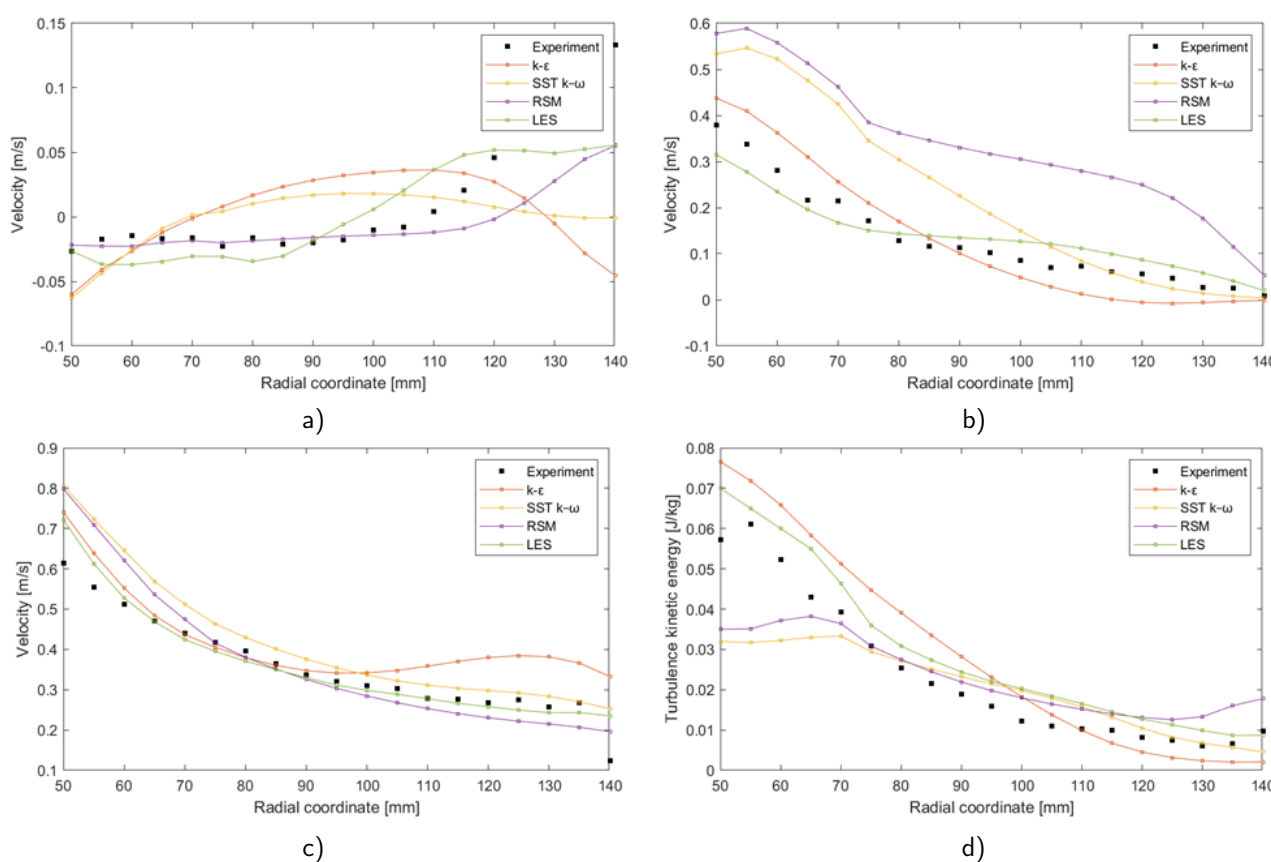


Figure 10. Comparison of measured and calculated average values: a) axial velocity, b) radial velocity, c) tangential velocity, d) kinetic energy of turbulence.

models significantly overestimated the mixing power, with relative errors for $k-\epsilon$, SST $k-\omega$, and RSM reaching 119.1%, 100.5%, and 94.9%, respectively. Only the LES model predicted the power consumption with high accuracy, yielding a relative error of merely 3.4%.

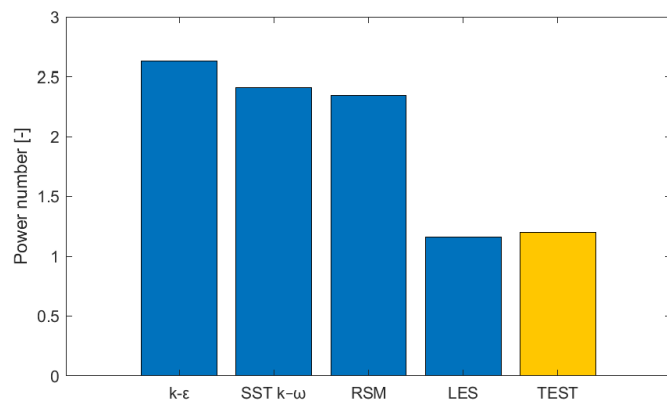


Figure 11. Comparison of the power values obtained in numerical simulations with the experimental value.

The excessive turbulent viscosity generated by RANS models distorted both the radial discharge jet and tangential circulation. This over-diffusion alters the local flow angle relative to the rotating blades, exacerbating flow separation and artificially increasing the pressure differential between the front and back surfaces of the Rushton blades. Additionally, the failure of RANS models to accurately capture the deep vortex funnel leaves an unphysical column of liquid above the impeller plane. This additional fluid mass exerts an elevated hydrostatic and inertial resistance on the primary recirculation loops. The combined effect of inflated blade pressure drag and excessive liquid head above the impeller leads to an overprediction of the integrated shaft torque, directly driving the overestimation of the global power number.

Figure 12 displays the instantaneous distribution of the free surface in a vertical projection. The liquid–gas interface was visualized using an isosurface generated at a liquid volume fraction of 0.5. The analysis of these distributions indicates

that as the complexity of the turbulence model increases, the predicted vortex funnel morphology progressively aligns with the experimental observations shown in Fig. 13. Notably, circumferential asymmetry is only observable in the vortex funnel predicted by the LES model, which is in excellent agreement with the findings from the experimental study.

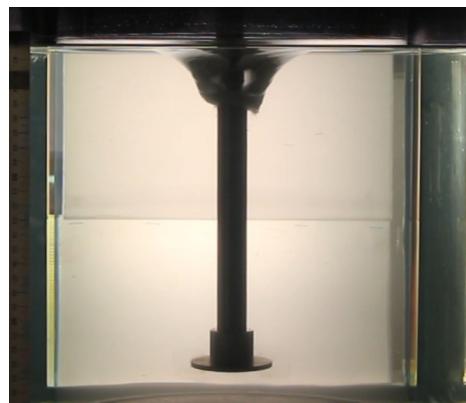


Figure 13. A picture of the instantaneous shape of the vortex funnel at the test stand.

Figure 14 presents the time-averaged profiles of the vortex funnel for each turbulence model, alongside the experimentally obtained profile for comparison. The mean vortex shapes in the simulations were determined by averaging the liquid volume fraction in each computational cell at every time step over the final 10 seconds of the simulation. Subsequently, a contour line representing a mean volume fraction of 0.5 was extracted from the vertical cross-section.

The experimental distribution was imported into the post-processor as a spline connecting the coordinates derived from the vortex shape analysis performed in MATLAB (The MathWorks, Inc. 2020). Analysis of the results in Fig. 14 indicates that the time-averaged vortex funnel profiles for the RANS models do not deviate significantly from their corresponding instantaneous distributions. Furthermore, it is observed that as the complexity of the turbulence model increases, the

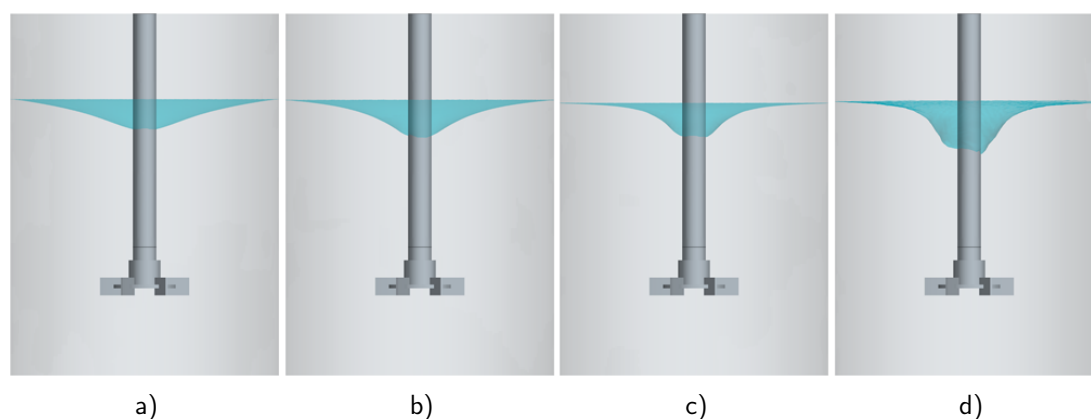


Figure 12. Visualization of the free surface in a vertical cross-section: a) $k-\epsilon$, b) SST $k-\omega$, c) RSM, d) LES.

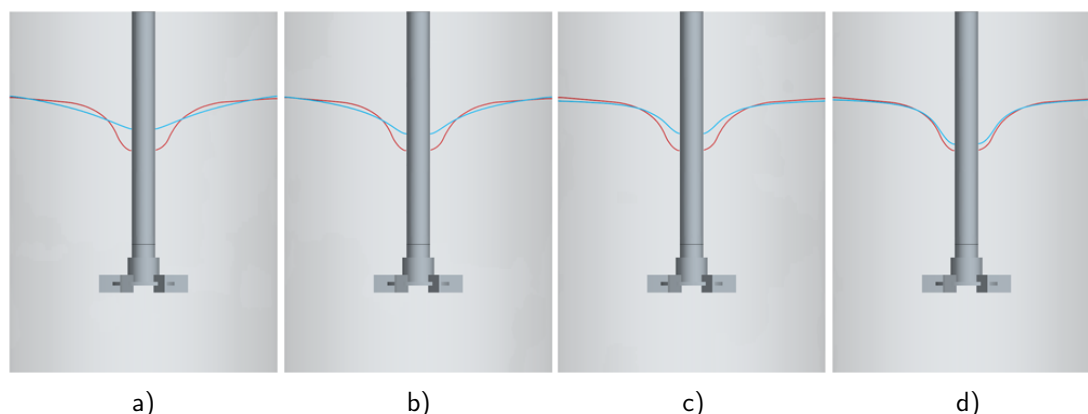


Figure 14. Time-averaged shape of a vortex funnel. The blue line represents the simulation result and the red line represents the experimental result. Turbulence models: a) $k-\varepsilon$, b) SST $k-\omega$, c) RSM, d) LES.

predicted vortex shape aligns progressively better with the experimental results. The LES model demonstrates very high consistency with the experimental data, with the exception of the region in the immediate vicinity of the shaft, where a slight underestimation of the vortex depth is observed. Results indicate that the likely cause of such a substantial overestimation of the mixing power by the URANS models ($k-\varepsilon$, SST $k-\omega$, RSM) is the excessive production of turbulent viscosity (μ_t). This could have led to a significant suppression of vortex structures, consequently increasing the drag forces generated on the impeller. The poorly resolved hydrodynamics could, in turn, be the reason for the inaccurate velocity field prediction and an overly shallow vortex funnel.

In summary, it can be concluded that RANS-based turbulence models are inadequate for predicting power consumption and velocity field distributions in unbaffled stirred tanks characterized by strong swirling flows. Furthermore, these models prove unsuitable for the accurate identification of the free-surface morphology.

5. CONCLUSIONS

The investigation of the unbaffled stirred tank with a centrally located impeller revealed significant limitations of RANS-based turbulence models under conditions of strong, axisymmetric swirling flow. All analyzed models within this group ($k-\varepsilon$, SST $k-\omega$, RSM) led to a substantial overestimation of the power number, with relative errors ranging from 95% to over 119%, effectively rendering them inadequate as predictive tools for engineering applications. Furthermore, these models were unable to correctly capture the velocity field structure, and their predictions regarding the morphology and depth of the forming vortex funnel showed poor correlation with experimental data. In contrast, the LES model demonstrated clear superiority, predicting the mixing power with high precision (a relative error of 3.4%) and accurately reproducing velocity distributions. Additionally, LES captured the

geometry of the vortex funnel with high fidelity. These results confirm the adequacy of the LES approach for modeling flows characterized by strong turbulence anisotropy and a dynamic free surface.

Regarding computational costs and resources, the study demonstrated that achieving high-fidelity results is intrinsically linked to substantial computational demands. LES simulations, which were the only ones to provide reliable results in complex configurations, required approximately twice the computational time compared to the most advanced RANS models. The execution of these analyses was possible only through the use of High-Performance Computing (HPC) infrastructure, utilizing between 480–720 processor cores for dozens of hours per single simulation. A key optimization strategy was the implementation of Adaptive Mesh Refinement (AMR), which enabled intelligent grid density management – maintaining refinement only in the critical region of the liquid-gas interface – thereby making these demanding simulations practically feasible. Although this work utilized dedicated HPC infrastructure, such calculations are increasingly viable for industrial practice through widely available cloud computing resources.

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SYMBOLS

b	blade height, m
d	impeller diameter, m
d_d	disc diameter, m
D	tank diameter, m
h	impeller off-bottom clearance, m
H	liquid level at rest, m

k	turbulence kinetic energy, m^2/s^2
n	rotational speed, RPM
N	number of samples, –
N_P	power number, $N_P = \frac{P}{\rho n^3 d^5}$, –
Re	Reynolds number, $Re = \frac{\rho n d^2}{\mu}$, –
t	time, s
u	fluid speed, m/s
w	blade width, m

Greek symbols:

Δx	mesh element size (spatial resolution)
μ	dynamic viscosity, $\text{Pa} \cdot \text{s}$
ρ	density, kg/m^3

Abbreviations:

AMR	Adaptive Mesh Refinement
CFL	Courant–Friedrichs–Lewy number
LDA	Laser Doppler Anemometry
LES	Large Eddy Simulation
RANS	Reynolds-Averaged Navier–Stokes
RES	Resolved
RSM	Reynolds Stress Model
SGS	Sub-Grid Scale

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