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ON FLOW SIMULATION STRATEGY FOR INDUSTRIAL MIXING VESSELS

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Abstract

The CFD-based analyses, optimizations, and troubleshooting of industrial-scale mixing tanks require a substantially simplified yet sufficiently accurate simulation strategy. Although there are numerous numerical studies on the simulation of various mixing vessels, most lack validation; based on a thorough review of studies reporting validated results, it is difficult to recommend a simulation methodology. This contribution summarizes a three-year effort to develop and validate such a recommended methodology. The methodology provides recommendations on mesh density, mesh structure, and the choice of turbulence model. The resulting strategy is first based on simulations of the flow field in a cylindrical baffled vessel, for which there is sufficient experimental data in the literature. Next, the strategy is validated using original experimental data obtained from a rectangular mixing tank with single- and double-impeller arrangements, two impeller types, and three impeller speeds.

Keywords: industrial-scale simulation, turbulence model choice, mixing vessel simulation

1 Motivation

This contribution reports on the development and validation of a simulation strategy applicable to the analysis, optimization, and troubleshooting of large-scale mixing vessels used in the production industry, particularly in water treatment facilities (WTFs). To present a motivation for this kind of research and illustrate the typical layout of the mixing vessel found in the water treatment industry, let's consider a stirred flocculation tank used in the *WTF Tlumačov, Czech Republic*, which was the subject of our academia-industrial collaboration five years ago. The vessel in question is a rectangular tank 8.7 m × 4.6 m × 2.7 m, equipped with two hyperbolic impellers of 1.5 m in diameter, positioned near the tank's floor, in the vessel's axis at the x-coordinates of 1.75 m and 6.1 m, respectively; the impellers rotate in the opposite direction. The inflow to the tank is approx. 50 L/s, providing the mean residence time of approx. half an hour. However, the observations of local operators led to the conclusion that the mixing inside the vessels is not optimal, with a substantial part of the inflow bypassing the mixed flocculation zone.

The question at that time was whether we could simulate the flow characteristics inside the tank and potentially propose changes in impeller position and rotation rate, which would improve the suboptimal function of the flocculation stage. Concerning the flow problem size and large characteristic times, we designed these simulations as *steady-state*, solving the Reynolds-Averaged Navier-Stokes equations (RANS), testing the three commonly used turbulence closures: (i) standard $k-\epsilon$ model for its simplicity, (ii) $k-\omega$ model for its expected better ability to catch the flow separation near impellers, and (iii) $k-\omega$ SST model, being considered as the industrial standard.The resulting flow fields are illustrated in Figure 1. As shown, the flow fields are quite different, predicting also substantially different mean flow paths and mean shear rate acting on suspended particles - flocs. Surprisingly, even with a thorough literature review on simulation strategy for mixing vessels, particularly of that size, we didn't find any conclusive recommendations not only for the turbulence model choice, but also for the simulation settings, e.g., the mesh density requirements or impeller motion modeling. To (at least partially) fill this knowledge gap, we started a research project aiming to describe and validate a recommended methodology for simulations of large mixing vessels.

2 Introduction

By production capacity, the water treatment industry is the largest in the world. In both drinking water and wastewater treatment facilities, mixing is an essential operation used for proper chemical homogenization, microbial culture distribution, batch aeration, and, in the latter treatment steps, the aggregation of impurities

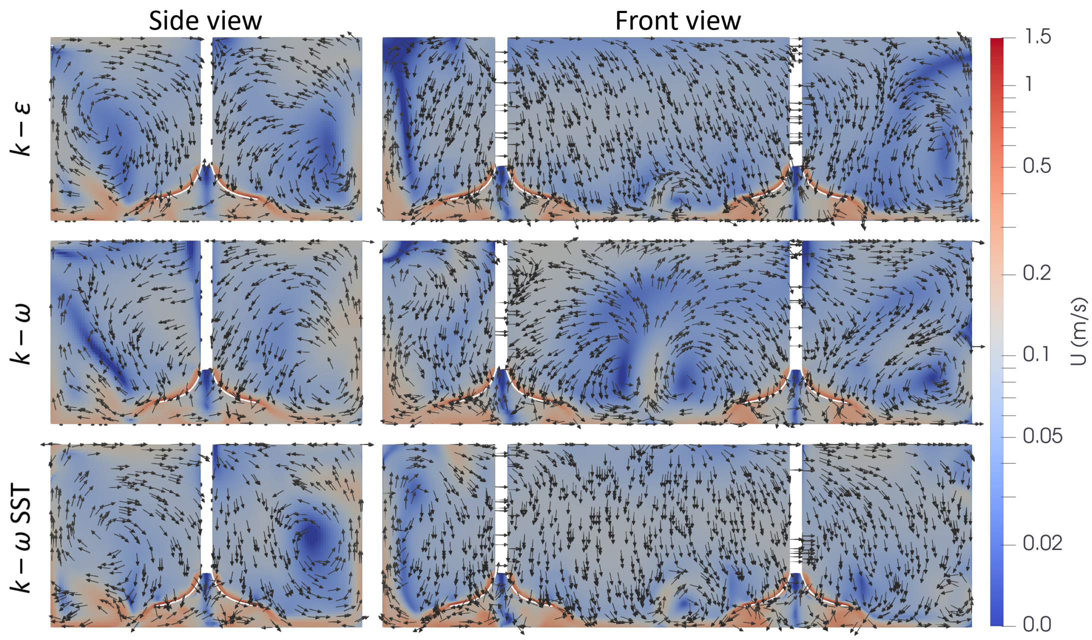

Figure 1: The flow fields predicted for an industrial-scale flocculation tank located at WTP Tlumacov, Czech Republic, using three common RANS turbulence models.

into separable flocs. The energy requirements for mixing and related processes reach from 25 % to 50 % of facilities' total energy demands [1, 2]. Therefore, their optimization can yield substantial savings in operational costs.

When focusing on mixing optimization, computational fluid dynamics (CFD) methods can serve as a valuable design and analytical tool, as shown in [3]. However, most research focuses on a very limited range of vessel configurations, specifically baffled cylindrical vessels with a centrally mounted impeller - disc turbine, pitched-blade turbine, or propellers — of volumes ranging from 1 to 100 L, furher denoted as the *standard arrangement*. Reports on CFD simulations of larger vessels ($\approx 1 - 100$ m^3) or vessels with different arrangements (rectangular, unbaffled, with asymetrically mounted impellers) are scarce and often lack any experimental validation, even though such vessels are frequently used in the production industry.

Such a narrowing of the research field enables the use of computationally expensive simulation approaches, e.g., large-eddy/detached-eddy simulations (LES/DES) or direct numerical simulations (DNS), yielding high-fidelity predictions of both flow fields and turbulence characteristics, as reported in [4, 5]. On the other hand, it weakens the connection between the research field and industrial applications, for which the high-fidelity simulations - transient, with a high mesh resolution - may be too expensive, or even impossible [6]. For such simulations, the simplified approaches based on the Reynolds averaging (RANS models) are usually required. However, researchers disagree on whether such an approach can yield sufficiently accurate results and, if so, which of the available RANS models should be used.

For example, an extensive review of Murthy and Joshi [4, 7, 8] documents that using RANS modeling with the standard $k - \epsilon$ turbulence model is highly inaccurate, especially for radial flow impellers; yet, some compromise results can be achieved when the Reynolds stress model (RSM) is used instead of $k - \epsilon$. This finding is further supported by later work of Lane [9], who prefers using the $k - \omega$ SST model. On the other hand, Coroneo et al. [10] and Singh et al. [11] conclude that the $k - \epsilon$ model is sufficiently accurate if the mesh is of sufficient resolution.

This contribution summarizes our recent work on assessing affordable modeling strategies for large-scale mixing vessels [12, 13, 14]. It aims to document a recommended methodology for affordable simulations that achieves the best possible compromise between simulation costs and accuracy. In order to keep focus on the practical application, the sought strategy is based on the stationary *steady-state* approach with possible switch to transient formulation of solved equations (unsteady RANS, URANS) utilized when no other strategy yields satisfactory results. The strategy was first built and validated based on the *standard vessel arrangement*, using the experimental data taken from the literature. Next, the know-how was validated for the simulation of a flow in a rectangular tank equipped with one and two radial and axial impellers.

3 Mesh construction

The steady-state formulation of the flow problem requires the stationary model of impeller motion. Although some authors tried to directly prescribe the impeller motion by means of boundary conditions, the classical and well-established approach consists of formulating the solved equations in the rotating frame of reference with an angular velocity corresponding to the impeller speed. These formulations - single rotating frame (SRF) and multiple rotating frames (MRF) - were tested against transient simulations with actual mesh movement, and it was found that there is practically no difference in the obtained results once the transient data were averaged.

However, the MRF-based method requires splitting the mesh into two aligned parts - stationary and rotating; the position of the MRF interface and quality of the mesh there were found to be essential in order to achieve reliable results. The sensitivity of the results on the interface position is illustrated on predicted profiles of turbulent viscosity in Figure 2 for four different interface radii. It is evident that for the interface too close to the impeller, the profiles are strongly affected, while with the interface situated at a larger distance, the profiles coincide; similar behavior was recently reported in [15].

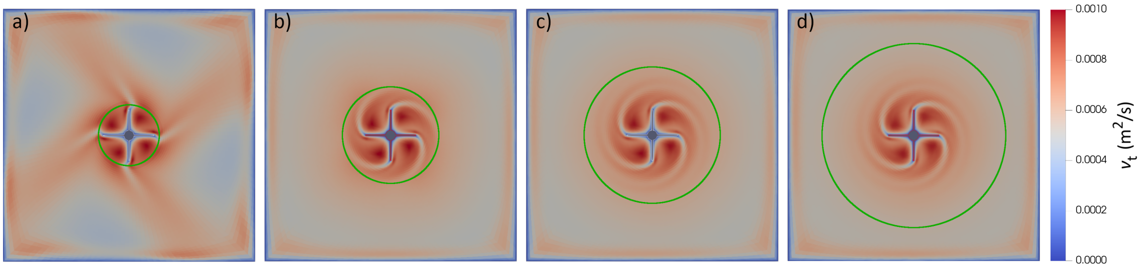

Figure 2: Illustration of the impact of MRF zone diameter on predicted profiles of predicted turbulent viscosity. The green line indicates the position of MRF zone interface.

Alongside the interface position, its shape is also important. This results from the handling of the momentum flux calculation across the interface,

$$\rho \mathbf{U}_{\text{int}} \left(\mathbf{U}_{\text{int}} \cdot \mathbf{n}_{\text{int}} \right) = \rho \mathbf{U}_{\text{int}} \left[\mathbf{U}^{\Omega}_{\text{int}} \cdot \mathbf{n}_{\text{int}} + \left(\boldsymbol{\omega} \times \mathbf{r}_{\text{int}} \right) \cdot \mathbf{n}_{\text{int}} \right] \tag{1}$$

where $\boldsymbol{\omega}$ represents the angular velocity vector, $\mathbf{n}_{\text{int}}$ is the interface normal vector, ρ is the fluid density, $\mathbf{r}_{\text{int}}$ is the position vector of the interface, relative to the center of rotation, and $\mathbf{U}^{\Omega}_{\text{int}}$ and $\mathbf{U}_{\text{int}}$ are the velocity vectors in the rotating and inertial frames of reference. In the Ansys Fluent implementation of the MRF, the second term in the square braces is neglected; in the OpenFOAM, this term is implemented to all faces in the MRF zone, including the interface ones, having the ambient property being inside and outside the rotating zone. In both implementations, the non-zero term $(\boldsymbol{\omega} \times \mathbf{r}_{\text{int}}) \cdot \mathbf{n}_{\text{int}}$ results in non-physical momentum source, which may substantially affect the velocity profiles at the interface. Its effect is evident even in the highly chaotic flow of the standard vessel arrangement; in the more structured flow of a larger vessel, the correction can completely alter the flow field not only in the impeller vicinity but also in the remainder of the vessel volume.

To suppress the effects of MRF interface position and shape on the results, the recommended strategy is to create the MRF interface in the shape of **a perfect cylinder** of diameter $\approx 1.3 - 1.5$ times that of the impeller and height of $\approx 2 - 3$ times the height of the impeller, for which the correction term (1) is zero. Based on our experience, the recommended structure of the mesh, illustrated in Figure 3 consists of at least two parts: (i) the cylindrical inner part housing the impeller, preferably constructed using the *bell-shaped O-grid layout*, (ii) the outer mesh around the inner part, housing the remainder of the vessel. The size and number of cells are highly case-dependent; however, it was shown that even for relatively small vessels ($\approx 10 - 20$ L), a mesh of ≈ 2 million cells is required for RANS simulations. That finding contrasts with substantially lower mesh densities used in the studies reporting insufficient RANS models' accuracy [4].

4 Turbulence model - standard vessel analysis

The accuracy and practical applicability of RANS models for mixing vessels' flow characterization were tested on a standard vessel arrangement using the experimental data of Wu and Patterson [16] for the near-

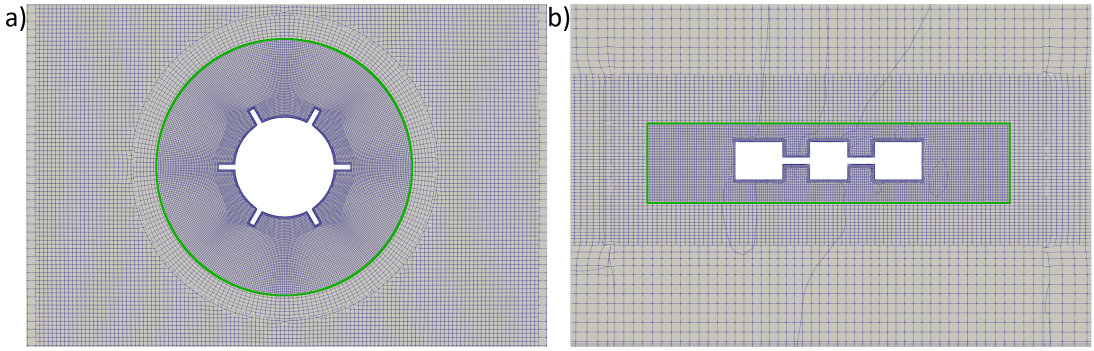

Figure 3: Recommended design of the mesh structure for MRF-based simulations. a) top-view, b) side view. The green circle marks the MRF interface position.

impeller region and Murthy and Joshi [4] for the whole vessel's profile. Four turbulence models have been assessed using the open-source library *OpenFOAM v. 23.12* and a partially structured mesh of ≈ .2.5 M of cells: (i) standard $k-\epsilon$ model, (ii) standard $k-\omega$ model, (iii) the latest version of $k-\omega$ SST model, and (iv) the SSG variant of a Reynolds Stress Model (RSM). All steady-state simulations began with a first-order upwind scheme; after initial flow development, the scheme was switched to a second-order upwind and continued until a steady state was achieved (as indicated by iteration-independent profiles). In addition, the detailed transient simulation based on the DDES formulation of the $k-\omega$ SST model was performed using a substantially denser mesh (≈ 18 M cells) to evaluate the limits of CFD capabilities in flow characterization.

First, it was found that simulations based on the $k-\omega$ SST model and the SSG-RSM models cannot converge to a steady-state solution, regardless of the numerical schemes, mesh density, or solver settings. While for the $k-\omega$ SST model, this can be aided by averaging the velocity profiles obtained at different iterations (≈ 30,000 RANS iterations were required) or profiles calculated using the transient approach (≈ 5 s of URANS simulation), no reliable and stable method was found for the RSM model. The results obtained using the four remaining turbulence models are shown in Figure 4.

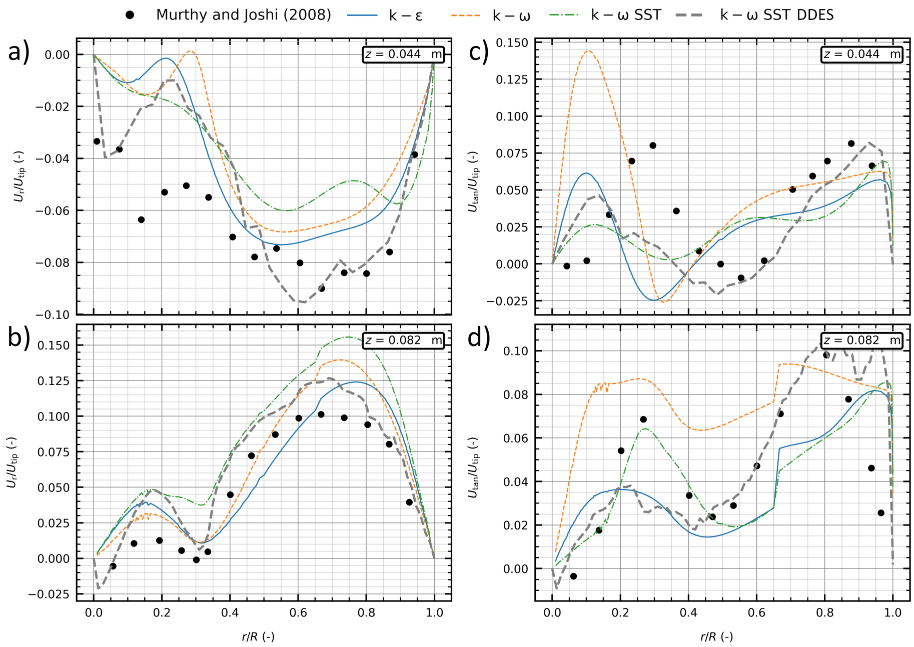

Figure 4: The comparison of the radial (left) and tangential (right) velocity profiles calculated for a cylindrical baffled vessel stirred with the Rushton turbine. Data calculated for two height coordinates using three RANS turbulence models compared to the experimental data presented in [4] and to predictions obtained with a transient simulation using a substantially more refined mesh and the $k-\omega$ SST DDES turbulence model.

It is evident that the computational complexity reflects the quality of the predicted results. The best agreement between simulated and experimental profiles is obtained with the most computationally expensive DDES simulation. Among the RANS turbulence models, the $k-\omega$ SST model, which requires temporal or iteration-based averaging, fits the experimental data both close to and far from the impeller with the lowest relative deviation. The worst results were obtained with the $k-\omega$ model; it performs comparatively well for predicting the radial and axial components of the flow velocity, but consistently overpredicts the tangential component and the turbulent kinetic energy. Based on these findings, the $k-\omega$ SST model is recommended for simulations, for which a sufficient number of iterations can be calculated (tens of thousands were required for standard vessel arrangement); otherwise, the standard $k-\epsilon$ model seems to provide a good compromise between the accuracy and computational cost. This somewhat justifies the approach of numerous researchers who use the $k-\epsilon$ model without experimental validation of the results obtained.

5 Turbulence model - pilot-scale tank verification

To extend the conclusions on the suitability of turbulence models for non-standard vessel arrangements, experimental data on the mean flow field in a rectangular pilot-plant vessel (200 L) were obtained using a modified particle tracking velocimetry (PTV) method and compared to the predicted flow fields [13]. The PTV method modification enabled simultaneous measurement of the mean velocity profiles in half of the tank (0.6 m × 0.4 m, averaged over 50 s). The results obtained using all three RANS models are shown in Figure 5.

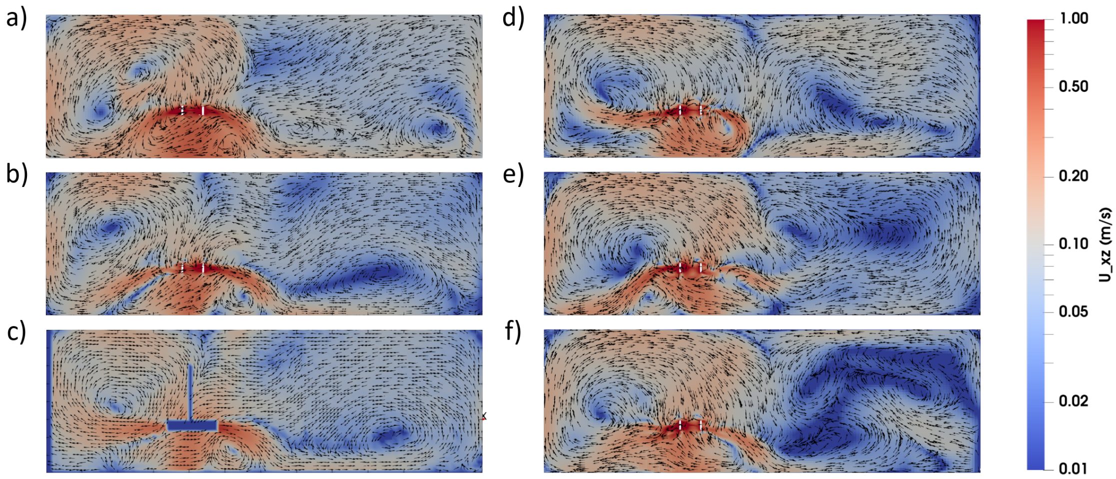

Figure 5: Velocity profiles predicted for a pilot-scale rectangular tank mixed with a single Rushton turbine at 3.45 rps. The profiles calculated using three common turbulence models are compared to the experimental data obtained using the modified PTV method. a) profiles predicted using $k-\omega$ model, b) profiles predicted using $k-\epsilon$ model, c) experimental profiles measured using the modified PTV technique [13], d)-f) illustration of unsteady profiles calculated using the $k-\omega$ SST model at the iterations: 30,000, 40,000, and 50,000, respectively.

They confirm the conclusions made based on the standard vessel simulations: the $k-\omega$ model exhibits the lowest reliability in the flow field prediction, and the $k-\omega$ SST model is highly unstable, requiring a substantial increase in computational costs if the reliable *frozen-field* profiles are sought. Simulations using the mesh structure described earlier and the standard $k-\epsilon$ model yielded velocity profiles in surprisingly good agreement with the experimental data. This agreement was further confirmed across three impeller speeds (Re 165,000, 300,000, and 460,000), two impeller types (Rushton turbine, pitched-blade turbine), and one- and two-impeller arrangements [14].

6 Conclusions

The flow simulation strategy for large, industrially-relevant mixing tanks was developed based on the thorough analysis of relevant literature, extensive numerical investigation of the impact of individual simulation aspects - mesh structure and density, MRF zone geometry, numerics, and turbulence model choice - and own experimental data. Based on all the obtained results, it is concluded that: 1. The representative predictions of mixing vessels' flow fields can be obtained using the steady-state simulations. 2. The standard $k - \epsilon$ model is suitable for accurate, convergent predictions of the flow field when a sufficiently detailed mesh is used. 3. The computational mesh should be constructed with emphasis on the perfectly cylindrical shape of the MRF zone interface to avoid instabilities on that interface, strongly affecting the flow field in the whole vessel.

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