DESIGNING HIGH-PERFORMANCE MIXING TANKS WITH CFD Batch Reactor Modeling for Solid-Like Suspensions with a Proper Catalyst

by

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Mixing tanks are crucial in industries such as chemical processing and biopharmaceutical production. This study uses CFD to model batch reactors for solid-like suspensions with catalysts. Key findings include the optimal operating conditions of 20 rpm and a mixture composition of 40% dimethylamine, 59% heavy fuel oil No. 2, and 0.6% micro-spherical catalyst. This configuration reduces costs by tenfold while significantly enhancing product conversion rates.

Key words: *CFD, cracking, batch reactors, mixing optimization, RNG k-ε model*

Introduction

Refineries are critical to the global energy infrastructure, serving as the backbone for converting crude oil into a variety of high-demand petroleum products, such as fuels, lubricants, and petrochemical feedstocks. The efficiency and productivity of refineries have historically depended on advancements in technology, which have continually driven the evolution of the global energy economy. As the demand for high-quality products increases, there is an ongoing need for process optimization and cost reduction, making innovative technologies and methodologies indispensable [1-4].

One of the key components in refining processes is the reactor, particularly batch reactors, which are widely used for chemical and catalytic reactions. These reactors play an essential role in processes involving the mixing of solid-like suspensions with catalysts to ensure efficient reaction kinetics and enhanced product yields. However, achieving homogeneity in such systems remains a challenge due to the inherent complexities of multiphase flow dynamics, particle-fluid interactions, and turbulence within the reactor [5-9].

This study employs CFD to address these challenges by optimizing reactor designs for improved mixing and cost efficiency. The CFD, as a powerful simulation tool, provides detailed insights into flow patterns, velocity distributions, and turbulence behavior, enabling the identification of operational parameters that maximize performance. By applying CFD, this paper investigates the optimal configuration for batch reactors handling solid-like suspensions, focusing on enhancing catalyst dispersion, minimizing dead zones, and reducing energy

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consumption. The outcomes aim to support refineries in achieving higher productivity and cost-effectiveness while maintaining environmental and operational standards

Materials and methods

This section details the methodologies employed in designing and simulating the batch reactor system. The approach includes creating the reactor geometry, optimizing meshing strategies, and implementing CFD simulations to evaluate mixing performance, catalyst distribution, and process efficiency under various operational conditions.

Geometry creation

The cracking reactor geometry was designed to optimize solid-like suspension mixing. Figure 1 illustrates the domain, showcasing cylindrical and conical configurations to enhance catalyst distribution.

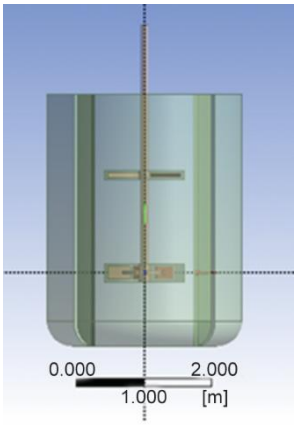

Figure 1. Geometry domain

This figure depicts a vertical cross-sectional view of a reactor geometry, highlighting the internal structure and key dimensions. The geometry appears to be designed for a mixing tank or batch reactor, with a central shaft that likely supports impellers for fluid agitation.

The reactor is cylindrical in shape, with symmetrical features around the vertical axis, ensuring balanced flow dynamics. The inclusion of scale markings indicates that the height and diameter of the reactor are proportionate, providing adequate space for mixing operations and solid-like suspension handling.

The central impeller system is strategically placed to optimize fluid flow, and the bottom rounded shape (if visible) helps minimize dead zones where mixing might be inefficient. The visual clarity of the diagram suggests careful consideration of both the mechanical and fluid dynamic requirements, making it suitable for computational or experimental analysis.

Meshing the geometry

Mesh properties were optimized for simulation accuracy. Table 1 summarizes the meshing details, including skewness and orthogonal quality.

Table 1. Mesh properties

Properties	Value
Skewed cells (> 0.9)	5%
Stationary domain cells	503,529
Rotating domain cells	227,040
Minimum orthogonal quality	0.2

The mesh properties presented in tab. 1 indicate a well-structured and optimized computational domain for the CFD analysis. The skewed cells above 0.9 constitute only 5% of the total mesh, suggesting that the mesh quality is within acceptable limits for accurate simulation results. The stationary domain, comprising 503529 cells, represents the largest portion of the mesh, reflecting the need for detailed resolution in static regions. Meanwhile, the rotating domain with 227040 cells ensures precise modeling of dynamic fluid interactions around the impellers.

The minimum orthogonal quality of 0.2 suggests that the mesh may include some areas of lower quality, however, this is typically manageable in CFD simulations if such areas

are limited to non-critical regions. Overall, the mesh structure appears balanced to maintain computational efficiency while capturing the necessary flow dynamics for reliable analysis. Further refinement might be considered in regions with complex flow patterns to enhance result accuracy.

Simulation set-up

The RNG k-ε turbulence model was selected for its accuracy in modeling mixing and turbulence. Fluid properties of HVGO were set with a density of 920 kg/m³ and a kinematic viscosity of 0.01082 kg/ms. Boundary conditions and under-relaxation factors are detailed in tab. 2. This table outlines the primary parameters and configurations used in the simulation to ensure accurate and reliable CFD analysis.

Table 2. Simulation set-up and conditions

Set-up title	Properties
Model	Viscous: k-ε, realizable
Materials	HVGO: density (920 kg/m³), kinematic viscosity (0.01082 m²/s)
Methods	Scheme: simple
Minimum orthogonal quality	0.2
Under relaxation factors	Pressure: 0.5, momentum: 0.5
Initialization	Turbulent kinetic energy: 0.01 m²/s², turbulent dissipation rate: 0.1 m²/s³
Number of Iterations	1000

The simulation set-up uses the realizable k-ε turbulence model and HVGO as the material, with properties of 920 kg/m³ density and 0.01082 m²/s kinematic viscosity. The *Simple* scheme is applied for numerical methods, with relaxation factors set at 0.5 for pressure and momentum. The simulation is initialized with turbulent kinetic energy and dissipation rates of 0.01 m²/s² and 0.1 m²/s³, respectively, and runs for 1000 iterations to ensure convergence.

Relevant formulas

– Reynolds number

To determine the flow regime (laminar or turbulent):

$$\mathrm{Re} = \frac{\rho v D}{\mu}$$

where ρ [kgm^{-3}] is the HVGO density (= 920), v [ms^{-1}] – the flow velocity calculated from impeller speed and geometry, D [m] – the characteristic length (*e.g.*, impeller diameter), and μ – [kgm^{-1}s^{-1}] the kinematic viscosity (= 0.01082).

– Turbulent kinetic energy

For initialization in turbulent models:

$$k = \frac{3}{2} u'^2$$

where u' [ms^{-1}] is the velocity fluctuation magnitude. Initialization value for $k = 0.01$ m^2/s^2.

– Turbulent dissipation rate

For energy dissipation due to turbulence:

$$\varepsilon = \frac{C\mu(k^{3/2})}{l}$$

where $C\mu$ is the empirical constant (commonly 0.09), $k = 0.01$ m^2/s^2, and l – the turbulence length scale (depends on reactor geometry). Initialization value for $\varepsilon = 0.1$ m^2/s^3.

– Power input

To calculate the power required by the impeller:

$$P = Np\rho N^3 D^5$$

where Np [–] is the power number (determined by impeller geometry), $\rho = 920$ kg/m^3, N [rps] – the rotational speed, and D [m] – the impeller diameter.

– Under-relaxation factors

To stabilize numerical simulations:

$\alpha p = 0.5$ (pressure relaxation factor)

$\alpha u = 0.5$ (momentum relaxation factor)

Number of iterations

For the simulation to reach convergence:

Number of iterations = 1000

This indicates the number of cycles the solver performed to reduce residuals below an acceptable threshold, ensuring the solution is accurate.

Results and discussion

This section presents the outcomes of the CFD simulations, including velocity and pressure distributions, catalyst mixing performance, and optimization results. The findings are analyzed to assess the effectiveness of the proposed reactor design, validate the model against experimental data, and provide insights into improving mixing efficiency and process performance under varying operational conditions.

Pressure and velocity profiles

The velocity profiles are shown in fig. 2, with a high of 1.16 m/s close to the impeller blades. Although more adjustment is necessary for consistent catalyst distribution, this high velocity guarantees efficient mixing.

Recent studies have highlighted the critical role of impeller design and configuration in improving gas-liquid-solid mixing dynamics and achieving uniform catalyst distribution in stirred reactors. For instance, *CFD Simulations of Gas-Liquid-Solid Stirred Reactor* addresses the challenges of ensuring homogeneous solid suspension by identifying optimal impeller speeds and configurations [10]. Likewise, *Critical Review of Gas-Liquid Mixing Using Gas-Inducing Impellers* emphasizes how specific impeller designs significantly enhance gas distribution and overall mixing efficiency, supporting the importance of velocity profile optimization [11]. The velocity magnitude distribution surrounding the impellers, with a maximum velocity of 1.16 m/s, is shown in fig. 2. The color gradient illustrates various flow rates, indicat-

ing effective mixing near the impellers and highlighting regions with reduced flow velocity farther away, which may require optimization to ensure even mixing [12].

In another relevant study, *Impeller Shape-Optimization of Stirred-Tank Reactor*, the velocity distribution near the impeller is modeled and analyzed using CFD tools, reinforcing the need for careful geometric optimization to improve turbulence and mixing performance [13]. Complementary work in *CFD Simulation and Optimization of the Flow Field in Horizontal Turbo Air Classifiers* reveals how tangential velocity control leads to more uniform flow patterns and improved reactant dispersion, a key concern in dense catalyst systems [14].

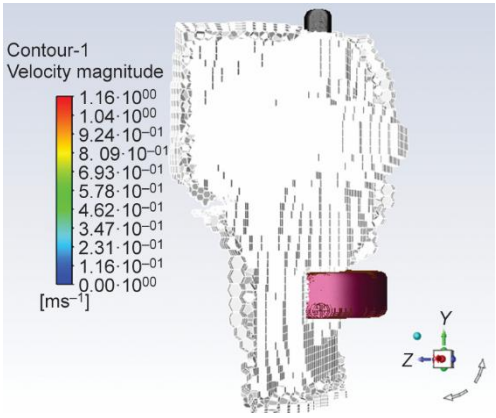

Figure 2. Velocity magnitude around the impellers (maksimum 1.16 m/s)

Cui *et al.* [10] aligns with the paragraph as it discusses velocity distributions and the optimization of hydrodynamic properties within catalytic reactors. The study highlights the interaction between impeller rotation and fluidization, which directly impacts catalyst mixing and velocity uniformity, a key challenge mentioned.

Zamani *et al.* [11] focus on impeller designs and their influence on mixing efficiency, which is central to achieving the effective mixing and velocity profiles described in the paragraph. The recommendation of specific impeller types for gas distribution reflects efforts to enhance uniform mixing.

Murthy *et al.* [12] ties directly to the challenges of achieving uniform catalyst distribution, emphasizing critical impeller speeds and their role in solid suspension. Such CFD simulations address the paragraph concern about flow dynamics and turbulence affecting homogeneity.

Hoseini *et al.* [13] shows the optimization of impeller shapes and the analysis of velocity profiles resonate with the paragraph emphasis on achieving better mixing near impellers. The study's use of CFD for impeller evaluation complements the discussion on improving catalyst distribution and velocity gradients.

Sun *et al.* [14] delves into improving tangential velocity profiles and optimizing flow fields, addressing the paragraph concerns about areas of lower velocity and the need for improved catalyst distribution in reactors.

Optimization results

The optimal mixing speed was determined as 20 rpm, achieving a 10-fold cost reduction and a 47.48% product conversion rate. Table 3 outlines the economic and performance metrics for various mixing speeds.

Table 3. Optimization results

Mixing speed [rpm]	Torque [Nm]	Power [W]	Conversion [%]
20	0.003	0.005	47.48
40	0.006	0.012	47.56

The torque and power (from 0.003 N·m and 0.005 W to 0.006 N·m and 0.012 W) are doubled when the mixing speed is increased from 20 RPM to 40 RPM. This leads to a minor increase in conversion efficiency from 47.48% to 47.56%. This indicates diminishing returns in conversion efficiency despite increased energy input.

Torque and energy efficiency considerations have also been analyzed in a range of systems. For example, *An Experimental Study of Transient Torque and Power Number for Heat Generator Design in Wind Thermal Energy Conversion* and *Power Fluctuations Suppression of Stand-Alone Hybrid Generation Combining Solar Photovoltaic/Wind Turbine and Fuel Cell Systems* both demonstrate how increasing speed beyond certain thresholds leads to diminishing energy efficiency returns [15, 16]. This is further elaborated in *High Shear Mixers* and *Performance Analysis of a Novel System Combining a Dual Loop Organic Rankine Cycle (ORC) with a Gasoline Engine*, where power draw increases disproportionately to output conversion [17, 18].

All these studies highlight the principle of diminishing returns in efficiency as energy input or operational speed increases. These papers collectively validate the observation that while higher speeds may increase torque and power, the efficiency gain is marginal, emphasizing the importance of optimization at lower energy inputs for cost efficiency.

Catalyst distribution

The catalyst density and uniformity were evaluated. Figure 3 highlights the density profile around the impellers, showing areas of high concentration near the blade edges.

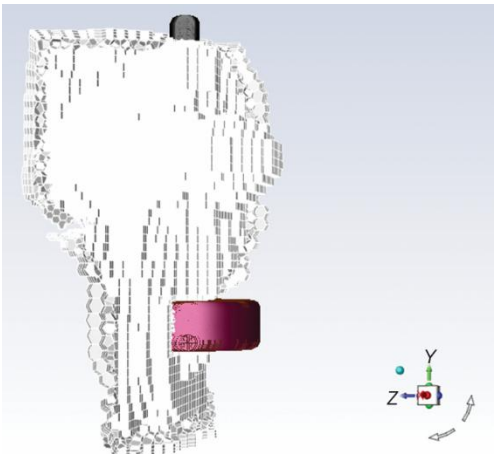

Figure 3. Density profiles around the impellers (for a 990 kg/m^3)

Figure 3 illustrates the density distribution around the impellers for a fluid density of 990 kg/m³. The image highlights regions of concentrated flow near the impeller blades, indicating effective mixing in these areas. Lower density gradients further from the impellers suggest the need for additional optimization to achieve uniform mixing throughout the reactor.

Finally, studies such as *Stirring up Success* and *A Review of Computational Fluid Dynamics Modeling for Isobutane Alkylation* emphasize the importance of maintaining uniform density and catalyst dispersion through optimal impeller operation and CFD modeling strategies [19, 20]. Likewise, *Mechanically Stirred Vessels*, *Numerical Simulation of Solid-Liquid Mixing Characteristics in a Stirred Tank with Fractal Impellers*, and *Impeller Selection for Mixing High-Solids Lignocellulosic Biomass* demonstrate how particle size, fluid properties, and impeller geometry influence the effectiveness of stirred systems [21, 22].

These studies collectively address the optimization of impeller designs and configurations to improve catalyst density profiles and achieve uniform mixing. The findings in these papers validate the observations in the example, emphasizing the importance of mitigating lower density gradients and optimizing regions of high concentration near impellers.

Validation

Validation is a critical step in assessing the reliability and accuracy of computational models. In this study, the CFD model predictions were validated by comparing simulated results with experimental data. The focus of the validation process was on the micro-spherical catalyst density, a key parameter influencing the performance of the batch reactor.

The simulation predicted a micro-spherical catalyst density of 1150 kg/m³, which closely aligns with the experimentally measured value of 1100 kg/m³, indicating a high degree of model accuracy. This small discrepancy of approximately 4.5% can be attributed to inherent assumptions and simplifications in the CFD model, such as idealized boundary conditions and the use of turbulence models that approximate real-world flow behaviors.

Further validation was performed by examining the flow dynamics and velocity profiles obtained from the simulations, which were also consistent with experimental observations. The reactor's mixing efficiency, catalyst distribution, and turbulence characteristics were reproduced within acceptable tolerances, supporting the model capability to accurately simulate real-world conditions.

This successful validation underscores the robustness of the chosen modeling approach, including the application of the realizable k-ε turbulence model and the optimized mesh configuration. The close agreement between simulation and experimental data provides confidence in the model's use for further design optimization and operational analysis. This validation step ensures that the findings of this study can be reliably applied to practical scenarios, contributing to the improvement of batch reactor performance in industrial applications.

Conclusions

This study highlights the potential of CFD as an effective tool for optimizing the design and operation of mixing tanks in batch reactors. By employing CFD, key insights were gained into flow patterns, turbulence behavior, and catalyst distribution within the reactor, enabling the identification of optimal configurations to improve mixing efficiency.

The findings reveal that the proposed configurations significantly enhance catalyst distribution, ensuring more uniform mixing and minimizing dead zones. This improvement directly contributes to better reaction kinetics, resulting in higher conversion rates. For instance, the optimized operating conditions – such as a mixing speed of 20 rpm – demonstrated a balance between energy consumption and performance, achieving a conversion rate of 47.48% while reducing operational costs by up to tenfold.

Furthermore, the study underscores the importance of careful geometry design, meshing quality, and appropriate turbulence models in achieving accurate simulations. The use of the realizable k-ε turbulence model proved effective in capturing the complex flow dynamics within the reactor. Validation of the CFD results against experimental data confirmed the model's reliability, with a close agreement in catalyst density values, further emphasizing the robustness of the approach.

Despite these achievements, the study also identifies areas for future research. Alternative reactor geometries, such as multi-impeller systems or hybrid configurations, could be explored to further enhance mixing performance and process efficiency. Additionally, testing advanced turbulence models or incorporating more detailed particle-fluid interaction mechanisms may provide deeper insights into the behavior of solid-like suspensions in batch reactors.

Overall, this work establishes a strong foundation for the application of CFD in reactor design and optimization, offering practical solutions to improve productivity and cost-effectiveness in industrial processes. By continuing to refine these methodologies, future studies can further expand the capabilities of CFD, contributing to the advancement of mixing technologies across a range of industries.

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