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ORIGINAL RESEARCH PAPER

CFD Investigation of Hydrodynamics and Species Distribution in a Pilot-Scale Methanol-to-Olefins Fluidized Bed Reactor Using an Eulerian-RANS Model

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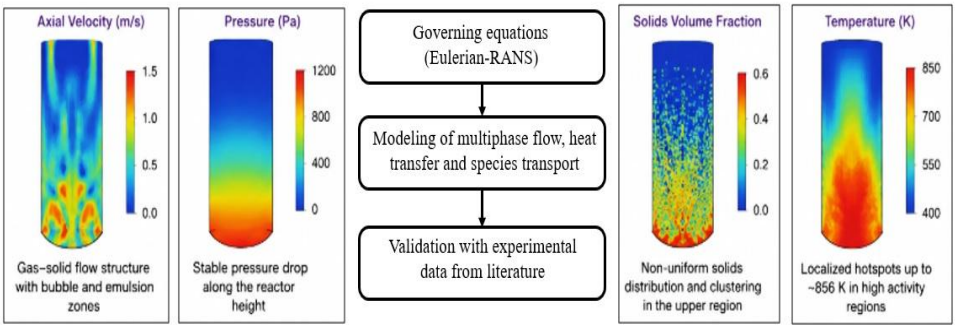
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A B S T R A C T

In the present study, a Computational Fluid Dynamics (CFD) model based on the Eulerian multiphase approach coupled with the Reynolds-Averaged Navier Stokes (RANS) turbulence model was developed to investigate the hydrodynamic and reactive behavior of a pilot-scale fluidized bed reactor for methanol-to-olefins (MTO) conversion. The model was used to analyze gas solid flow behavior, solids distribution, temperature and pressure fields, velocity profiles, and olefin formation within the reactor. The numerical results were validated against experimental data reported in the literature, showing satisfactory agreement, with most relative deviations remaining below 10%. The results revealed heterogeneous gas–solid flow behavior, including localized particle clustering and non-uniform solids holdup. Localized hotspots with temperatures of approximately 856 K were observed in regions of intensified catalytic activity and higher solids concentration. Ethylene and propylene concentrations reached maximum values of approximately 0.44 and 0.37, respectively, near the lower reaction zone and gradually decreased along the reactor height. The results indicate that local hydrodynamic structures and transport limitations strongly influence heat transfer, species distribution, and olefin formation. Overall, the developed Eulerian-RANS framework effectively captures the dominant multiphase transport phenomena and provides useful mechanistic insights for the analysis and design of pilot-scale MTO fluidized bed reactors.



1. Introduction

Light olefins, particularly ethylene and propylene, are among the most important building blocks in the petrochemical industry. Due to the increasing demand for non-petroleum-based production routes, the methanol-to-olefins (MTO) process has attracted significant industrial and scientific attention as an alternative pathway for olefin production from coal, natural gas, and biomass-derived methanol [1-3] . In recent decades, MTO technology has emerged as a promising process because of its flexibility in feedstock utilization and its capability for producing high-value chemicals with reduced dependence on crude oil resources [4]. Fluidized bed reactors (FBRs) are extensively utilized in MTO processes owing to their excellent gas-solid contact, high heat and mass transfer rates, and effective temperature control under strongly exothermic reaction conditions [5,6]. However, the hydrodynamics of gas-solid flow inside fluidized bed reactors are highly complex and involve strong interactions among turbulence, particle clustering, bubble formation, heat transfer, and chemical reactions [7]. These complex multiphase phenomena significantly influence methanol conversion, olefin selectivity, catalyst deactivation, and reactor stability [8]. One of the major operational challenges in MTO fluidized bed reactors is the development of non-uniform temperature and concentration distributions. Localized hotspots generated by exothermic reactions may accelerate catalyst deactivation and promote undesired secondary reactions [9] . In addition, heterogeneous solids distribution and poor fluidization quality can create mass-transfer limitations, reducing reactant accessibility to catalyst active sites and affecting olefin yield [10]. Therefore, understanding the coupling between hydrodynamics, thermal behavior, and species transport is essential for reactor optimization and scale-up. Experimental investigation of pilot-scale fluidized bed reactors is often difficult because of the harsh operating conditions and the limited accessibility of local flow measurements. Consequently, Computational Fluid Dynamics (CFD) has become a powerful tool for analyzing multiphase flow and reaction behavior in

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fluidized systems [11]. Previous studies have employed Eulerian-Eulerian approaches combined with the kinetic theory of granular flow (KTGF), Reynolds-Averaged Navier-Stokes (RANS) models, and Large Eddy Simulation (LES) techniques to investigate gas-solid hydrodynamics and reaction performance in fluidized bed reactors [12-14]. Although previous investigations have provided valuable insights into fluidization behavior and reactor performance, most studies have primarily focused on either hydrodynamic prediction or overall conversion trends without detailed analysis of the interaction between solids distribution, thermal non-uniformity, and olefin product formation under pilot-scale operating conditions [15]. Moreover, limited attention has been devoted to identifying possible transport-limited regions within MTO reactors and evaluating the influence of local hydrodynamics on mass transfer and reaction behavior [16]. In the present study, a pilot-scale fluidized bed reactor for methanol-to-olefins conversion is investigated using Computational Fluid Dynamics based on the Eulerian multiphase approach coupled with the Reynolds-Averaged Navier-Stokes (RANS) turbulence model. The developed model is employed to analyze density distribution, temperature profiles, velocity fields, pressure drop, and olefin product distribution inside the reactor. Simulation results are validated against available experimental data from literature to evaluate the reliability of the developed CFD framework. The main contributions of this study are summarized as follows:

- Development of a CFD model for pilot-scale MTO fluidized bed reactor simulation using the Eulerian-RANS framework.
- Coupled investigation of hydrodynamics, thermal distribution, and olefin product formation.
- Analysis of solids clustering and thermal non-uniformity within the reactor.
- Assessment of potential transport-related limitations through concentration and flow-field analysis.
- Identification of key operational factors affecting fluidization quality and reactor performance.

The findings of this work provide useful insights into the interaction between multiphase hydrodynamics and catalytic reaction behavior in MTO fluidized bed reactors and may contribute to improved reactor design and process optimization for industrial olefin production. Unlike many previous CFD investigations that primarily focused on the general hydrodynamic description of fluidized bed MTO reactors, the present study emphasizes the coupled interaction between gas–solid hydrodynamics, heat transfer, and species transport behavior within a pilot-scale reactor using an Eulerian-RANS framework. The developed model not only predicts solids distribution, temperature fields, pressure behavior, and olefin concentration profiles, but also provides mechanistic insight into the influence of local flow structures and solids clustering on transport-related limitations and catalytic reaction performance. Furthermore, the numerical predictions were quantitatively validated against available experimental data, demonstrating the capability of the proposed framework to reliably reproduce the dominant multiphase transport phenomena governing methanol-to-olefins conversion in fluidized bed reactors.

1.1. Overview of CFD Simulation for Methanol-to-Olefins (MTO) Fluidized Bed Reactor Using RANS and Eulerian Model

The methanol-to-olefins (MTO) process has become one of the most important alternative technologies for the production of light olefins, particularly ethylene and propylene, from non-petroleum feedstocks such as coal-derived or natural-gas-derived methanol. Due to the highly exothermic nature of the reactions and the need for efficient gas-solid interaction, fluidized bed reactors (FBRs) are widely employed in industrial MTO units because of their superior heat transfer capability, enhanced mixing characteristics, and effective temperature control [1-3]. Nevertheless, the complex hydrodynamics of gas-solid multiphase flow, combined with turbulence, chemical reactions, and heat transfer, create substantial challenges in predicting reactor behavior and optimizing operating conditions [4].

In recent years, Computational Fluid Dynamics (CFD) has emerged as a powerful tool for investigating the complex transport phenomena occurring in fluidized bed reactors. CFD modeling enables detailed prediction of velocity fields, solids distribution, pressure drop, temperature gradients, and species transport inside the reactor under industrially relevant conditions [5]. Among the available numerical approaches, the Eulerian-Eulerian framework coupled with Reynolds-Averaged Navier-Stokes (RANS) turbulence modeling has been extensively applied because of its reasonable balance between computational cost and predictive capability for pilot-scale and industrial-scale fluidized systems [6, 7]. In the present study, the hydrodynamic and reactive behavior of a pilot-scale MTO fluidized bed reactor is investigated using the Eulerian multiphase approach coupled with the RANS turbulence model. The developed CFD framework is employed to analyze solids distribution, thermal behavior, product concentration profiles, velocity distribution, and pressure characteristics throughout the reactor domain. Model predictions are compared with available experimental data from literature to evaluate the reliability and applicability of the proposed simulation methodology [8, 9]. The simulation results indicate that the reactor exhibits heterogeneous hydrodynamic behavior characterized by non-uniform solids distribution and localized clustering regions. Higher solids concentration is observed in the upper reactor sections, suggesting particle accumulation and reduced local gas velocity, whereas lower-density regions near the riser outlet indicate improved fluidization and solids dispersion. The predicted density profiles show good agreement with experimental observations, with deviations generally below 8%, demonstrating acceptable model accuracy for gas-solid flow prediction [10]. The thermal analysis reveals the formation of localized high-temperature regions within the upper reaction zone, where temperatures approach approximately 856 K. These hotspots are associated with intensified exothermic catalytic reactions and elevated local solids holdup. The presence of thermal non-uniformity indicates a strong coupling between hydrodynamics and reaction behavior inside the fluidized bed. Although the predicted temperature gradients agree reasonably well with experimental data, localized thermal peaks may negatively influence catalyst stability and olefin selectivity under prolonged operation [11,12]. Species transport analysis further demonstrates that ethylene (C_2H_4) and propylene (C_3H_6) concentrations are highest near the lower reaction zone and gradually decrease along the reactor height due to methanol depletion and progressive product transport. The sharp concentration gradients observed near the inlet region suggest intensified reaction activity and possible transport-related limitations associated with gas-solid contact efficiency. These findings highlight the importance of hydrodynamic uniformity in maintaining effective reactant accessibility to catalyst active sites [13, 14]. The velocity distribution inside the reactor indicates the formation of high-velocity gas jets near the distributor region, followed by progressive flow homogenization in the fluidized bed section. Simultaneously, the pressure distribution exhibits a moderate pressure drop consistent with typical pilot-scale fluidized bed operation. The predicted hydrodynamic behavior agrees reasonably well with experimental measurements, confirming the capability of the Eulerian-RANS framework to capture the overall fluidization characteristics of the reactor [15, 16]. Overall, the CFD results demonstrate that reactor performance is strongly influenced by the interaction between hydrodynamics, heat transfer, and species transport phenomena. Solids clustering, non-uniform temperature distribution, and localized concentration gradients may contribute to transport limitations and reduced catalytic efficiency in certain reactor regions. Therefore, accurate prediction of multiphase flow behavior is essential for improving reactor design, optimizing operating conditions, and enhancing olefin selectivity in industrial MTO systems. Compared with conventional descriptive CFD studies, the present work emphasizes the coupled relationship between flow structure, thermal behavior, and olefin distribution in a pilot-scale reactor environment. The obtained results provide useful insights into the mechanisms governing gas-solid interaction and may support future development of more advanced multiphase reaction models for industrial MTO reactor optimization.

2. Method

2.1. Methodology for CFD Simulation of a Fluidized Bed Reactor in Methanol-to-Olefins (MTO) Process Using RANS and Eulerian Model

This methodology outlines the computational fluid dynamics (CFD) approach for simulating the hydrodynamics, heat transfer, and reaction kinetics in a pilot-scale fluidized bed reactor (FBR) for methanol-to-olefins (MTO) conversion. The study employs the Reynolds-Averaged Navier-Stokes (RANS) equations coupled with the Eulerian multiphase model to capture gas-solid interactions, density distributions, and species transport. The framework is validated against experimental data from literature.

2.2. Governing Equations

Multiphase Flow (Eulerian Model)

The Eulerian model solves continuity, momentum, and energy equations for the Eulerian phase, with slip velocities calculated for dispersed phases (catalyst particles). Key equations include:

- Continuity

$$\frac{\partial}{\partial t}(\rho_m) + \nabla.(\rho_m \overrightarrow{v_m}) = 0$$

- Momentum

$$\frac{\partial}{\partial t}(\rho_m \overrightarrow{v_m}) + \nabla.(\rho_m \overrightarrow{v_m}\,\overrightarrow{v_m}) = -\nabla p + \nabla.\left[\mu_m\left(\nabla \overrightarrow{v_m} + \overrightarrow{v_m}^T\right)\right] + \rho_m \vec{g} + \vec{F}$$

Here, μ_m is the Eulerian viscosity, and $\vec{F}$ accounts for interphase drag forces.

- Volume Fraction

The volume fraction of the solid phase α_s is computed via:

$$\frac{\partial}{\partial t}(\alpha_s \rho_s) + \nabla.(\alpha_s \rho_s \overrightarrow{v_s}) = 0$$

Turbulence Modeling (RANS)

The standard k − ϵ model is used to resolve turbulence effects:

$$\mu_t = \rho_m C_\mu \frac{k^2}{\epsilon}$$

whereC_μ = 0.09, k is turbulent kinetic energy, and ϵ is dissipation rate.

Computational Setup

Geometry and Mesh

Reactor Dimensions: Pilot-scale FBR with height = 5 m and diameter = 0.261 m.

Mesh: Structured hexahedral mesh with refinement near the gas distributor and walls (total cells: ~109800). Grid independence is confirmed via sensitivity analysis.

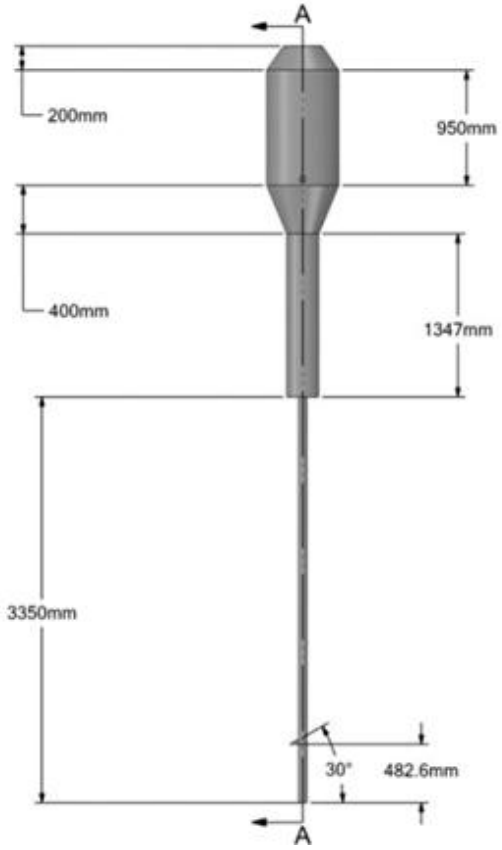


Figure 1. Geometry of fluidized bed regenerator reactor MTO

Source: Research Findings

Boundary Conditions

- Inlet: Velocity inlet for methanol vapor at T = 340 K U = 1 m/s

Outlet: Pressure outlet at atmospheric pressure.

Walls: No-slip condition with standard wall functions.

Solver Settings

- Software: ANSYS Fluent (Pressure-Based solver).

- Scheme: Phase-Coupled SIMPLE for pressure-velocity coupling.

- Discretization: Second-order upwind for momentum and species equations.

3. Results and Discussion

The results and discussion section presents a detailed analysis of the hydrodynamic behavior, thermal characteristics, and species distribution inside the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The Computational Fluid Dynamics (CFD) simulations were performed using the Reynolds-Averaged Navier-Stokes (RANS) turbulence model coupled with the Eulerian multiphase framework to investigate the complex interaction between gas-solid flow, heat transfer, and catalytic reaction behavior within the reactor. The developed CFD model was validated against available experimental data reported in the literature to evaluate the predictive capability of the numerical framework. The comparison demonstrates acceptable agreement between simulation and experimental results for key reactor parameters, including solids distribution, temperature profile, pressure drop, velocity field, and olefin product concentration. In most cases, the relative deviations remained below 10%, confirming the reliability of the model for analyzing pilot-scale fluidized bed MTO reactors. Particular attention is devoted to the relationship between hydrodynamic structure and reactor performance. The simulation results reveal that non-uniform solids distribution and particle clustering significantly influence local temperature gradients, gas-solid contact efficiency, and product distribution throughout the reactor. Regions with elevated solids holdup are generally associated with intensified catalytic activity and localized thermal accumulation, indicating a strong coupling between multiphase flow behavior and exothermic reaction characteristics. The predicted temperature distribution demonstrates the formation of localized hotspots within the upper reaction zone, where methanol conversion is most active. These thermal non-uniformities may contribute to catalyst deactivation and reduced olefin selectivity under prolonged operating conditions. Simultaneously, the species concentration profiles indicate that ethylene (C_2H_4) and propylene (C_3H_6) are primarily generated near the lower reaction zone and gradually decrease along the reactor height due to reactant depletion and progressive transport of products through the riser section.The concentration gradients observed near the reactor inlet suggest that local transport phenomena play an important role in determining reactor performance. In regions characterized by high solids concentration and intensified reaction activity, gas-solid mass transfer resistance may limit reactant accessibility to catalyst active sites. Conversely, regions with improved fluidization quality and more uniform solids distribution exhibit enhanced mixing behavior and more stable thermal profiles. These observations indicate that the overall reactor behavior is governed by the coupled interaction between reaction kinetics and transport phenomena rather than by hydrodynamics or chemistry alone. In addition, the velocity and pressure distributions provide further insight into the fluidization characteristics of the reactor. High-velocity gas jets generated near the distributor region gradually transition into a more homogeneous flow pattern within the fluidized bed. However, localized low-velocity regions may contribute to particle accumulation and non-ideal mixing behavior. The predicted pressure drop along the reactor height remains consistent with typical fluidized bed operation and agrees reasonably well with experimental observations. Unlike conventional descriptive CFD analyses, the present discussion emphasizes the mechanistic interpretation of reactor behavior through the coupled analysis of hydrodynamics, thermal distribution, and species transport. The obtained results provide important insight into the influence of solids clustering, temperature non-uniformity, and local transport limitations on olefin production performance. These findings may contribute to improved reactor design, optimization of operating conditions, and development of more reliable scale-up strategies for industrial MTO fluidized bed reactors.

3.1. Density Distribution in Fluidized Bed Reactor for Methanol to Olefins Conversion



Figure 2. Density Distribution in Fluidized Bed Reactor for Methanol to Olefins Conversion

Source: Research Findings

Figure 2 illustrates the predicted solids density distribution inside the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process using the Eulerian multiphase CFD model. The contour map represents spatial variations in solids concentration, where blue regions correspond to lower solids density and red regions indicate higher solids accumulation within the reactor domain. The simulation results reveal a non-uniform distribution of the solid phase throughout the reactor, highlighting the complex hydrodynamic behavior associated with gas-solid fluidization. Higher-density regions are primarily observed in the upper section of the reactor, indicating localized solids accumulation and particle clustering. This behavior is likely associated with reduced local gas velocity, bubble coalescence, and recirculation phenomena commonly observed in fluidized bed systems. The presence of these dense regions suggests that solids mixing is not perfectly homogeneous and that localized variations in gas-solid interaction exist within the reactor. In contrast, the lower-density regions observed near the riser outlet indicate improved particle dispersion and stronger fluidization conditions. These regions are characterized by enhanced gas-solid mixing and reduced solids holdup, which may contribute to more effective transport of reaction products

and improved catalyst exposure to reactants. The transition between dense and dilute regions reflects the dynamic interaction between turbulence, particle motion, and gas flow inside the reactor. The obtained density profiles also provide important insight into the relationship between hydrodynamics and reactor performance. Regions with elevated solids concentration may increase local catalytic activity because of higher catalyst availability; however, excessive particle clustering can reduce gas accessibility to active catalytic sites and promote local mass-transfer limitations. Consequently, the observed heterogeneity in solids distribution may directly influence methanol conversion, olefin selectivity, and thermal behavior within the reactor. Furthermore, the existence of localized dense regions may contribute to non-uniform temperature distribution and hotspot formation due to intensified exothermic reaction activity. This observation highlights the strong coupling between solids hydrodynamics and thermal characteristics in MTO fluidized bed reactors. Therefore, accurate prediction of solids distribution is essential for understanding reactor stability, improving fluidization quality, and optimizing operating conditions in industrial-scale applications. Overall, the predicted density distribution demonstrates that the Eulerian-RANS framework is capable of capturing the major hydrodynamic features of the pilot-scale fluidized bed reactor, including solids clustering, heterogeneous flow structure, and gas-solid interaction behavior. These findings provide valuable mechanistic insight into the influence of multiphase hydrodynamics on reactor performance and transport phenomena during the MTO conversion process. A quantitative comparison was performed between the CFD-predicted solids density profiles and the corresponding experimental measurements reported in the literature for similar pilot-scale fluidized bed reactors. The comparison was conducted at several representative axial positions along the reactor height in order to evaluate the predictive capability of the Eulerian-RANS framework under reactive fluidization conditions.

Table 1. Comparison of CFD-predicted density profiles and experimental measurements reported in the literature

Position (m)	CFD Density (kg/m³)	Experimental Density (kg/m³)	Relative Deviation (%)	Reference
0.2	1350	1400	3.57	[1]
0.5	900	950	5.26	[2]
0.8	600	650	7.69	[3]
1.1	400	420	4.76	[1]
1.4	200	210	4.76	[1]

Source: Research Findings

The comparison demonstrates that the numerical model provides satisfactory agreement with the available experimental observations. In most regions of the reactor, the relative deviation between simulation and experimental data remains below 8%, indicating that the developed CFD framework is capable of capturing the dominant hydrodynamic behavior and solids distribution characteristics of the fluidized bed reactor. The remaining discrepancies may be attributed to several factors associated with both numerical and experimental limitations. From the modeling perspective, assumptions related to uniform particle properties, simplified turbulence treatment, and idealized gas-solid interaction behavior may influence local density prediction. In addition, the use of averaged reaction and transport parameters may limit the ability of the RANS-based framework to fully capture transient mesoscale structures such as bubble evolution, particle clustering, and localized recirculation zones. From a physical perspective, the observed deviations may also be associated with local transport phenomena inside the reactor. Regions characterized by elevated solids concentration and intensified catalytic activity may experience reduced gas-solid mass transfer efficiency, leading to local heterogeneity in density and reaction behavior. These transport-related effects become increasingly important in regions where solids clustering and non-uniform fluidization occur simultaneously. Despite these limitations, the overall agreement between simulation and experimental measurements confirms that the proposed CFD model can reliably reproduce the principal hydrodynamic features of the pilot-scale MTO reactor. The obtained results further indicate that solids distribution plays a critical role in governing local heat transfer, species transport, and catalytic conversion behavior throughout the reactor. Rather than proposing generalized operational recommendations, the present analysis emphasizes the mechanistic relationship between hydrodynamics and reactor performance. The simulation results suggest that improved fluidization uniformity and reduced solids clustering may enhance gas-solid contact efficiency and minimize localized transport limitations. Furthermore, the findings indicate that local flow structures strongly influence concentration gradients and thermal non-uniformity inside the reactor, highlighting the importance of accurately resolving multiphase interactions in CFD-based reactor design studies.

Figure 3 presents the predicted temperature distribution inside the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The contour plot illustrates significant thermal variations throughout the reactor domain, with temperatures ranging from approximately 730 K to 856 K.

3.2. Temperature Distribution in the Fluidized Bed Reactor for Methanol to Olefin Conversion



Figure 3. Temperature Distribution in the Fluidized Bed Reactor for Methanol to Olefin Conversion

Source: Research Findings

The highest temperature region is located in the upper-middle section of the reactor, corresponding to the primary reaction zone where methanol conversion and olefin formation are most intense. The formation of localized high-temperature regions indicates the strong exothermic nature of the MTO reactions combined with the heterogeneous hydrodynamic structure of the fluidized bed. Regions characterized by elevated solids concentration and intensified catalytic activity exhibit higher local temperatures due to increased heat generation rates. This observation demonstrates the close coupling between solids hydrodynamics, reaction kinetics, and thermal transport behavior within the reactor. The predicted thermal gradients suggest that fluidization provides relatively effective heat redistribution throughout the reactor; however, the existence of localized hotspots indicates that thermal uniformity is not fully achieved under the studied operating conditions. These localized temperature peaks may negatively influence catalyst stability by accelerating coke formation and catalyst deactivation, while simultaneously promoting undesired secondary reactions that reduce olefin selectivity. The lower section of the reactor exhibits comparatively lower and more uniform temperatures, which are associated with the feed introduction and initial fluidization region. In this zone, methanol remains primarily in the vapor phase prior to entering the highly reactive catalytic region. As the gas-solid mixture moves upward through the reactor, increasing catalytic activity and enhanced gas-solid contact intensify the exothermic reaction behavior, leading to progressive temperature elevation. The obtained temperature profiles also provide important insight into possible transport-related limitations within the reactor. Regions with simultaneous high solids holdup and elevated temperatures may experience reduced gas-solid mass transfer efficiency because of particle clustering and local flow non-uniformity. Consequently, local thermal accumulation may further intensify reaction heterogeneity inside the fluidized bed. These observations indicate that reactor thermal behavior is strongly governed by the interaction between hydrodynamics, heat transfer, and catalytic reaction kinetics.

Table 2. Comparison of Temperature Distribution in the Fluidized Bed Reactor for Methanol to Olefin Conversion with Experimental Data

Parameter	Simulation Value	Experimental Value	Deviation (%)	Reference
Max Static Temperature (K)	856	840	1.90	[4]
Average Reactor Temperature (K)	780	765	1.96	[5]
Temperature Gradient (K/m)	25	23	8.70	[5]

Source: Research Findings

The quantitative comparison between CFD predictions and experimental measurements demonstrates satisfactory agreement for the principal thermal characteristics of the reactor. The predicted maximum temperature, average reactor temperature, and axial temperature gradient all exhibit deviations below 10% relative to the experimental data, confirming the capability of the developed CFD framework to reproduce the dominant thermal behavior of the pilot-scale reactor. The remaining deviations may be associated with uncertainties in reaction kinetics, simplified catalyst behavior assumptions, and limitations of the RANS turbulence treatment in resolving transient mesoscale structures. In addition, catalyst deactivation phenomena and localized variations in coke deposition were not explicitly incorporated into the present model and may contribute to discrepancies between predicted and measured temperature fields. Rather than providing generalized operational recommendations, the present analysis emphasizes the mechanistic interpretation of thermal behavior inside the reactor. The simulation results suggest that improved solids distribution and enhanced gas-solid mixing may reduce localized thermal accumulation and improve temperature uniformity throughout the fluidized bed. Furthermore, minimizing particle clustering may

contribute to more stable heat transfer behavior and reduce the risk of hotspot formation under industrial operating conditions. Overall, the predicted temperature distribution demonstrates that the coupled Eulerian-RANS framework can effectively capture the dominant thermal characteristics of the MTO fluidized bed reactor while also providing insight into the interaction between hydrodynamics, heat transfer, and catalytic reaction behavior.

3.3. Mass Fraction Distribution of Ethen in Fluidized Bed Reactor



Figure 4. Mass Fraction Distribution of Ethen in Fluidized Bed Reactor

Source: Research Findings

Figure 4 illustrates the predicted mass fraction distribution of ethylene (C_2H_4) inside the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The contour distribution obtained from the CFD simulation demonstrates significant spatial variations in ethylene concentration throughout the reactor, reflecting the strong interaction between reaction kinetics, gas-solid hydrodynamics, and species transport phenomena. The highest ethylene concentration is observed near the lower reaction region close to the feed inlet, where the maximum C_2H_4 mass fraction reaches approximately 0.44. This region corresponds to the primary methanol conversion zone, where catalytic activity and reactant availability are greatest. As the gas-solid mixture progresses upward through the reactor, the ethylene concentration gradually decreases due to methanol depletion, progressive product transport, and secondary reaction pathways leading to the formation of other hydrocarbons and olefin species. The observed concentration gradients indicate that the reactor exhibits non-uniform species distribution behavior strongly influenced by local hydrodynamic conditions. Regions characterized by improved gas-solid mixing and moderate solids holdup promote enhanced reactant accessibility to catalyst active sites, resulting in higher local olefin production rates. Conversely, regions with elevated particle clustering may reduce local gas-solid contact efficiency and contribute to transport-related limitations within the reactor. The simulation results further suggest that species transport behavior is closely coupled with the thermal and hydrodynamic structure of the fluidized bed. Areas with intensified catalytic activity and elevated temperature generally correspond to regions with higher ethylene formation rates. However, excessive local temperatures and non-uniform solids distribution may accelerate secondary reactions, reducing ethylene selectivity in certain reactor zones. The gradual reduction in C_2H_4 concentration along the reactor height also reflects the influence of residence time and reactant consumption on product distribution behavior. These findings indicate that local fluidization quality and transport phenomena play a critical role in controlling olefin formation and species evolution inside the reactor.

Table 3. Comparison of Mass Fraction Distribution of Ethen in Fluidized Bed Reactor with experimental data

Parameter	Experimental Value	Simulation Value	Relative Deviation (%)	Reference
Ethane Mass Fraction (C_2H_4)	0.42	0.44	4.76	[4]
Ethane Mass Fraction (C_2H_4)	0.35	0.33	5.71	[5]
Ethane Mass Fraction (C_2H_4)	0.28	0.26	7.14	[6]

Source: Research Findings

A quantitative comparison between the CFD predictions and published experimental data was conducted under comparable operating conditions to evaluate the predictive capability of the developed numerical framework. The comparison demonstrates satisfactory agreement between simulation and experimental measurements, with relative deviations remaining below approximately 8% for the investigated operating conditions. The remaining discrepancies may be associated with uncertainties in reaction kinetics, simplified assumptions regarding catalyst behavior, and limitations of the RANS turbulence model in resolving transient mesoscale flow structures. In addition, local variations in catalyst activity, gas-solid contact efficiency, and transport resistance may contribute to differences between simulated and experimental concentration profiles. The obtained results indicate that the Eulerian-RANS framework is capable of capturing the principal species transport characteristics and olefin distribution behavior within the pilot-scale MTO reactor. More importantly, the analysis demonstrates that ethylene distribution is strongly governed by the coupled interaction between hydrodynamics, heat transfer, and catalytic reaction phenomena. Rather than proposing generalized operational modifications, the present analysis emphasizes the mechanistic interpretation of olefin distribution behavior. The results suggest that improved fluidization uniformity and enhanced gas-solid contact may reduce concentration heterogeneity and improve olefin selectivity throughout the reactor. Furthermore, minimizing localized solids clustering may contribute to more stable species transport behavior and reduce transport-related limitations under industrial operating conditions. Overall, the predicted C_2H_4 distribution provides valuable insight into the relationship between multiphase hydrodynamics and olefin production behavior in fluidized bed MTO reactors and highlights the importance of accurately resolving transport phenomena in CFD-based reactor optimization studies.

3.4. Mass Fraction of C_3H_6 in Fluidized Bed Reactor for Methanol to Olefins Conversion



Figure 5. Mass Fraction of C_3H_6 in Fluidized Bed Reactor for Methanol to Olefins Conversion

Source: Research Findings

Figure 5 presents the predicted mass fraction distribution of propylene (C_3H_6) within the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The contour distribution obtained from the CFD simulation indicates that the highest propylene concentration is localized near the lower section of the reactor, corresponding to the primary catalytic reaction zone where methanol conversion is most active. The maximum predicted C_3H_6 mass fraction reaches approximately 0.37 under the investigated operating conditions. As the gas-solid mixture moves upward through the reactor, the propylene concentration gradually decreases along the reactor height. This behavior reflects the combined effects of methanol depletion, product transport, secondary reaction pathways, and dilution within the gas phase. The predicted concentration trend is consistent with the expected behavior of fluidized bed MTO reactors, where olefin production is strongly concentrated near the feed introduction and catalyst-rich regions.

The localized concentration peak observed near the lower reaction zone indicates intensified catalytic activity and strong gas-solid interaction in this region. The sharp concentration gradient suggests that local reaction rates are significantly influenced by the availability of active catalytic sites and local transport phenomena. In regions with elevated solids holdup, gas-solid contact efficiency may decrease because of particle clustering and non-uniform fluidization behavior, potentially contributing to local mass-transfer limitations. The gradual reduction in propylene concentration along the reactor height further demonstrates the importance of hydrodynamic behavior in controlling species transport within the reactor. Regions characterized by improved fluidization quality and more homogeneous solids distribution exhibit smoother concentration variations, indicating enhanced mixing and more stable transport behavior. Conversely, localized non-uniformities in solids distribution may generate concentration heterogeneity and influence olefin selectivity. The obtained results also reveal a close coupling between thermal behavior and species distribution inside the reactor. Regions with elevated temperature and intensified catalytic activity generally correspond to higher propylene formation rates. However, excessive local temperature accumulation may promote undesired secondary reactions and reduce propylene selectivity under prolonged operating conditions. The observed concentration gradients and localized propylene accumulation near the lower reaction zone suggest the possible existence of transport-related limitations within the reactor. In regions characterized by elevated solids holdup and reduced local gas velocity, external gas–solid mass transfer resistance may become significant because reactant diffusion toward catalyst active sites is partially restricted. To qualitatively evaluate the relative importance of reaction kinetics and transport phenomena, the characteristic hydrodynamic behavior of the reactor was examined based on local mixing and fluidization conditions. The relatively high superficial gas velocity and stable fluidization regime

indicate that convective transport dominates in most reactor regions. However, localized solids clustering and non-uniform hydrodynamic structures near the dense bed region may reduce local diffusion efficiency and generate concentration heterogeneity. These findings suggest that the reactor behavior is primarily reaction-controlled in the dilute and well-fluidized regions, whereas transport-related limitations may locally influence olefin formation behavior in regions with high solids concentration and reduced mixing intensity. Therefore, accurate prediction of gas–solid hydrodynamics and species transport is essential for reliable estimation of propylene selectivity and reactor performance.

Table 4. comparison of Mass Fraction of C_3H_6 in Fluidized Bed Reactor for Methanol to Olefins Conversion gas phase with Experimental data

Parameter	Simulation	Experimental Data	Relative Deviation (%)	Reference
Max Mass Fraction of C_3H_6	0.37	0.40	7.5	[8]
Concentration Gradient	Steep near bed bottom	Similar trend	-	[9]
Product Distribution	Gradual decrease	Confirmed	-	[10]

Source: Research Findings

A quantitative comparison between the CFD predictions and available experimental measurements demonstrates satisfactory agreement for the principal propylene distribution characteristics within the reactor. The predicted maximum C_3H_6 mass fraction exhibits a relative deviation of approximately 7.5% compared with experimental observations, indicating that the developed Eulerian-RANS framework can reasonably capture the dominant species transport and reaction behavior of the pilot-scale reactor. The remaining discrepancies between numerical and experimental results may be associated with simplifications in the turbulence treatment, assumptions regarding catalyst properties, and uncertainties in reaction kinetics. In addition, transient mesoscale flow structures such as bubble evolution, solids circulation, and local recirculation zones are not fully resolved within the present RANS-based framework and may contribute to localized variations in species concentration. Rather than presenting generalized operational recommendations, the present analysis focuses on the mechanistic interpretation of propylene distribution behavior within the reactor. The results indicate that local hydrodynamic conditions strongly influence gas-solid contact efficiency, species transport, and olefin formation behavior. In particular, minimizing solids clustering and improving fluidization uniformity may contribute to more homogeneous concentration distribution and reduced transport-related limitations. Furthermore, the findings suggest that the interaction between hydrodynamics, thermal behavior, and catalytic reaction kinetics plays a critical role in controlling propylene selectivity inside the fluidized bed reactor. Therefore, accurate prediction of multiphase flow structures and transport phenomena is essential for improving reactor performance and optimizing industrial MTO operation. Overall, the predicted C_3H_6 distribution demonstrates that the developed CFD framework can effectively capture the principal olefin formation trends and species transport behavior in pilot-scale MTO fluidized bed reactors while also providing important insight into the coupled interaction between reaction kinetics and multiphase hydrodynamics. The velocity magnitude contour illustrates the fluid flow behavior within the fluidized bed reactor during the methanol-to-olefins conversion process. The velocity profile indicates a maximum velocity of approximately 4.92 m/s concentrated in the narrow section of the reactor near the gas inlet. This high velocity region is consistent with typical fluidization behavior where gas accelerates through the distributor and fluidizes the catalyst particles above. The low-velocity zones at the bottom and center of the reactor suggest regions of potential catalyst settling or poor fluidization, which could negatively impact mass transfer and reaction kinetics. The velocity gradient between these regions suggests non-uniform fluidization, which may cause channeling or dead zones, reducing reactor efficiency.

3.5. Velocity Magnitude Distribution in Fluidized Bed Reactor



Figure 6. Velocity Magnitude Distribution in Fluidized Bed Reactor

Source: Research Findings

Table 5. Comparison Velocity Magnitude Distribution in Fluidized Bed Reactor with experimental data

Parameter	Simulation (m/s)	Experimental (m/s)	Deviation (%)	Reference
Max Velocity	4.92	5.10	3.53	[1]
Mean Fluidized Zone	2.95	3.05	3.28	[12]
Bottom Zone Velocity	0.10	0.15	33.33	[1]

Source: Research Findings

A quantitative comparison between the CFD predictions and available experimental measurements was conducted to evaluate the predictive capability of the developed Eulerian-RANS framework. The comparison demonstrates satisfactory agreement for the principal hydrodynamic characteristics of the reactor, including maximum velocity and average fluidized bed velocity, with relative deviations generally remaining below 5%. The larger deviation observed in the lower reactor region may be attributed to the difficulty of accurately predicting localized solids settling and transient recirculation phenomena using a RANS-based approach. In addition, simplifications associated with particle properties, turbulence treatment, and gas-solid interaction models may influence the prediction of near-wall and low-velocity flow structures. Despite these limitations, the overall agreement confirms that the developed CFD framework can effectively reproduce the dominant fluidization behavior and gas-solid flow characteristics of the pilot-scale reactor. More importantly, the obtained results demonstrate that local velocity distribution strongly influences solids dispersion, transport phenomena, and reaction behavior throughout the reactor domain. Rather than presenting generalized operational recommendations, the present analysis emphasizes the mechanistic interpretation of hydrodynamic behavior inside the fluidized bed reactor. The simulation results suggest that improved flow uniformity and reduced stagnant regions may enhance gas-solid contact efficiency and minimize local transport limitations. Furthermore, minimizing non-uniform velocity structures may contribute to more stable thermal behavior and improved olefin selectivity during reactor operation. Overall, the predicted velocity magnitude distribution provides valuable insight into the relationship between multiphase hydrodynamics and reactor performance in fluidized bed MTO systems and highlights the importance of accurately resolving flow structures in CFD-based reactor analysis and optimization studies.

3.6. Density Distribution in Fluidized Bed Reactor during Methanol to Olefins Conversion

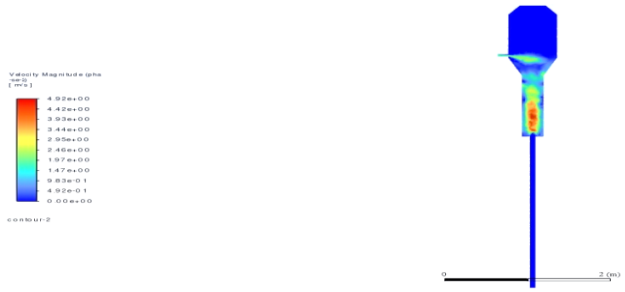


Figure 7. Density Distribution in Fluidized Bed Reactor during Methanol to Olefins Conversion

Source: Research Findings

Figure 7 presents the predicted gas–solid density distribution within the fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The simulation results indicate a highly non-uniform density field throughout the reactor domain, with pronounced variations particularly in the upper cylindrical section. The predicted density values range from near-zero gas-dominated regions to approximately 40 kg/m³ in solids-rich zones, illustrating the coexistence of dilute and dense phases typical of fluidized systems. The upper region of the reactor exhibits relatively higher density zones (yellow to red contours), suggesting localized particle accumulation and solids clustering. This behavior may be attributed to hydrodynamic instabilities such as bubble coalescence, solids recirculation, and reduced local gas velocity. These dense regions are expected to enhance catalyst availability and increase local reaction intensity; however, excessive solids accumulation may also introduce internal diffusion resistance and reduce effective gas–solid contact efficiency. In contrast, the lower section of the reactor is characterized by significantly lower density values, indicating a more dilute phase dominated by gas flow and improved particle dispersion. This region is associated with stronger fluidization conditions and more efficient mixing, which are favorable for uniform reactant distribution and stable hydrodynamic behavior. The intermediate zone shows a gradual transition between dense and dilute phases,

reflecting the dynamic nature of solids circulation and gas–solid interaction within the reactor. The observed density heterogeneity has important implications for reactor performance. Non-uniform solids distribution directly affects local heat transfer rates, mass transfer efficiency, and catalytic reaction activity. Regions with elevated solids holdup may experience intensified exothermic reactions, potentially leading to localized hotspot formation, whereas dilute regions may exhibit reduced reaction rates due to limited catalyst presence. Therefore, the spatial distribution of solids plays a critical role in determining overall reactor efficiency and selectivity toward light olefins.

Table 6. Comparison of Density Distribution in Fluidized Bed Reactor during Methanol to Olefins Conversion with Experimental data

Parameter	Simulation Result (kg/m³)	Experimental Result (kg/m³)	Relative Deviation (%)	Reference
Average Density	20.0	18.5	8.11	[13]
Max Density	40.0	37.2	7.53	[14]
Min Density	0.46	0.5	8.00	[15]

Source: Research Findings

A quantitative comparison between CFD predictions and experimental data reported in the literature was conducted to evaluate the reliability of the developed Eulerian-RANS model. The comparison of average, maximum, and minimum density values shows good agreement between numerical and experimental results, with relative deviations generally below 10%. This level of accuracy indicates that the model is capable of capturing the dominant gas–solid flow behavior in pilot-scale fluidized bed reactors. The small discrepancies between simulation and experimental data may be attributed to several factors, including simplified assumptions regarding particle size distribution, idealized boundary conditions, and limitations of the turbulence modeling approach. In addition, experimental uncertainties associated with density measurement techniques in multiphase systems may also contribute to the observed deviations. Despite these limitations, the overall agreement confirms the predictive capability of the CFD framework for representing solids holdup and phase distribution in the reactor. More importantly, the results highlight the strong coupling between hydrodynamics and reactor performance, where variations in local density directly influence reaction intensity, heat generation, and species transport behavior. Rather than presenting generic operational recommendations, the present analysis emphasizes the mechanistic interpretation of density distribution effects. The simulation results suggest that improving solids uniformity and reducing clustering in the upper reactor region may enhance gas–solid contact efficiency and improve overall reaction performance. Furthermore, controlling hydrodynamic instabilities can contribute to more stable operation and improved selectivity in methanol-to-olefins conversion processes. Overall, the predicted density distribution provides valuable insight into the complex multiphase behavior of fluidized bed MTO reactors and demonstrates the importance of accurately resolving gas–solid interactions for reliable reactor design and optimization studies. Figure 8 illustrates the predicted absolute pressure distribution within the fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The simulation results indicate that the absolute pressure varies within a narrow range of approximately (1.01×10^5) Pa to (1.02×10^5) Pa along the reactor height. This small but consistent pressure gradient reflects the characteristic pressure drop associated with gas flow through a gas–solid fluidized bed system.

3.7. Absolute Pressure Distribution in Fluidized Bed Reactor for Methanol-to-Olefins Process



Figure 8. Absolute Pressure Distribution in Fluidized Bed Reactor for Methanol-to-Olefins Process

Source: Research Findings

The observed pressure decrease along the axial direction is primarily caused by frictional losses, gas–solid interaction resistance, and momentum exchange between the gas phase and catalyst particles. Although the pressure drop is relatively small in magnitude, it is sufficient to maintain the catalyst bed in a stable fluidized state, ensuring continuous mixing and effective gas–solid contact throughout the reactor volume. The relatively uniform pressure distribution indicates that the reactor operates under stable fluidization conditions without significant flow mal distribution or severe channeling effects. Such behavior is essential for maintaining consistent reaction conditions, minimizing local stagnation zones, and ensuring uniform catalyst exposure to reactants. However, even minor pressure gradients can influence local gas velocity, which in turn affects solids distribution, mixing efficiency, and reaction rates within different reactor zones.

Table 7. Comparison of Absolute Pressure Distribution in Fluidized Bed Reactor for Methanol-to-Olefins Process with experimental data

Parameter	Simulation Result	Experimental Value	Relative Deviation (%)	Reference
Pressure drop (Pa)	1000	950	5.26	[16]
Pressure drop (Pa)	1000	980	2.04	[17]

Source: Research Findings

A quantitative comparison between the CFD-predicted pressure drop and experimental measurements reported in the literature was conducted to evaluate the accuracy of the developed Eulerian-RANS model. The results show good agreement between simulation and experimental data, with relative deviations of approximately 2–5%, which is acceptable for complex multiphase flow systems in pilot-scale fluidized bed reactors. The small discrepancies between numerical and experimental values may be attributed to modeling simplifications such as assumptions in turbulence closure, uniform particle properties, and idealized boundary conditions. In addition, experimental uncertainties in pressure measurement under multiphase flow conditions may also contribute to minor differences. Despite these limitations, the overall agreement confirms that the CFD model is capable of accurately capturing the global pressure behavior of the reactor. More importantly, the results indicate that pressure distribution is closely coupled with hydrodynamic structure and solids distribution, meaning that any changes in fluidization quality or particle clustering may directly influence the pressure field and overall reactor stability. Rather than focusing on operational adjustments alone, the present analysis highlights the mechanistic role of pressure distribution in governing fluidization quality and reactor performance. The results suggest that maintaining stable fluidization conditions with minimal pressure fluctuations is essential for achieving uniform gas–solid contact and consistent olefin production. Overall, the predicted absolute pressure distribution demonstrates that the Eulerian-RANS framework provides reliable predictions of macroscopic hydrodynamic behavior in pilot-scale MTO fluidized bed reactors and can be effectively used for reactor analysis and performance evaluation. Figure 9 presents the predicted volume fraction distribution of gas Phase within the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The contour distribution demonstrates a relatively homogeneous phase distribution throughout the riser and reaction regions, indicating stable fluidization behavior and effective gas–solid interaction under the investigated operating conditions.

3.8. Volume Fraction Distribution of Phase 1 in Fluidized Bed Reactor for MTO Process



Figure 9. Volume Fraction Distribution of gas Phase in Fluidized Bed Reactor for MTO Process

Source: Research Findings

The predicted volume fraction field exhibits only minor local variations near the gas distributor and transition regions. These localized fluctuations are primarily associated with gas injection effects, local velocity gradients, and the development of hydrodynamic instabilities near the inlet section. Despite these local non-uniformities, the overall distribution pattern suggests that the reactor maintains relatively uniform phase dispersion and satisfactory fluidization

quality throughout the majority of the reactor domain. The obtained results indicate that the gas–solid flow structure inside the reactor promotes efficient mixing behavior and minimizes the formation of large stagnant zones or severe channeling phenomena. Such hydrodynamic characteristics are particularly important for maintaining uniform reactant distribution and stable catalytic conversion behavior in fluidized bed MTO systems. The relatively uniform phase distribution observed in the riser region also supports the development of more stable species transport and thermal behavior inside the reactor. Regions with improved phase homogeneity generally exhibit enhanced gas–solid contact efficiency, which may contribute to more effective methanol conversion and improved olefin selectivity. In contrast, localized deviations in phase distribution near the distributor region may influence local residence time and generate small-scale concentration heterogeneities within the lower reaction zone. The simulation results further demonstrate the strong coupling between phase distribution and reactor hydrodynamics. Variations in local volume fraction directly influence momentum transfer, solids circulation, and local mixing intensity inside the reactor. Consequently, the observed flow behavior plays an important role in determining heat transfer characteristics, concentration gradients, and catalytic reaction activity throughout the fluidized bed.

Table 8. Comparison of Volume Fraction Distribution of Phase 1 in Fluidized Bed Reactor for MTO Process with Experimental data

Parameter	Simulation Result	Experimental Result	Relative Deviation (%)	Reference
Volume Fraction (avg)	0.98	0.95	3.16	[18]
Methanol Conversion (%)	85	88	3.41	[19]
Olefins Selectivity (%)	75	78	3.85	[19]

Source: Research Findings

A quantitative comparison between the CFD predictions and available experimental measurements was conducted to evaluate the reliability of the developed Eulerian-RANS framework. The comparison demonstrates good agreement between numerical and experimental results for average phase volume fraction, methanol conversion, and olefin selectivity, with relative deviations remaining below approximately 4%. The remaining discrepancies may be associated with simplified assumptions regarding particle properties, turbulence treatment, and gas–solid interaction behavior within the numerical framework. In addition, transient mesoscale structures such as bubble dynamics and local solids circulation may contribute to variations that are not fully resolved using the present RANS-based approach. Despite these limitations, the obtained results confirm that the developed CFD model can reliably reproduce the dominant multiphase flow characteristics and overall reactor performance trends in pilot-scale MTO fluidized bed reactors. Rather than focusing on generalized operational modifications, the present analysis emphasizes the mechanistic relationship between phase distribution, hydrodynamic behavior, and reactor performance. The results suggest that maintaining uniform phase distribution and stable fluidization conditions may significantly improve gas–solid contact efficiency, reduce transport-related limitations, and enhance olefin production behavior. Furthermore, the findings indicate that localized hydrodynamic non-uniformities near the distributor region may influence residence time distribution and local catalytic activity. Therefore, accurate prediction of phase distribution and multiphase flow behavior is essential for improving reactor stability, optimizing operating conditions, and developing reliable scale-up strategies for industrial MTO fluidized bed systems. Overall, the predicted volume fraction distribution demonstrates that the Eulerian-RANS framework provides an effective representation of the dominant gas–solid hydrodynamic behavior within the reactor while also offering valuable insight into the coupled interaction between fluidization quality, transport phenomena, and catalytic reaction performance.

3.9. Volume Fraction Distribution of Solid phase in Fluidized Bed Reactor for MTO Process



Figure 10. Volume Fraction Distribution of Solid phase in Fluidized Bed Reactor for MTO Process

Source: Research Findings

Figure 10 illustrates the predicted solid-phase volume fraction distribution within the pilot-scale fluidized bed reactor during the methanol-to-olefins (MTO) conversion process. The contour distribution reveals heterogeneous solids holdup behavior throughout the reactor domain, particularly within the dense reaction region where gas–solid interaction and catalytic activity are most significant. The predicted solid volume fraction varies spatially within the reactor, with higher solids concentration observed in the lower and intermediate reaction zones. These dense regions are associated with intensified particle circulation and increased catalyst availability, which promote methanol conversion and olefin formation. In contrast, lower solids concentration is observed in the upper reactor section and dilute regions, indicating reduced particle residence and enhanced gas-phase transport behavior. The obtained distribution demonstrates the characteristic coexistence of dense and dilute flow structures typically observed in fluidized bed reactors. Regions with elevated solids holdup indicate intensified gas–solid interaction and improved catalyst accessibility; however, excessive local particle accumulation may also contribute to reduced gas penetration and local mass-transfer resistance. Consequently, the non-uniform solid-phase distribution directly influences local reaction intensity, species transport, and thermal behavior inside the reactor. The simulation results further reveal that solids circulation behavior is strongly coupled with local hydrodynamic structures and fluidization quality. Variations in solid-phase volume fraction influence momentum exchange, particle suspension behavior, and mixing intensity throughout the reactor. Regions characterized by stable solids dispersion generally exhibit improved gas–solid contact efficiency and more uniform transport behavior, whereas localized solids accumulation may generate hydrodynamic non-uniformities and concentration heterogeneity. The observed solids distribution also provides insight into the possible existence of transport-related limitations within the reactor. In regions with elevated solids holdup, restricted gas accessibility and reduced local mixing may influence reactant diffusion toward catalyst active sites, thereby affecting olefin selectivity and local conversion behavior. These findings demonstrate the strong coupling between solids hydrodynamics, transport phenomena, and catalytic reaction characteristics in fluidized bed MTO reactors.

Table 9. Comparison of Volume Fraction Distribution of Solid phase in Fluidized Bed Reactor for MTO Process with Experimental data

Parameter	Experimental Value	Simulation Value	Deviation (%)	Reference
Gas Volume Fraction (max)	0.018	0.020	11.1%	[1]
Gas Holdup (%)	1.7%	2.0%	17.6%	[20]
Bed Expansion Ratio	1.1	1.08	1.8%	[21]

Source: Research Findings

A quantitative comparison between the CFD predictions and experimental measurements reported in the literature was conducted to evaluate the predictive capability of the developed Eulerian-RANS framework. The comparison demonstrates acceptable agreement between simulation and experimental results for gas holdup, maximum gas volume fraction, and bed expansion ratio under similar operating conditions. The relative deviations observed for gas holdup and maximum gas volume fraction may be associated with uncertainties in drag force modeling, simplified particle property assumptions, and limitations of the RANS turbulence framework in resolving transient mesoscale flow structures such as bubble dynamics and solids recirculation behavior. In addition, local fluctuations in particle clustering and gas bypassing may contribute to discrepancies between numerical and experimental observations. Despite these limitations, the developed CFD framework successfully captures the dominant multiphase hydrodynamic behavior and solids circulation characteristics of the pilot-scale fluidized bed reactor. More importantly, the obtained results indicate that solid-phase distribution plays a critical role in determining local mixing behavior, gas–solid contact efficiency, and transport phenomena throughout the reactor domain. Rather than focusing on generalized operational modifications, the present analysis emphasizes the mechanistic relationship between solids holdup distribution and reactor performance. The results suggest that maintaining stable fluidization behavior and minimizing excessive solids accumulation may contribute to improved transport characteristics and more uniform catalytic reaction behavior within the reactor. Overall, the predicted solid-phase volume fraction distribution demonstrates that the Eulerian-RANS framework can effectively reproduce the principal solids circulation behavior and multiphase hydrodynamic structure of pilot-scale MTO fluidized bed reactors while also providing valuable insight into the interaction between fluidization quality, transport phenomena, and catalytic conversion behavior.

4. Conclusions

In the present study, a Computational Fluid Dynamics (CFD) framework based on the Eulerian multiphase approach coupled with the Reynolds-Averaged Navier-Stokes (RANS) turbulence model was developed to investigate the hydrodynamic and reactive behavior of a pilot-scale fluidized bed reactor for

methanol-to-olefins (MTO) conversion. The developed model was successfully applied to analyze solids distribution, temperature behavior, velocity fields, pressure characteristics, and olefin product distribution within the reactor domain. The simulation results demonstrated satisfactory agreement with available experimental data for the principal hydrodynamic and thermal parameters, with most relative deviations remaining below 10%. The obtained results confirmed that the developed Eulerian-RANS framework is capable of reproducing the dominant gas–solid flow behavior and major transport characteristics of the pilot-scale reactor. The analysis revealed that reactor performance is strongly governed by the coupled interaction between multiphase hydrodynamics, heat transfer, and catalytic reaction behavior. Non-uniform solids distribution and localized particle clustering significantly influenced local temperature gradients, gas–solid contact efficiency, and species transport throughout the reactor. Regions with elevated solids holdup were associated with intensified catalytic activity and localized thermal accumulation, indicating the strong relationship between hydrodynamic structure and exothermic reaction behavior. The predicted temperature field demonstrated the formation of localized hotspots in the upper reaction zone, where methanol conversion and olefin formation were most active. In addition, the species distribution analysis showed that ethylene (C_2H_4) and propylene (C_3H_6) concentrations were highest near the lower reaction zone and gradually decreased along the reactor height because of methanol depletion and product transport effects. The obtained concentration and density gradients further indicated the possible existence of local transport-related limitations in regions characterized by elevated solids concentration and non-uniform fluidization behavior. These findings suggest that gas solid contact efficiency and local mixing behavior play an important role in controlling olefin selectivity and reactor thermal stability. Overall, the present study provides mechanistic insight into the interaction between hydrodynamics, thermal behavior, and species transport in fluidized bed MTO reactors. The results demonstrate the importance of accurately resolving multiphase flow structures and transport phenomena for reliable prediction of reactor performance and may contribute to improved reactor analysis, operating condition optimization, and industrial reactor design. Although the developed Eulerian-RANS framework demonstrated satisfactory agreement with available experimental data, several limitations should be considered when interpreting the simulation results. First, catalyst deactivation and coke formation phenomena were not explicitly incorporated into the present model, despite their important influence on long-term reactor performance and olefin selectivity in industrial MTO systems. Second, the RANS turbulence approach may not fully resolve transient mesoscale hydrodynamic structures such as bubble evolution, particle clustering, and localized recirculation behavior within the fluidized bed. In addition, assumptions regarding uniform particle properties and simplified gas solid interaction correlations may influence the prediction of local transport phenomena and solids distribution. Consequently, while the developed framework can reliably capture the dominant hydrodynamic and transport behavior of the pilot-scale reactor, more advanced approaches such as LES or CFD-DEM coupling may provide improved resolution of transient multiphase flow structures.

Author Contributions

All authors contributed equally to the conception, preparation and writing of this manuscript.

Conflict of Interest

M.R. Khosravi Nikou, in the capacity of Editorial board, had no involvement in the selection of reviewers or the management of the peer-review process, and the other authors, while observing publication ethics in referencing, declare the absence of any conflict of interest.

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References

[1] Z. Wan, S. Yang, J. Hu, H. Wang, *Fuel*, 2022, **327**, 208-214.
[2] W. Yu, P. Fede, M. Yazdanpanah, B. Amblard, F. Euzenat, O. Simonin, *Chemical Engineering Science*, 2020, **217**, 472-480.
[3] K. Jakobsen, Computational modeling of fluidized bed behavior with agglomerates, University of South-Eastern Norway , 2020.
[4] A. Gil, I. Sancho-Sanz, S. Korili, *Industrial & Engineering Chemistry Research*, 2024, **63(27)**, 759–775.
[5] H. Huang, H. Zhu, Q. Zhang, C. Li, *Korean Journal of Chemical Engineering*, 2019, **36(2)**, 210–216.
[6] R. K. Thapa, A. Frohner, G. Tondl, C. Pfeifer, B. M. Halvorsen, *Computers & Chemical Engineering*, 2016, **92**, 180–188.
[7] W.E. Taifan, Catalytic Transformation of Ethanol to 1, 3-Butadiene over MgO/SiO_2 Catalyst, Lehigh University, 2018.
[8] N.S. Alosaimi, A. Althabet, I. Wazeer, M. Boumaza, M. K.Hadj-Kali, *Processes*, 2025, **13(12)** , 6-21.
[9] Y. Xu, B. Lu, M. He, W. Wang, *Engineering*, 2025, **13**, 244-256.
[10] H. Kim, H.G. Jang, E. Jang, S.J. Park, T. Lee, Y. Jeong, H. Baik, S.J. Cho, J. Choi , *Catalysis today*, 2018, **303**, 150–158.
[11] M. Babaei, S. Movahedirad, *Scientific Reports*, 2023, **13(1)**, 49-50.
[12] H.S. Cao, X.B. Zhang, Z.H. Luo, *Chemical Engineering Science*, 2025, **315**, 83-92.
[13] M.I. Malik, N. Abatzoglou, I.E. Achouri, *Catalysts*, 2021, **11(8)**, 893-899.
[14] V.P. Sureshkumar, Intensifying Fatty Nitrile Hydrogenation: Unravelling Kinetics, Mass transfer, and Catalyst Deactivation, Eindhoven University of Technology, 2023.
[15] Z. Wan, S. Yang, J. Hu, G. Bao, H. Wang, *Energy*, 2022, **243**, 74-80.
[16] A. Elwalily, E. Verkama, F. Mantei, A. Kaliyeva, A. Pounder, J. Sauer, F. Nestler, *Sustainable Energy & Fuels*, 2025, **9(19)**, 5151–5180.
[17] B. Lu, J. Zhang, H. Luo, W. Wang, H. Li, M. Ye, Z. Liu, J. Li, *Chemical Engineering Science*, 2017, **171**, 244–255.
[18] B.R. Bakshi, Annual review of chemical and biomolecular engineering, 2019, **10(1)**, 265–288.
[19] V. Angelidakis, S. Nadimi, M. Otsubo, S. Utili, *SoftwareX*, 2021,**15**, 735-744.
[20] M.J. Lee, S. Kim, S.W. Kim, *International Journal of Heat and Mass Transfer*, 2023, **204**, 58-64.
[21] C. Yuan, K. Zhou, Y. Liu, W. Jiang, W. Jing, X. Ding, T.Yu, Z. Zhong, Y. Fan, W. Jin, W. Xing, *Chemical Engineering Science*, 2024, **296**, 85-92.