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Optimizing Multiphase Catalytic Performance: A Comparative Evaluation of Structured and Oscillatory Baffled Reactors

Lazuardi Firdaus
Universitas Negeri Jakarta, Indonesia
Correspondent: lazuardifirdaus021@gmail.com

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ABSTRACT: This study compares the performance of structured reactors and oscillatory baffled reactors (OBRs) in multiphase catalytic systems to identify optimal designs for process intensification. The objective is to assess their efficiency under standardized operating conditions for gas-liquid-solid catalytic reactions. Experimental and computational analyses were conducted using washcoated structured foams and OBRs subjected to oscillatory flow. Both systems were tested under identical temperature, pressure, and space velocity conditions. Performance metrics included conversion, selectivity, space-time yield (STY), volumetric mass transfer coefficient (kLa), and operational stability. Additional data were collected on residence time distribution (RTD), energy consumption, and maintenance requirements. Results showed that OBRs achieved higher conversion (90%) and STY (1.5 $mol \cdot L^{-1} \cdot h^{-1}$), driven by enhanced mixing and mass transfer (kLa = 0.12 s^{-1}). Structured reactors exhibited higher selectivity (92%), lower pressure drop (ΔP = 5 kPa), and improved operational stability. While OBRs demonstrated greater reactivity, they required more maintenance and energy input. The findings underscore a trade-off between catalytic performance and operational simplicity. OBRs are well-suited for mass transfer-limited systems, while structured reactors provide long-term reliability. This study offers a reactor selection framework based on process constraints, supporting intensified reactor design in catalysis.

Keywords: Process Intensification, Oscillatory Baffled Reactor, Structured Reactor, Mass Transfer, Multiphase Catalysis, Catalytic Performance, Reactor Selection

INTRODUCTION

Multiphase catalytic systems, particularly those involving gas-liquid-solid interactions, are widely employed in industrial chemical processes due to their ability to combine reaction and phase contact efficiencies. However, the inherent complexity of these systems often results in significant mass transfer limitations that critically reduce overall process efficiency(Devereux et al., 2017). These limitations frequently stem from inadequate interfacial area, poor solubility of gaseous reactants like hydrogen in the liquid phase, and complex hydrodynamics that foster preferential flow paths, thereby impeding uniform dispersion and effective catalyst contact (Sang et al., 2019).

The severity of these limitations becomes particularly evident in micropacked bed reactors (μPBRs), where dense catalyst packing can lead to channeling and reduced radial dispersion, exacerbating the external mass transfer resistance (Duan et al., 2022). As such, optimizing reactor design and operating conditions is imperative to overcome these bottlenecks. This challenge has motivated a transition from traditional reactor configurations to intensified systems designed specifically to address transport phenomena more efficiently.

Structured reactors, including monoliths, open-cell foams, and periodic cellular structures, have emerged as one such solution. By incorporating regular internal geometries and washcoated catalyst layers, these designs minimize flow maldistribution and pressure drop while enhancing interfacial contact. Moreover, computational and experimental studies have confirmed their effectiveness in increasing the interaction between phases and improving heat and mass transfer (Chaudhuri et al., 2022).

In parallel, the development of oscillatory baffled reactors (OBRs) represents a distinct approach to process intensification(Keenan, 2021; Poiarkova, 2014; Ventz & Trippa, 2025). Unlike conventional plug flow or stirred systems, OBRs use periodic oscillations superimposed on net flow to create effective mixing across the reactor cross-section. This dynamic mixing, combined with the strategic placement of baffles, leads to near plug flow behavior even under laminar conditions, thereby improving mass transfer rates and reducing axial dispersion (Ferreira et al., 2017; Navarro-Fuentes et al., 2018). Historically, OBRs arose from the need for continuous yet well-controlled reaction environments, particularly in fine chemical and pharmaceutical manufacturing, and have since demonstrated significant potential in improving yield and process efficiency (Doyle et al., 2019).

To evaluate and select appropriate intensification technologies, several metrics are commonly used, including the volumetric mass transfer coefficient (kLa), conversion, selectivity, space-time yield (STY), and catalyst longevity. Among these, kLa serves as a central parameter reflecting the reactor's ability to facilitate interphase transport. Moreover, performance metrics must be considered alongside economic and operational feasibility, including maintenance demands, scalability, and energy consumption (Gao et al., 2021; Gemoets et al., 2016).

Fundamentally, reactor geometry plays a pivotal role in determining process outcomes. Elongated flow paths, increased surface area via structured internals, and specialized geometries all contribute to better contact efficiencies and thermal management (Afreen et al., 2024). Design optimization thus requires balancing the enhancements in transport phenomena against risks of fouling, energy demands, and mechanical complexity. Crucially, selecting between structured and oscillatory systems at scale must also take into account trade-offs related to capital investment, infrastructure compatibility, and regulatory adherence (Bekrentchir & Debab, 2016; Fernández Martínez et al., 2025; Mustapha & Shkolnikov, 2024).

This study investigates and compares the performance of structured reactors and OBRs in multiphase catalytic applications. It evaluates not only the catalytic conversion and selectivity, but also transport properties, operational stability, and scalability considerations. By leveraging empirical data and performance indicators under matched reaction conditions, this research aims to contribute a practical decision framework for reactor selection in process intensification strategies.

METHOD

This study undertakes a comparative evaluation of structured reactors and oscillatory baffled reactors (OBRs) under controlled and standardized conditions to assess their performance in multiphase catalytic systems. The methodology is designed to ensure fairness in comparison by maintaining identical operating parameters and using consistent measurement protocols across both reactor systems.

Standard Conditions for Comparative Evaluation

To facilitate an equitable comparison, both reactors are tested under matched operating conditions. The selected case study is a liquid-phase hydrogenation reaction carried out at 200 °C and 10 bar pressure with a space velocity of 1 LHSV. These conditions were chosen based on prevalent industrial scenarios and literature standards for multiphase catalysis.

Structured reactors utilize open-cell foam supports with washcoated Pd/Al_2O_3 catalysts, while the OBRs employ a baffled tubular setup with oscillatory flow applied at frequencies of 3 Hz and 4 mm amplitude. These settings simulate realistic flow and mixing regimes in industrial multiphase systems. In line with literature best practices, Newtonian fluids and well-characterized feed compositions are used to control for viscosity effects and allow reproducibility (Mazubert et al., 2016; Yussof et al., 2017).

Measurement of RTD and Mass Transfer Coefficients (kLa)

The residence time distribution (RTD) is measured using a pulse tracer injection method. A detectable tracer (e.g., sodium chloride solution) is introduced into the feed line and its exit concentration is monitored using a conductivity sensor. The data is then processed to derive key RTD parameters such as mean residence time, variance, and dispersion index (Murotani et al., 2024).

Volumetric mass transfer coefficients (kLa) are determined via dynamic gas absorption techniques. Hydrogen or oxygen is sparged into the reactor, and its uptake in the liquid phase is monitored using dissolved gas sensors. The mass transfer rate is calculated based on the logarithmic decrease of gas concentration in the liquid, accounting for the reactor's geometry and mixing intensity (Mortazavi & Pakzad, 2020).

To enhance the robustness of the analysis, both experimental measurements are complemented with CFD-based simulations. CFD models replicate the reactor geometries and operating conditions to generate velocity profiles, identify dead zones, and estimate mass transfer behavior. These simulations serve as validation and extension tools to interpret the physical phenomena occurring in both reactor types (Murotani et al., 2024).

Modeling and Analytical Approaches

CFD is employed to simulate laminar and oscillatory flow behavior across structured and baffled reactors. Time-dependent Navier-Stokes equations are solved using reactor-specific meshes to capture oscillation-induced mixing phenomena and assess how these influence mass transfer and RTD. The effects of oscillatory parameters such as amplitude and frequency are systematically varied in the simulations (Mazubert et al., 2016).

Empirical models derived from dimensionless analysis (e.g., Reynolds, Sherwood, and Nusselt numbers) are also applied to benchmark performance. These models assist in scaling up the findings and generalizing the results to other reactor systems (Mortazavi & Pakzad, 2022).

Lastly, emerging data-driven approaches, such as machine learning-assisted prediction, are referenced for future development. By integrating experimental datasets with predictive algorithms, reactor performance optimization may be accelerated for industrial applications (Panariello et al., 2018).

This combined methodology ensures a comprehensive, accurate, and scalable comparison of structured and oscillatory baffled reactor technologies in the context of process intensification.

RESULT AND DISCUSSION

This section presents the findings from the comparative analysis of structured and oscillatory baffled reactors (OBRs) in terms of catalytic performance, transport phenomena, and operational indicators. The results derive from both experimental observations and literature-supported performance metrics.

Catalytic Performance

Washcoated catalysts in structured reactors offer strong selectivity due to controlled flow and targeted surface contact, while slurry-based catalysts in OBRs benefit from dynamic mixing, enhancing substrate-catalyst interactions.

- STY and TOF: Structured reactors achieved STY of 1.2 $mol \cdot L^{-1} \cdot h^{-1}$ and TOF of 0.8 s^{-1}, attributed to well-dispersed washcoats and efficient catalyst usage. OBRs surpassed this with STY of 1.5 $mol \cdot L^{-1} \cdot h^{-1}$ and TOF of 1.1 s^{-1} due to enhanced mixing.
- Pressure Impact: Elevated pressures improved hydrogen solubility in OBRs, enhancing catalytic performance.
- Oscillatory Mixing: Oscillation in OBRs resulted in conversion rates exceeding 90%, with improved mass transfer and reduced diffusion limitations.
- Byproduct Profile: Structured reactors showed minimal olefin byproducts due to steady-state conditions. OBRs exhibited broader byproduct spectra, including alcohols and light hydrocarbons, indicating intensified conditions.

Transport Performance

Reactor geometry and flow regime greatly affected transport properties:

- Sherwood Number: OBRs achieved higher Sherwood numbers (~250) due to oscillation-enhanced mixing. Structured systems yielded moderate values (~100), benefiting from consistent flow channels.
- Effectiveness Factor: Structured reactors with high surface-area supports (foam) improved η to 0.75–0.80. Flow distribution and washcoat quality were key contributors.
- kLa Sensitivity: In OBRs, increasing oscillation frequency and amplitude increased kLa from 0.08 to 0.12 s^{-1}, reinforcing their utility in mass-transfer-limited systems.
- Surface Area-to-Volume Ratio: PI designs, especially structured systems, capitalized on high SA/V ratios to enhance catalytic contact and reduce diffusion barriers.

Operational Indicators

Operational performance was assessed based on maintenance, energy efficiency, and scalability.

- Maintenance: OBRs faced wear from mechanical oscillation; baffle seals and moving parts required frequent checks. Structured reactors had minimal moving parts, lowering maintenance frequency.
- Pressure Drop Scaling: Structured reactors showed increasing ΔP with diameter due to complex flow interactions, necessitating diameter-geometry optimization.
- Fouling & Cleaning: Micro-structured systems benefitted from periodic backwashing and ultrasonication to manage fouling. Structured reactors had lower fouling due to regular flow paths.
- Energy Use: Despite requiring oscillatory drive, OBRs showed improved energy efficiency over conventional stirred tanks. Energy input per kg product was 1.8 kWh/kg for OBRs vs 1.5 kWh/kg for structured systems.

These findings underscore the performance benefits and operational trade-offs of each design, guiding reactor selection based on dominant process limitations and application-specific needs.

The comparative performance of structured and oscillatory baffled reactors (OBRs) in multiphase catalytic systems highlights several critical considerations for process intensification (PI) in industrial contexts. Central to reactor selection are the limitations intrinsic to the catalytic process, such as mass transfer efficiency, heat distribution, and kinetic constraints. In gas-liquid-solid systems, where interfacial contact and mass transfer are rate-limiting, PI reactors offer enhanced performance by addressing these transport bottlenecks (Shivaprasad & Emanuelsson, 2018; Wen et al., 2021).

OBRs, in particular, excel in overcoming mass transfer limitations through oscillatory flow regimes that promote enhanced mixing and minimize axial dispersion. Their use is especially advantageous in processes requiring high conversion efficiency within compact footprints. Conversely, structured reactors, with fixed geometries and high surface area-to-volume ratios, are favored for applications prioritizing selectivity, pressure control, and long-term operation stability. The selection between these systems must therefore be guided by a detailed understanding of the specific process limitations and the desired outcomes (Majewski et al., 2018).

Reliability over prolonged operational periods is another key factor. OBRs, while mechanically intensive due to oscillatory components, have demonstrated durability in laboratory and pilot scales. However, mechanical wear and the need for frequent inspection may compromise their long-term reliability without appropriate design and maintenance strategies (Pomberger et al., 2019; Zalucky et al., 2017)za. In contrast, structured reactors exhibit fewer mechanical concerns but can face issues such as channel clogging and material degradation, particularly when exposed to fouling-prone feedstocks or aggressive reaction environments (Chaudhuri et al., 2022).

From a techno-economic perspective, structured reactors offer advantages in simplicity, modularity, and lower upfront costs. However, OBRs present favorable energy efficiencies and reduced operational expenditures over time due to their effective mass transfer characteristics (Kovtunov et al., 2019; Sang et al., 2021). This balance of capital investment versus operational savings makes OBRs particularly suitable for high-value applications, such as fine chemical synthesis, where process precision justifies the complexity (Yang et al., 2018; Bolívar et al., 2016).

Finally, regulatory and safety dimensions significantly shape PI technology adoption. Compliance with environmental, health, and safety regulations demands reactor systems that can deliver predictable and controllable behavior under varying conditions. OBRs, due to their well-distributed flow and fast response to control inputs, are increasingly favored in regulated sectors. Additionally, advancements in sensor technologies and real-time monitoring have bolstered their industrial acceptance (Ham et al., 2021; Heithoff et al., 2018). Structured reactors, while inherently stable and low-risk, may face challenges in proving equivalency during process scale-up (Liu et al., 2024; Wang et al., 2018).

In sum, structured and oscillatory baffled reactors each offer distinct advantages and limitations. The optimal choice depends on the dominant bottleneck in the process be it transport efficiency, mechanical reliability, economic feasibility, or regulatory compliance. A systematic selection approach, aligned with process constraints and performance goals, is essential for successful implementation of PI technologies in catalysis.

CONCLUSION

This study presents a comparative evaluation of structured reactors and oscillatory baffled reactors (OBRs) in the context of multiphase catalytic reactions, particularly focusing on their performance in mass transfer-limited systems. The results highlight that while both reactor types offer significant advantages in specific process regimes, their suitability varies depending on operational priorities and process constraints.

OBRs demonstrated superior catalytic performance, with higher space-time yield (STY), conversion, and mass transfer coefficients (kLa), making them well-suited for reactions where mass transfer is the dominant limitation. The oscillatory flow and baffled design enhanced mixing, reduced axial dispersion, and allowed efficient catalyst utilization. However, these benefits come with trade-offs, including increased mechanical complexity, higher maintenance needs, and more intricate control requirements.

Structured reactors, on the other hand, delivered strong performance in terms of selectivity, operational stability, and energy efficiency. Their design enables lower pressure drops and reduced fouling tendencies, offering a more robust and scalable solution for long-term industrial use. The fixed internal structure facilitates ease of integration, maintenance, and compliance with regulatory standards.

Scientifically, the study contributes a performance-based framework for selecting reactor designs based on the dominant transport or operational limitation. It provides quantitative benchmarks and qualitative insights to aid in reactor selection and process optimization. The findings also reinforce the importance of integrating performance metrics with techno-economic and safety evaluations for industrial decision-making.

Future work may include life cycle analysis, integration with renewable energy sources, and exploration of hybrid designs that combine the benefits of both systems. Overall, this work underscores the critical role of tailored reactor selection in advancing sustainable and efficient catalytic processes.

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