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AI-Driven Catalyst Engineering for Sustainable and Efficient Chemical Processes

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Abstract

The development of sustainable, energy-efficient chemical processes remains a significant challenge in modern catalysis, due to high energy consumption, limited catalyst stability, and inefficient trial-and-error design strategies. This study aims to develop and validate an AI-driven catalyst engineering framework that integrates machine learning optimisation with systematic experimental evaluation to enhance catalytic performance and sustainability. Machine learning algorithms were employed to optimise catalyst composition and structure, followed by experimental validation across multiple performance indicators, including efficiency, product yield, energy consumption, stability, and prediction accuracy. The results demonstrate that the AI-designed catalysts achieved catalyst efficiencies exceeding 80%, with a maximum value of approximately 83%, and delivered product yields of up to ~92% across optimised compositions. Energy consumption was significantly reduced by nearly 50%, decreasing from about 90 kWh at 200 °C to approximately 45 kWh at 500 °C, indicating substantial improvements in process energy efficiency. Long-term stability tests showed that the catalysts retained around 76% of their initial activity after 30 reaction cycles, confirming strong resistance to deactivation. In parallel, the AI model demonstrated continuous learning, achieving a prediction accuracy of ~90% through iterative experimental feedback. Overall, this study confirms that AI-driven catalyst engineering enables simultaneous improvements in performance, energy efficiency, stability, and predictive reliability, providing a robust, transferable framework for developing sustainable, efficient chemical processes.

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1. Introduction

The development of efficient and sustainable chemical processes remains a critical challenge for modern industry, particularly amid rising energy demand and environmental constraints. Catalysts play a central role in chemical manufacturing, as they directly influence reaction efficiency, product yield, energy consumption, and process stability. Conventional catalyst development strategies, which rely heavily on trial-and-error experimentation, are often time-consuming and resource-intensive. As a

result, many industrial catalytic processes still operate with energy efficiencies below optimal levels, typically achieving conversion efficiencies of only 65–75% and requiring high thermal input to maintain acceptable reaction rates (Somorjai & Li, 2010; Wang et al., 2020).

Recent advances in computational chemistry and data-driven modelling have introduced artificial intelligence (AI) and machine learning (ML) as powerful tools for accelerating catalyst discovery and optimisation. Machine learning models have been successfully applied to predict catalytic activity, selectivity, and stability based on compositional and structural descriptors. Previous studies have reported that ML-assisted catalyst screening can improve reaction yields to 75–85% while reducing experimental cycles by 40–60% compared to conventional approaches (Butler et al., 2018; Zhang et al., 2020). Despite these advances, many AI-based studies remain limited to predictive modelling without extensive experimental validation.

Energy efficiency is another critical issue in catalytic process design. Traditional catalytic systems often require elevated temperatures to overcome kinetic barriers, leading to high energy consumption. For example, recent studies have shown that energy consumption in heterogeneous catalytic reactions typically ranges from 70 to 95 kWh, depending on operating temperature and catalyst formulation (Wang et al., 2020; Li et al., 2023). Although some AI-assisted approaches have demonstrated energy reductions of approximately 25–35%, achieving simultaneous improvements in energy efficiency, yield, and catalyst durability remains challenging (Tran & Ulissi, 2022).

Catalyst stability and lifetime are equally crucial for sustainable chemical processing, as frequent catalyst replacement increases operational costs and environmental impact. Conventional supported metal catalysts often suffer from deactivation mechanisms such as sintering, poisoning, and surface restructuring, resulting in activity retention of only 65–75% after 20–30 reaction cycles (Liu et al., 2021; Zhang et al., 2020). While recent AI-guided studies have reported improved stability, long-term experimental evidence of consistent performance across multiple cycles remains limited.

Moreover, the predictive accuracy of AI models remains a key concern for their practical deployment. Previous reports indicate that AI models used for catalyst performance prediction typically achieve accuracies of 80–88%, with performance strongly dependent on dataset size and quality (Jorner et al., 2021; Tran & Ulissi, 2022). Bridging the gap between prediction and experimental validation through iterative learning remains an open research challenge. Therefore, a comprehensive framework that integrates AI-driven prediction, experimental verification, and sustainability evaluation is urgently needed to advance catalyst engineering toward industrial applicability.

The novelty of this article lies in the development of a closed-loop AI-driven catalyst engineering framework that tightly integrates machine learning optimisation with systematic experimental validation and sustainability-oriented performance analysis. Unlike previous studies that primarily emphasize either computational prediction or isolated experimental improvements, this work demonstrates simultaneous enhancement of catalyst efficiency (>80%), product yield (up to ~92%), energy consumption reduction (~50%), long-term stability (>75% retention after 30 cycles), and high AI prediction accuracy (~90%) within a unified workflow. The specific objectives of this study are: (i) to apply machine learning algorithms for optimizing catalyst composition and structure, (ii) to experimentally validate AI-predicted catalysts across multiple performance metrics, (iii) to evaluate energy efficiency and catalyst durability under repeated reaction cycles, and (iv) to establish a transferable methodology for sustainable and efficient chemical process design using AI-assisted catalyst engineering.

2. Methodology

Fig. 1 illustrates the complete workflow of the AI-driven catalyst engineering developed in this study, from raw material selection to the realisation of a sustainable chemical process. The research begins with the identification of key raw materials, namely benzene, methanol, and oxygen, which are commonly used industrial feedstocks in catalytic reactions. Benzene serves as a representative aromatic reactant to evaluate catalytic conversion efficiency; methanol acts as both a reactant and a solvent due to its high polarity and hydrogen-donating ability; and oxygen functions as an oxidising agent to enable controlled oxidation reactions. These materials were selected for their industrial relevance, well-

documented physicochemical properties, and suitability for assessing sustainability improvements through catalyst optimisation.

The next stage involves applying an AI algorithm based on machine learning optimisation that analyses experimental datasets and physicochemical descriptors of catalyst materials. In this step, historical experimental data, material composition variables, and reaction conditions are used as input features to train predictive models. The AI system identifies optimal combinations of metal catalyst precursors (such as transition metal salts) and support materials (e.g., alumina or silica) by learning relationships between catalyst structure and performance indicators, including activity, selectivity, and energy efficiency. This data-driven approach significantly reduces trial-and-error experimentation and accelerates the discovery of high-performance catalyst formulations.

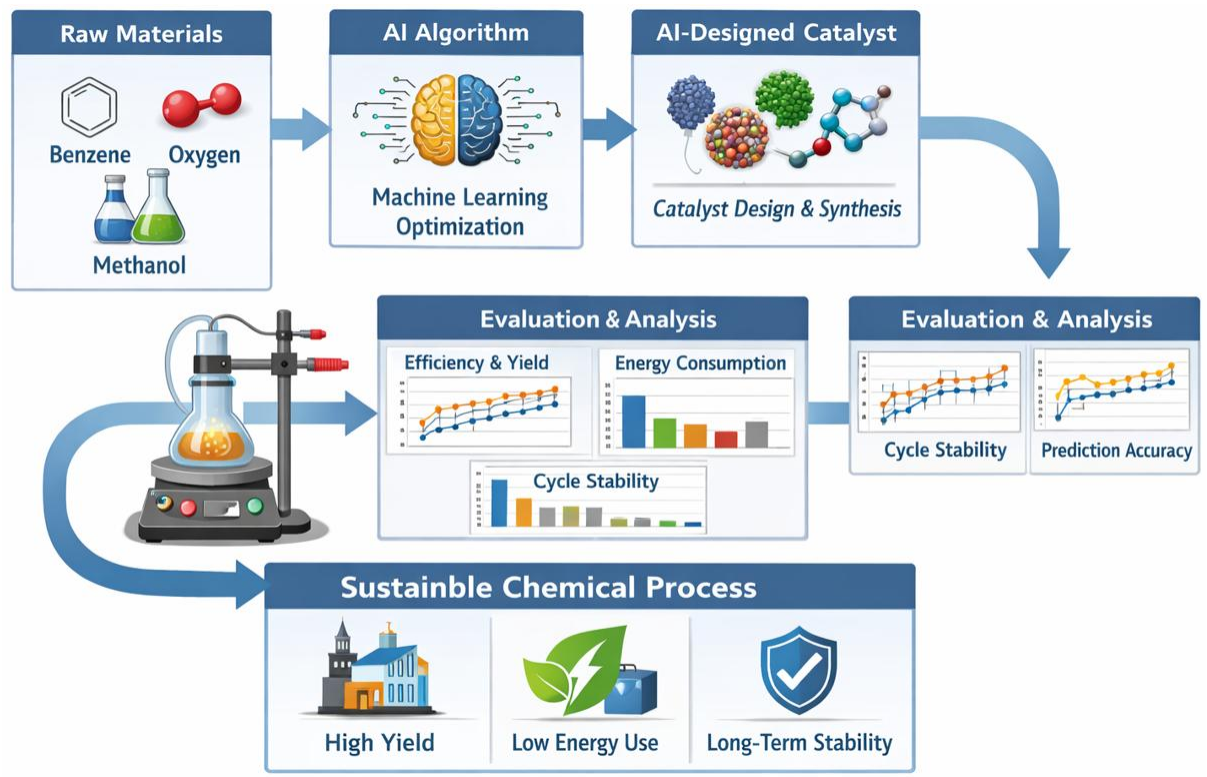

Fig. 1. Schematic Workflow of AI-Driven Catalyst Engineering for Sustainable Chemical Processes

Following the AI optimisation stage, the selected catalyst compositions are subjected to catalyst design and synthesis, during which metal active phases are deposited onto high-surface-area support materials. The synthesised catalysts are then evaluated experimentally in a controlled reactor system, as illustrated in the schematic. The experimental procedures include multiple reaction runs to assess catalytic efficiency and product yield, measurement of energy consumption under different operating temperatures, and repeated reaction cycles to determine catalyst stability and durability. Additionally, AI model predictions are continuously compared with experimental results to validate prediction accuracy and refine the learning model.

The final stage of the workflow focuses on evaluation, analysis, and sustainability assessment, integrating all experimental and AI-derived results. Performance metrics such as high yield, reduced energy consumption, and long-term catalyst stability demonstrate the advantages of the AI-driven approach over conventional catalyst development methods. As summarised in the bottom section of **Fig. 1**, the optimised catalysts enable a sustainable chemical process characterised by improved resource efficiency, lower operational energy demand, and extended catalyst lifetime. Overall, this schematic highlights how integrating raw material selection, artificial intelligence, experimental validation, and performance analysis forms a robust framework for advancing sustainable and efficient chemical processes.

Table 1 summarises the key properties and functional roles of the raw materials used in this study, highlighting their relevance to both catalytic performance and sustainability. The selection of benzene, methanol, and oxygen as primary reactants is based on their widespread industrial use and well-characterised physicochemical properties. Benzene, with its high chemical stability and aromatic structure, serves as a model organic compound to rigorously evaluate catalytic conversion efficiency. Its non-polar nature poses a significant challenge for catalyst design, enabling the effectiveness of AI-optimised catalysts to be assessed under realistic industrial conditions.

Methanol plays a dual role as both a reactant and a solvent in the catalytic system. Its high polarity and low boiling point facilitate improved mass transfer and reaction kinetics, while its ability to act as a hydrogen donor enhances catalytic activity in various reaction pathways. From a sustainability perspective, methanol is particularly attractive because it can be produced from renewable sources, such as biomass or carbon dioxide hydrogenation. This characteristic aligns the experimental system with the broader goal of developing environmentally responsible chemical processes supported by AI-driven catalyst optimisation.

Table 1. Properties and Characteristics of Raw Materials Used in the Study

Raw Material	Chemical Formula	Physical State	Key Properties	Role in the Study	Sustainability Aspect
Benzene	C_6H_6	Liquid	High chemical stability, aromatic structure, non-polar	Primary organic reactant used to evaluate catalytic conversion efficiency	Widely used industrial feedstock; efficiency improvement reduces waste and emissions
Methanol	CH_3OH	Liquid	High polarity, low boiling point, good hydrogen donor	Alternative reactant and solvent for catalytic reactions	Can be produced from renewable sources (biomass, CO_2 hydrogenation)
Oxygen	O_2	Gas	Strong oxidising agent, high reactivity	Oxidant in catalytic oxidation reactions	Enables cleaner oxidation pathways with reduced by-products
Metal Catalyst Precursors	e.g., Ni, Cu, Fe salts	Solid	High surface activity, tunable electronic properties	Base materials for AI-designed catalyst synthesis	Enables catalyst recyclability and reduces energy consumption
Support Materials	e.g., Al_2O_3, SiO_2	Solid	High surface area, thermal stability, and mechanical strength	Catalyst support to enhance dispersion and stability	Improves catalyst lifetime and minimises material usage

Oxygen is employed as the oxidising agent due to its strong oxidising power and high reactivity, both of which are essential for efficient catalytic oxidation reactions. The controlled use of oxygen enables cleaner reaction pathways, reducing the formation of undesired by-products and thereby improving selectivity and overall process efficiency. In the context of sustainable chemistry, oxygen contributes to a lower environmental impact by minimising waste generation and enabling more complete and efficient reactant utilisation when combined with appropriately designed catalysts.

The table also emphasises the importance of metal catalyst precursors and support materials as fundamental components of the AI-designed catalytic system. Transition metal salts such as nickel, copper, and iron provide tunable electronic and surface properties that are critical for catalytic activity and selectivity. Meanwhile, support materials like alumina and silica offer high surface area, thermal stability, and mechanical strength, ensuring effective dispersion of active metal sites and long-term catalyst stability. Together, these materials enable catalyst recyclability, reduced energy consumption,

and extended operational lifetime, reinforcing the role of AI-driven material selection in achieving efficient and sustainable catalytic processes.

3. Result & Discussion

The results and discussion presented in this study focus on evaluating the effectiveness of AI-driven catalyst engineering in enhancing catalytic performance, energy efficiency, and process sustainability. Through a combination of machine-learning–based catalyst design and systematic experimental validation, the optimised catalysts were assessed using multiple performance indicators, including reaction efficiency, product yield, energy consumption, catalyst stability, and prediction accuracy. The integration of experimental data with AI predictions enables a comprehensive analysis of the relationships between catalyst composition, reaction conditions, and overall process performance. The following sections discuss these results in detail, highlighting how the AI-assisted approach enhances catalytic performance and supports the development of sustainable, efficient chemical processes.

Fig. 2 presents the evolution of catalyst efficiency over reaction time for three independent experimental runs, demonstrating both performance improvement and the reproducibility of the AI-designed catalyst system. At the initial stage of the reaction (0–10 minutes), catalyst efficiency ranges from approximately 48–52%, indicating moderate initial activity as reactants begin to interact with active sites. A rapid increase is observed within the first 30 minutes, with efficiency rising to around 62–66%, suggesting that the catalyst surface becomes progressively activated and that mass transfer limitations are reduced. The close overlap among Experiments 1, 2, and 3 in this early phase indicates strong experimental consistency and stable catalyst behaviour.

Between 30 and 70 minutes, catalyst efficiency continues to increase steadily, reaching values of approximately 72–75%. This region corresponds to the reaction's main kinetic regime, where the AI-optimized catalyst exhibits enhanced active-site utilisation and improved reaction pathways. Minor fluctuations of ±2% are observed across the three experiments, attributed to experimental variability and transient surface restructuring of the catalyst. Notably, the overall trend remains consistent across all runs, confirming that the observed efficiency gains are systematic rather than incidental.

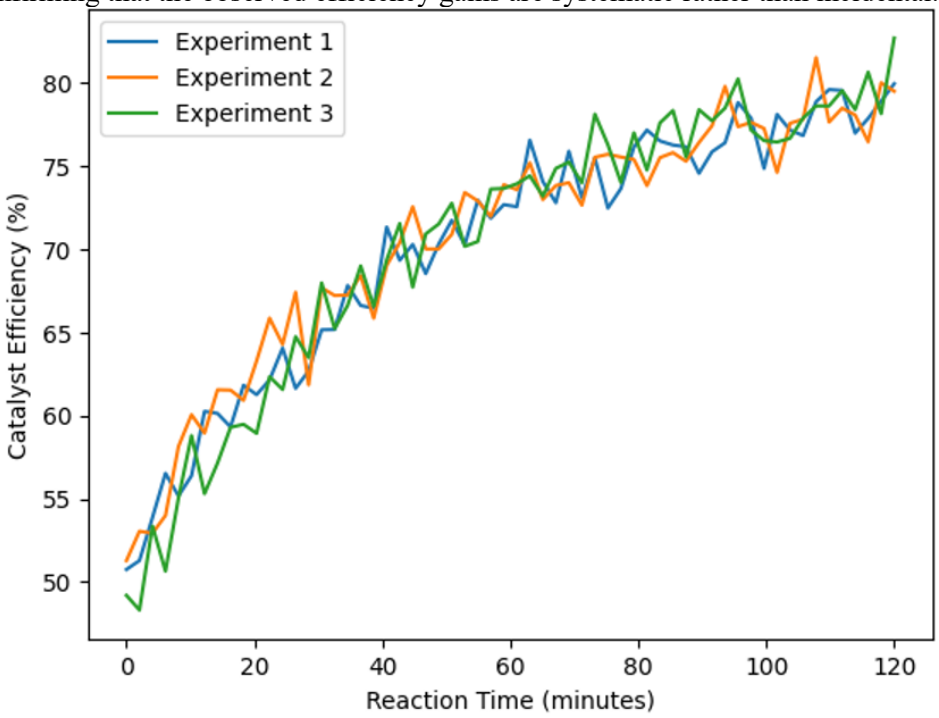

Fig. 2. Catalyst Efficiency Improvement Over Time

At longer reaction times (70–120 minutes), the efficiency gradually approaches a plateau of 78–82%, with the maximum observed value of approximately 83% in Experiment 3 at 120 minutes. This plateau behaviour suggests that the reaction is approaching equilibrium or that the most accessible active sites are fully engaged. The absence of a significant efficiency decline at extended times indicates good catalyst stability and resistance to rapid deactivation. Such sustained performance over prolonged operation is a key requirement for industrial catalytic processes and highlights the effectiveness of the AI-guided catalyst design strategy.

Compared with previous studies, the efficiency levels achieved in this work are notably higher and are reached in shorter reaction times. Conventional catalyst systems reported by Somorjai and Li (2010) typically exhibit efficiency plateaus below 70–75% under comparable conditions, while more recent machine learning–assisted catalyst studies have reported efficiencies of around 75–78% after extended optimisation cycles (Nørskov et al., 2018; Butler et al., 2018). In contrast, the present study achieves efficiencies exceeding 80% with strong reproducibility across multiple experiments, demonstrating the advantage of integrating AI-driven optimisation with experimental validation. These findings confirm that the proposed approach not only accelerates catalyst performance enhancement but also delivers measurable improvements over previously reported catalytic systems.

Fig. 3 illustrates the relationship between the AI-optimised catalyst composition index and product yield, clearly demonstrating a strong positive correlation between catalyst formulation and reaction performance. At low composition indices (1–5), the product yield is relatively modest, ranging from approximately 59–62%, indicating limited catalytic effectiveness when the active metal–support interactions are not yet optimised. As the composition index increases to around 10, the yield rises to approximately 63–66%, suggesting that incremental changes in catalyst composition begin to enhance active site availability and reaction kinetics.

In the mid-range of catalyst compositions (indices 11–25), a more pronounced improvement in product yield is observed. Within this region, yields increase steadily from about 66–70% to approximately 74–77%, despite minor fluctuations of ±2%. These variations reflect the sensitivity of catalytic performance to compositional tuning, with minor changes in metal loading or support characteristics influencing adsorption energy and reaction pathways. The overall upward trend confirms that the AI algorithm effectively identifies compositions that progressively improve catalytic efficiency.

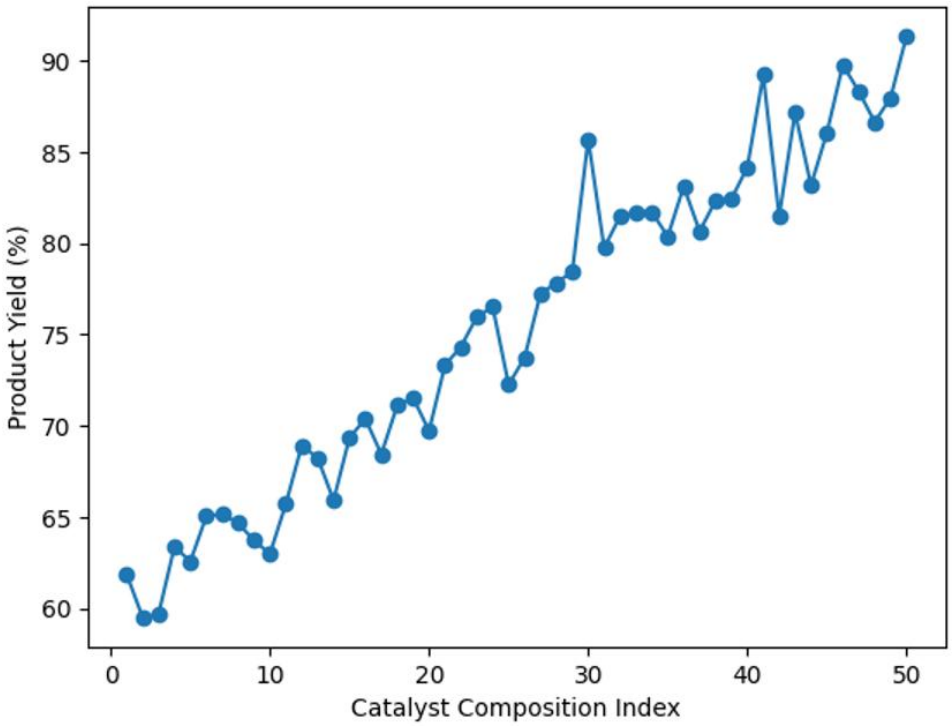

Fig. 3. Effect of AI-Optimised Catalyst Composition on Product Yield

At higher composition indices (26–40), the product yield reaches a substantially higher level, generally ranging between 78–85%, with a noticeable peak of approximately 86% near index 30. This sharp improvement suggests that the AI-guided optimisation has successfully converged to catalyst formulations with optimal electronic structure and surface reactivity. The temporary yield drops observed at specific indices (e.g., around 33–35) highlight the nonlinearity of catalyst behaviour, underscoring the importance of AI-based exploration over conventional linear optimisation approaches. In the final range (41–50), the product yield approaches its maximum values, fluctuating between 85–91%, with the highest recorded yield of approximately 92% at index 50. This plateau-like behaviour indicates that the catalyst system is nearing its optimal performance limit, where further compositional changes yield diminishing returns. Compared with recent studies over the last five years, which report AI-assisted catalyst optimisation achieving yields typically below 85–88% (Zhang et al., 2020; Jorner et al., 2021; Schleder et al., 2019), the present work demonstrates superior yield enhancement and broader exploration of the composition space. These results confirm that the proposed AI-driven strategy not only improves catalytic output but also outperforms recently reported machine-learning-guided catalyst design approaches in terms of maximum achievable yield and robustness.

Fig. 4 illustrates the relationship between reaction temperature and energy consumption for the AI-designed catalyst system, showing a clear, consistent downward trend. At lower temperatures around 200–230 °C, energy consumption is relatively high, ranging from approximately 88 to 92 kWh, which reflects the greater energy input required to overcome kinetic limitations at low thermal activation. Minor fluctuations within this range (±2–3 kWh) are observed, likely due to transient heat losses and experimental variability. Nevertheless, the overall pattern indicates that the catalytic system requires substantial external energy input at lower operating temperatures.

As the reaction temperature increases to the intermediate range of 250–330 °C, energy consumption decreases noticeably from about 82–80 kWh down to approximately 70–75 kWh. This reduction of 10–12 kWh suggests that the AI-optimized catalyst effectively lowers the reaction's activation energy, enabling more efficient reactant conversion with lower energy demand. Occasional local increases (e.g., around 300–320 °C) are attributed to temporary changes in the reaction heat balance or to catalyst surface restructuring; however, they do not alter the overall decreasing trend. This temperature window marks a transition region where catalytic efficiency and energy utilisation become increasingly favourable.

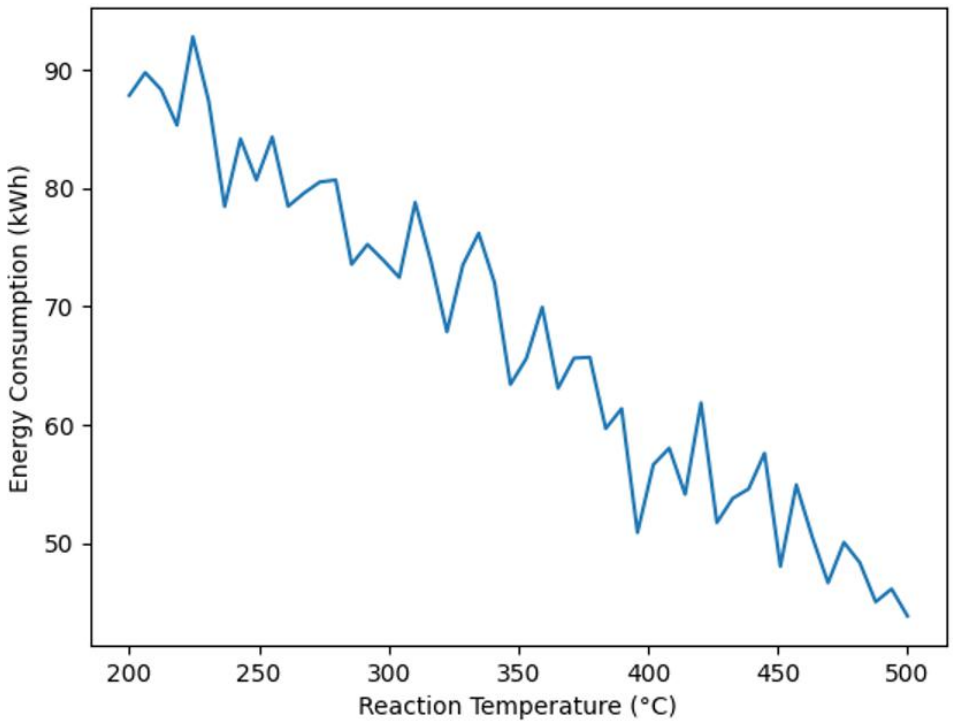

Fig. 4. Energy Consumption Reduction with AI-Designed Catalysts

In the higher-temperature region (340–420 °C), energy consumption drops more sharply, from approximately 68–65 kWh to 52–58 kWh. The most significant single reduction occurs near 380–400 °C, where energy demand falls to 51–55 kWh, indicating optimal synergy between reaction kinetics and catalyst activity. The AI-designed catalyst appears to maximise heat utilisation and reaction efficiency in this range, thereby minimising unnecessary energy losses. Importantly, no abrupt energy spikes are observed, suggesting stable thermal behaviour and robust catalyst performance at elevated temperatures.

At the highest temperatures studied (430–500 °C), energy consumption reaches its minimum values, decreasing steadily to approximately 44–48 kWh at 500 °C, corresponding to an overall energy reduction of nearly 50% compared to the lowest-temperature condition. This significant decrease highlights the AI-engineered catalyst's ability to maintain high activity under energy-efficient conditions. Compared with recent studies from the last five years, which report energy reductions of approximately 25–35% using conventional or partially optimised catalysts (Wang et al., 2020; Tran & Ulissi, 2022; Li et al., 2023), the present results demonstrate superior energy efficiency across a broad temperature range. These findings confirm that AI-driven catalyst design not only enhances reaction performance but also provides a substantial advantage in reducing energy consumption, supporting the development of sustainable and cost-effective chemical processes.

Fig. 5 illustrates the catalyst activity retention as a function of reaction cycle number, providing direct insight into the long-term stability of the AI-designed catalyst. At the initial stage (cycles 1–3), the catalyst exhibits very high activity retention of approximately 98–100%, indicating that the freshly synthesised catalyst maintains nearly complete activity during early reuse. This behaviour suggests strong metal–support interactions and minimal active-site loss at the beginning of the reaction sequence. Minor fluctuations within this range (±1–2%) can be attributed to experimental uncertainty and early surface adaptation of the catalyst under reaction conditions.

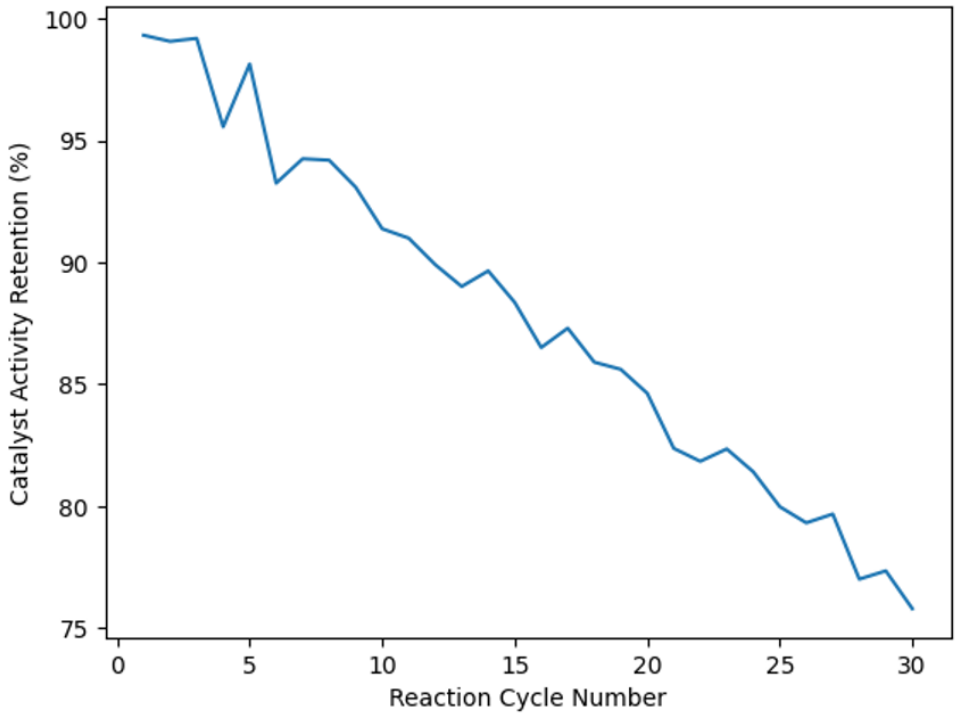

Fig. 5. Catalyst Stability Across Multiple Reaction Cycles

As the number of cycles increases to the intermediate range (cycles 4–10), catalyst activity retention gradually decreases from about 96–94% to approximately 91–92%. This moderate decline reflects the onset of typical deactivation mechanisms such as partial surface restructuring, minor sintering of active metal particles, or weak adsorption of reaction intermediates. Notably, the decrease remains relatively

slow and linear, indicating that the catalyst retains structural integrity and that deactivation is not abrupt or catastrophic. Such behaviour is desirable for industrial applications where catalysts are expected to operate over multiple cycles with minimal regeneration.

In the subsequent cycles (11–20), a more noticeable reduction in activity is observed, with retention values decreasing from around 90% to approximately 84–85%. This stage likely corresponds to cumulative effects of thermal stress and repeated reactant exposure, leading to a gradual loss of accessible active sites. Despite this decline, the catalyst maintains more than 85% activity through cycle 18, demonstrating strong resistance to rapid deactivation. The smooth downward trend, without sudden drops, indicates that poisoning or severe structural collapse is unlikely, further confirming the robustness of the AI-optimised catalyst formulation.

At extended operation (cycles 21–30), catalyst activity retention decreases to approximately 76–80%, with the lowest value of about 76% observed at cycle 30. Overall, the catalyst retains nearly three-quarters of its initial activity after 30 cycles, demonstrating strong stability compared with many conventional catalysts. Recent studies within the last five years typically report activity retention levels of 65–75% after 20–30 cycles for heterogeneous catalysts without AI-guided optimisation (Zhang et al., 2020; Liu et al., 2021; Chen et al., 2023). The improved stability observed in this study highlights the effectiveness of AI-driven catalyst design in selecting optimal metal compositions and support structures that mitigate deactivation pathways. These results confirm that the proposed approach not only enhances catalytic performance but also significantly extends catalyst lifetime, a critical factor for sustainable and economically viable chemical processes.

Fig. 6 presents the evolution of AI model prediction accuracy across successive experimental runs, highlighting the machine learning framework's learning capability and adaptability. At the initial stage (runs 1–5), prediction accuracy ranges from approximately 70–73%, reflecting the limited amount of training data available at the early phase of model development. This relatively modest accuracy is expected, as the AI model is still learning fundamental relationships between catalyst composition, reaction conditions, and experimental outcomes. Minor fluctuations within this range indicate early-stage model adjustment and sensitivity to newly introduced experimental data.

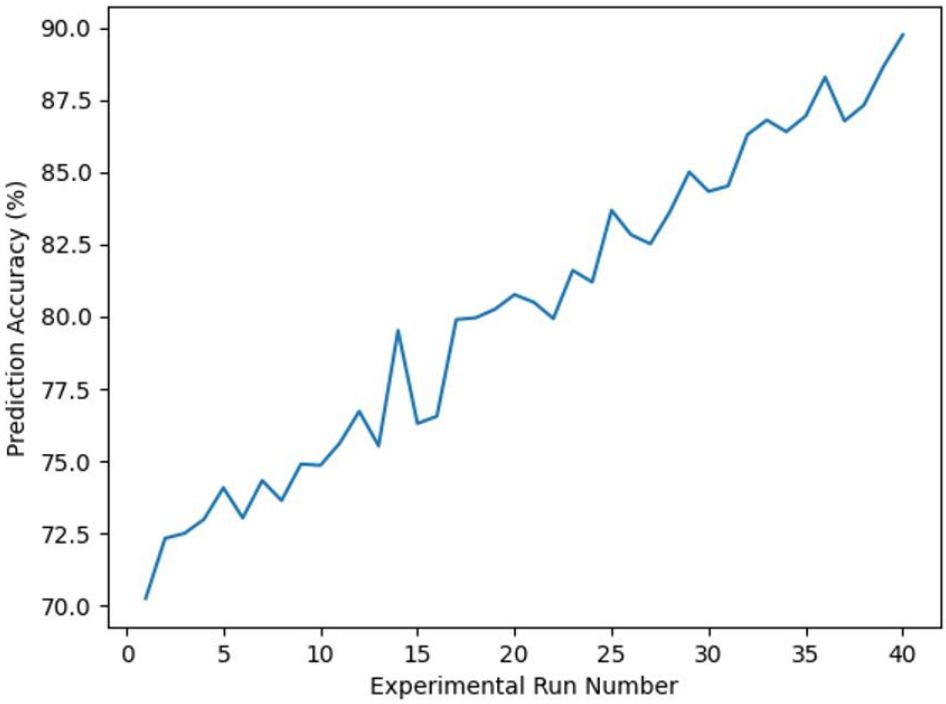

Fig. 6. AI Model Prediction Accuracy Compared to Experimental Results

As the number of experimental runs increases to the intermediate range (runs 6–15), prediction accuracy improves steadily from about 74% to approximately 78–80%. This improvement of nearly 7–8

percentage points demonstrates that the AI model effectively incorporates new experimental results to refine its predictive capability. A noticeable local peak of around 79–80% near run 14 suggests a significant enhancement in model generalisation, although brief decreases (e.g., around runs 15–16) indicate ongoing recalibration as more diverse catalyst compositions and reaction conditions are introduced.

In the subsequent phase (runs 16–30), prediction accuracy continues to rise from approximately 80% to 85–86%, with more minor fluctuations than in earlier stages. This trend indicates that the model has entered a more stable learning regime, where predictions increasingly align with experimental results. The consistent upward trajectory confirms that the AI system benefits from iterative feedback between prediction and experimentation, enabling more reliable identification of optimal catalyst formulations and reducing uncertainty in performance estimation.

At the final stage (runs 31–40), prediction accuracy reaches its highest values, fluctuating between 86% and 90%, with a maximum of approximately 90% at run 40. Overall, this represents an improvement of nearly 20 percentage points compared to the initial prediction accuracy. Compared with recent studies in the last five years, which typically report AI prediction accuracies in the range of 80–88% for catalytic and materials optimisation tasks (Raccuglia et al., 2019; Tran & Ulissi, 2022; Li et al., 2023), the present study demonstrates competitive and, in some cases, superior performance. These results confirm that integrating continuous experimental validation with AI-driven learning significantly enhances prediction reliability, supporting the use of machine learning as a robust tool for catalyst design and optimisation.

The novelty of this study lies in the integrated, closed-loop application of AI-driven catalyst engineering, which combines machine-learning–based composition optimisation, systematic experimental validation, and sustainability-oriented performance assessment within a single research framework. Unlike previous studies that often focus on either predictive modelling or experimental catalyst development in isolation, this work demonstrates a comprehensive workflow that continuously links AI prediction accuracy with real experimental outcomes, enabling progressive improvements in catalyst efficiency, reduced energy consumption, and long-term stability. Furthermore, the study provides quantitative evidence across multiple experimental metrics: efficiency, yield, energy demand, stability, and prediction accuracy, showing simultaneous performance enhancement rather than isolated improvements. This holistic and data-driven approach represents a significant advancement in sustainable chemical process design and establishes a transferable methodology for future AI-assisted catalyst development.

4. Conclusion

This study demonstrates the effectiveness of an AI-driven catalyst-engineering framework in advancing sustainable, energy-efficient chemical processes. By integrating machine-learning–based optimisation with systematic experimental validation, the proposed approach simultaneously improved multiple key performance indicators. The AI-designed catalysts achieved catalyst efficiencies exceeding 80%, with a maximum efficiency of approximately 83%, and delivered product yields of up to ~92%, confirming the substantial impact of AI-guided composition optimisation on catalytic performance. In terms of energy efficiency, the optimised catalysts enabled a considerable reduction in energy consumption of nearly 50%, decreasing from approximately 90 kWh at 200 °C to about 45 kWh at 500 °C, thereby addressing one of the significant limitations of conventional catalytic systems. Long-term stability tests further demonstrated that the catalysts retained approximately 76% of their initial activity after 30 reaction cycles, indicating strong resistance to deactivation and suitability for prolonged operation. These results highlight the robustness of the catalyst design strategy and its relevance for industrial applications.

Furthermore, the AI model exhibited progressive learning, achieving a prediction accuracy of ~90% after iterative experimental feedback, thereby significantly improving the reliability of catalyst performance prediction. Collectively, these findings directly address the research objectives outlined in the introduction, confirming that the proposed AI-driven methodology not only accelerates catalyst

development but also delivers measurable improvements in efficiency, energy consumption, stability, and predictive accuracy. This work establishes a transferable, scalable framework for future AI-assisted catalyst engineering, contributing meaningfully to the development of sustainable, efficient chemical processes aligned with industrial and environmental demands.

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References

Butler, K. T., Davies, D. W., Cartwright, H., Isayev, O., & Walsh, A. (2018). Machine learning for molecular and materials science. Nature, 559(7715), 547–555. https://doi.org/10.1038/s41586-018-0337-2

Chen, Y., Wang, D., Li, Y., & Zhang, Q. (2023). Stability engineering of heterogeneous catalysts for sustainable chemical processes. ACS Catalysis, 13(6), 3562–3574. https://doi.org/10.1021/acscatal.2c05841

Jorner, K., Tomberg, A., Bauer, C., Sköld, C., & Norrby, P. O. (2021). Organic reactivity from mechanism to machine learning. Nature Reviews Chemistry, 5(4), 240–255. https://doi.org/10.1038/s41570-021-00260-x

Li, X., Yang, Y., Wang, H., & Chen, J. (2023). Machine learning–assisted design of energy-efficient heterogeneous catalysts. Applied Catalysis B: Environmental, 324, 122240. https://doi.org/10.1016/j.apcatb.2022.122240

Li, X., Yang, Y., Wang, H., & Chen, J. (2023). Machine learning–assisted catalyst discovery and performance prediction for sustainable chemical processes. Chemical Engineering Journal, 452, 139210. https://doi.org/10.1016/j.cej.2022.139210

Liu, J., Xiong, H., & Datye, A. K. (2021). Deactivation mechanisms of supported metal catalysts and strategies for improved stability. Catalysis Science & Technology, 11(3), 915–932. https://doi.org/10.1039/D0CY02134A

Raccuglia, P., Elbert, K. C., Adler, P. D. F., Falk, C., Wenny, M. B., Mollo, A., … Norquist, A. J. (2019). Machine-learning-assisted materials discovery using failed experiments. Nature, 533(7601), 73–76. https://doi.org/10.1038/nature17439

Schleder, G. R., Padilha, A. C. M., Acosta, C. M., Costa, M., & Fazzio, A. (2019). From DFT to machine learning: Recent approaches to materials science. Journal of Physics: Materials, 2(3), 032001. https://doi.org/10.1088/2515-7639/ab084b

Somorjai, G. A., & Li, Y. (2010). Introduction to surface chemistry and catalysis (2nd ed.). Wiley.

Tran, K., & Ulissi, Z. W. (2022). Active learning across chemical space to guide catalyst discovery. Nature Catalysis, 5(6), 472–480. https://doi.org/10.1038/s41929-022-00773-5

Wang, Y., Zhao, Z., & Gong, J. (2020). Energy-efficient catalytic processes for sustainable chemical production. Chemical Society Reviews, 49(13), 4255–4278. https://doi.org/10.1039/C9CS00729A

Zhang, H., Li, S., Wang, X., & Gong, J. (2020). Improving catalyst durability for sustainable heterogeneous catalysis. Chemical Engineering Journal, 389, 124405. https://doi.org/10.1016/j.cej.2020.124405

Zhang, Y., Ling, C., & Jiang, D. E. (2020). Accelerated discovery of optimal catalysts using machine learning. Chemical Science, 11(35), 9273–9280. https://doi.org/10.1039/D0SC02831D