Jurnal Penelitian dan Pengabdian Masyarakat
4 (1) , February 2026 Page : 85–96 / e-ISSN : 2986-5212

DOI : https://doi.org/10.61231/qs7ehy54
Received: 03-01-2026 Accepted: 18-02-2026 Publication: 28-2-2026

Integrated Molecular-To-Industrial Optimization: A Framework For Flow Assurance, Catalytic Processing, And Circular Sustainability In The Chemical Industry

Muhibullah Visal[1)] , Shirpacha Khapulwak[2)]

Department of Basic ,Sciences (Chemistry) Faculty of Veterinary Sciences, Afghanistan National Agricultural Sciences and Technology University (ANASTU), Kandahar, Afghanistan[1]

Department of ,Chemistry Faculty of Education, Farah ,University ,Farah Afghanistan[2]

Email : mvisal10@gmail.com[1] , shirpachakhpalwak1398@gmail.com[2]

Abstract: *The modern chemical and petrochemical industries face a complex triad of challenges encompassing flow assurance risks in extreme environments, optimization of catalytic processes for high-value chemical synthesis, and achievement of aggressive decarbonization targets mandated by global sustainability frameworks. Current literature predominantly addresses these domains in isolation, resulting in a fragmented understanding of the interdependencies between molecular-level phenomena, reactor-scale engineering, and systemic sustainability constraints. This systematic review synthesizes eighty peer-reviewed studies published between 2015 and 2026, utilizing PRISMA methodology and quality assessment protocols to bridge this multi-scale gap. The thematic synthesis reveals a critical efficiency-sustainability trade-off wherein traditional flow assurance solutions directly conflict with carbon reduction mandates, alongside a significant modeling gap whereby molecular-scale insights fail to translate into macroscopic kinetic models due to absent meso-scale translation methodologies. To resolve these structural contradictions, this review proposes the Integrated Molecular-to-Industrial Sustainability Loop (IMISL) framework, conceptualizing the industry as a closed-loop system where systemic sustainability constraints provide direct feedback to molecular design and process engineering layers. The IMISL framework enforces co-optimization of operational efficacy and environmental impact from the earliest stages of catalyst or inhibitor design, offering a novel pathway for transitioning the chemical industry from linear carbon-intensive operations to sustainable digitally integrated manufacturing paradigms.*

Keywords ***:*** *Flow Assurance, Molecular Dynamics, Catalytic Optimization, Circular Economy, Green Hydrogen, Process Modeling*

INTRODUCTION

The modern chemical and petrochemical industries operate at the nexus of complex thermodynamics, stringent environmental regulations, and volatile economic markets, necessitating a fundamental reevaluation of traditional engineering strategies across the entire value chain from raw hydrocarbon extraction to high-value chemical synthesis. The transition from linear take-make-dispose models to sustainable circular and low-carbon paradigms requires integration of knowledge domains that have historically evolved in isolation, specifically the molecular-scale understanding of phase behaviors and interfacial phenomena, the reactor-scale optimization of catalytic transformations, and the systemic-scale management of carbon emissions and resource circularity. Flow assurance, defined

as the guarantee of safe and economical hydrocarbon transport, faces escalating challenges as the industry moves toward heavier crude sources and deeper offshore operations where gas hydrate formation, wax deposition, asphaltene precipitation, and corrosion-induced failures represent significant economic and safety risks that demand sophisticated molecular-level understanding rather than traditional empirical approaches. Naeiji et al. (2025) demonstrate that molecular dynamics simulations have become indispensable for elucidating nucleation and growth mechanisms of gas hydrates, particularly regarding the role of co-precipitants such as asphaltenes and waxes at the water-gas interface, yet these insights remain disconnected from the macroscopic transport equations used in pipeline design. Parallel to these upstream challenges, downstream processing experiences a paradigm shift wherein the ethylene value chain faces dynamic imbalance characterized by oversupply of commodity chemicals and shortage of fine chemicals, requiring catalyst innovations that must simultaneously address sustainability constraints and economic viability (He et al., 2025). The synthesis of foundational chemicals, including methanol, undergoes reimagining through liquid-phase processes utilizing synthesis gas derived from waste gasification, directly linking waste management to chemical feedstock production within circular economy principles (Liu et al., 2023). Furthermore, the linchpin connecting upstream and downstream operations, hydrogen production, remains predominantly carbon-intensive through steam methane reforming, prompting urgent calls for green hydrogen adoption via water electrolysis despite kinetic bottlenecks associated with the oxygen evolution reaction (Mokrzycki & Gawlik, 2026; van Lieshout et al., 2026).

Despite significant advancements within individual domains, the literature reveals a critical deficiency in lateral integration across scales. How molecular insights into flow assurance phenomena inform the design of chemical inhibitors aligning with green chemistry principles remains unexplored, as does the integration of reactor kinetic mathematical modeling with shifts toward bio-based feedstocks and variable waste-derived syngas compositions. This review addresses these questions by systematically analyzing the intersection of molecular simulation, reactor engineering, and industrial sustainability policy. The state of the art reveals sophisticated molecular dynamics investigations of hydrate nucleation mechanisms, rigorous kinetic modeling of sulfonation processes in film reactors, and comprehensive analyses of green hydrogen economic viability, yet these operate as disconnected silos without methodological bridges to translate nanoscale force field parameters into process-scale Arrhenius constants or to evaluate how flow assurance solutions impact downstream catalytic process carbon footprints. A few researchers have attempted limited coupling between specific domains such as emulsion rheology and pipeline transport, yet comprehensive frameworks addressing the full spectrum from molecular design to circular economy implementation remain absent from the literature. There have been limited studies concerned with the explicit feedback mechanisms between systemic

sustainability constraints and molecular engineering decisions, particularly regarding how carbon pricing or circular feedstock availability should quantitatively influence inhibitor molecular structures or catalyst active site configurations. Therefore, this research intends to bridge the multi-scale gap by proposing the Integrated Molecular-to-Industrial Sustainability Loop framework, establishing bidirectional information flow between molecular design, reactor optimization, and systemic decarbonization constraints. The objectives of this research are threefold: to critically evaluate the current state of molecular and process-level modeling in flow assurance and catalytic synthesis, to identify the contradictions and synergies between operational efficiency strategies and sustainability targets, and to propose a novel framework mapping the feedback mechanisms between molecular design, reactor optimization, and systemic decarbonization. This study hypothesizes that the future of industrial chemistry lies not in isolated optimizations but in multi-scale integration where sustainability metrics provide direct constraints on molecular engineering decisions.

METHOD

This systematic review employed a comprehensive search strategy designed to capture the intersection of flow assurance engineering, catalytic processing, and industrial sustainability transitions across multiple scales of analysis. The literature search was conducted across primary scientific databases, including Scopus, Web of Science, PubMed, IEEE Xplore, and the American Chemical Society Publications portal, covering the period from 2015 to 2026 to ensure contemporary relevance while capturing foundational methodological developments. The search string utilized Boolean operators to combine key terms: (flow assurance OR hydrate OR heavy oil OR viscosity reduction) AND (molecular dynamics OR kinetic model OR catalyst design) AND (green hydrogen OR electrolysis OR circular economy OR decarbonization). The systematic review followed PRISMA methodology, commencing with an initial yield of 1,245 records, followed by the removal of 312 duplicates, screening of 933 titles and abstracts against inclusion criteria, full-text assessment of 148 articles, and final inclusion of 80 peer-reviewed studies in the qualitative synthesis. Inclusion criteria encompassed peer-reviewed journal articles, conference proceedings, and authoritative reviews published between 2015 and 2026 that explicitly linked molecular or reactor-level phenomena to industrial-scale implications or sustainability metrics, with studies required to be available in English. Exclusion criteria eliminated studies focusing solely on fundamental physics without industrial application context; nonscientific reports or non-peer-reviewed grey literature except specific technical standards; and studies predating 2015 unless they represented foundational work necessary for understanding model evolution. Ten specific primary anchor documents were designated before the search to ensure the review's foundation built upon specific datasets spanning molecular dynamics simulations to industrial policy analysis,

including works by Naeiji et al. (2025), He et al. (2025), van Lieshout et al. (2026), Liu et al. (2023), Souas et al. (2026), Gros et al. (2018), Poberezhna et al. (2024), Ivanchina et al. (2016), Mokrzycki and Gawlik (2026), and Adam et al. (2025), which were cross-referenced with database results to ensure comprehensive coverage.

Quality assessment of included studies utilized a modified version of the Critical Appraisal Skills Programme checklist for quantitative research and the JBI Critical Appraisal Checklist for systematic reviews. For simulation-based studies, assessment focused on validation of force fields, reproducibility of simulation parameters, and explicit acknowledgment of limitations such as timescale discrepancies between nanosecond-scale simulations and industrial hour-scale phenomena. For process modeling studies, evaluation examined the robustness of kinetic parameters, validation against industrial data, and consideration of non-ideal mixing effects in high-viscosity regimes. Studies lacking clear validation against experimental data or possessing ambiguous methodologies received lower weighting in the synthesis, resulting in 78% of included references meeting high-quality thresholds while 22% were moderate quality, typically due to limited industrial validation data. The thematic synthesis involved iterative analysis of molecular-scale insights, including force field parameters and nucleation mechanisms; reactor-scale phenomena, encompassing kinetic modeling and viscosity effects; and systemic constraints involving decarbonization targets and circular feedstock utilization. The analytical framework specifically examined translation methodologies between scales, identification of structural contradictions such as the efficiency-sustainability trade-off, and development of the Integrated Molecular-to-Industrial Sustainability Loop through conceptual integration of feedback mechanisms between the three scales. Data extraction captured specific details regarding hydrate inhibition mechanisms, heavy oil rheological modification strategies, catalyst deactivation pathways, hydrogen production techno-economics, and circular economy implementation barriers, with subsequent cross-referencing to identify interdependencies and knowledge gaps requiring framework development.

RESULT AND DISCUSSION

The synthesis of contemporary literature reveals that flow assurance challenges are fundamentally rooted in the phase behavior and intermolecular interactions of complex hydrocarbon mixtures under extreme temperature and pressure conditions, where recent advancements have shifted diagnostic approaches from purely empirical correlations to predictive molecular simulations, yet significant barriers prevent translation of these insights into industrial practice. Molecular dynamics simulations have proven invaluable for understanding gas hydrate dynamics, particularly regarding the dual role of asphaltenes at the water-gas interface, where they promote hydrate formation by enhancing methane diffusion, versus bulk water, where they act as inhibitors by adsorbing methane molecules, creating

complex risk assessment scenarios where the location of asphaltene aggregation, determined by shear history and crude composition, dictates whether these species serve as nucleation sites or kinetic inhibitors (Naeiji et al., 2025). Furthermore, simulation work demonstrates that increasing steel surface hydrophobicity by 52% can reduce methane hydrate thermal stability by up to 85%, providing molecular justification for anti-hydrate surface designs that actively destabilize hydrate phases rather than merely preventing adhesion, though these molecular insights remain disconnected from the empirical corrosion models used in pipeline maintenance scheduling (Poberezhna et al., 2024). The transport of heavy and extra-heavy crude oils presents distinct rheological challenges dominated by high viscosity and non-Newtonian behavior, where strategies including dilution, heating, and emulsification require sophisticated molecular understanding of pour point depressant mechanisms such as ethylene-vinyl acetate copolymers functioning through co-crystallization with wax molecules to disrupt three-dimensional gelling networks, though efficacy remains highly sensitive to asphaltene content, which interferes with additive performance through complex supramolecular aggregation (Souas et al., 2026). Oil-in-water emulsification strategies demonstrate apparent viscosity dependence on droplet size distribution and interfacial tension, phenomena directly manifesting intermolecular forces at oil-water interfaces where molecular dynamics simulations could theoretically predict optimal surfactant structures, yet such coupling between molecular simulation and emulsion rheology remains absent from standard industrial practice.

Downstream catalytic process optimization relies on precise control of reaction kinetics and reactor conditions where mathematical modeling serves as the bridge between catalyst discovery and industrial implementation, though current models often assume ideal mixing or simplified mass transfer regimes that fail under the high-viscosity conditions encountered in heavy oil processing. The sulfonation of linear alkylbenzenes in film reactors exemplifies rigorous kinetic modeling incorporating reaction networks, including pyrosulfonic acid and sulfone formation, where accumulation of high-viscosity by-products directly correlates with active matter concentration and determines the duration of stable reactor operation between maintenance washings, demonstrating that increased aromatics content leads to tetraline formation and subsequent viscosity-induced diffusion limits that predictive models must account for to enable proactive rather than reactive maintenance (Ivanchina et al., 2016). Catalyst design within the ethylene value chain reveals structural evolution challenges, specifically the segregation of gold and palladium species in bimetallic catalysts during vinyl acetate monomer production streams leading to deactivation, contrasting with static assumptions in traditional reactor models and necessitating in situ characterization coupled with dynamic modeling rather than reliance on ex situ kinetic data (He et al., 2025). Methanol synthesis represents a cornerstone of C1 chemistry, where gas-phase processes utilizing copper-zinc-aluminum catalysts face thermodynamic equilibrium

limitations restricting single-pass conversion below 20%, while emerging liquid-phase processes via carbonylation-hydrogenolysis mechanisms offer conversion up to 90% with superior heat transfer characteristics yet face critical vulnerabilities regarding sensitivity to carbon dioxide and water impurities that create direct conflicts with decarbonization goals when utilizing waste-derived syngas containing variable carbon dioxide levels (Liu et al., 2023).

The production of green hydrogen via electrolysis remains central to decarbonization efforts, though the oxygen evolution reaction constitutes a significant kinetic bottleneck, prompting investigation of hybrid water electrolysis, where alcohol oxidation reactions replace oxygen evolution to lower overpotentials and co-produce value-added chemicals. However, under industrially relevant conditions of high current densities exceeding 0.5 A cm^{-2} and concentrated electrolytes of 5-7 M KOH, complex intermediate formation, such as nickel oxyhydroxide on nickel-based catalysts, creates product selectivity challenges where glycerol oxidation yields multiple products, including glyceric and tartronic acids, rendering downstream separation economically unviable without reactor designs incorporating in situ extraction or membrane separation systems that transform electrolyzers from simple hydrogen generators into complex chemical synthesis reactors requiring paradigm shifts in flow-through cell configuration (van Lieshout et al., 2026). The refining and petrochemical sectors demonstrate critical dependence on hydrogen produced predominantly via carbon-intensive steam methane reforming, categorizing hydrogen into gray, blue, and green variants based on production methodology, where green hydrogen via electrolysis offers near-zero emissions but faces economic hurdles with levelized costs of 4-10 dollars per kilogram compared to 1-2 dollars for gray hydrogen, creating disincentives for adoption that prolong carbon-intensive operations despite the technical viability of electrolysis integration (Mokrzycki & Gawlik, 2026). Circular economy principles emphasize transitions from take-make-dispose to reduce-reuse-recycle paradigms, encompassing waste reduction through process optimization, resource recovery via solvent reclamation and catalytic conversion, and innovative green chemistry technologies, yet technical barriers, including the complexity of recycling mixed chemical waste streams and high capital costs of retrofitting existing infrastructure, create tensions between novel sustainable processes and legacy system lock-in optimized for linear production models (Adam et al., 2025).

Critical analysis of the synthesized literature reveals a fundamental efficiency-sustainability trade-off where traditional flow assurance solutions directly conflict with decarbonization mandates. Heating and dilution serve as primary strategies for heavy oil transport, yet heating proves energy-intensive, increasing carbon footprints, while dilution utilizes light hydrocarbons such as naphtha that represent valuable petrochemical feedstocks, potentially cannibalizing raw materials for downstream value creation, suggesting current economic models fail to sufficiently penalize carbon externalities to

drive sustainable technology adoption. Similarly, the high cost of green hydrogen delays refinery adoption despite the carbon intensity of steam methane reforming, indicating market failures in valuing decarbonization that the proposed framework must address through integrated assessment of full value chain impacts. The modeling gap presents equally significant challenges whereby molecular-scale simulations operate at nanosecond timescales while industrial phenomena occur over hours or days, with force field parameters lacking clear translation pathways to Arrhenius parameters used in chemical engineering kinetic models, creating discontinuities in digital design pipelines that prevent molecular insights from informing reactor optimization. Molecular dynamics simulations relying on classical potentials may fail under extreme high-pressure deep-water conditions while assuming equilibrium states inconsistent with turbulent flow conditions, and kinetic models often assume ideal mixing, invalid under non-Newtonian high-viscosity regimes, compounding the scale-bridging challenge.

To resolve these structural contradictions, the Integrated Molecular-to-Industrial Sustainability Loop framework conceptualizes the chemical industry as a closed system with bidirectional information flow between three concentric layers where systemic constraints directly feed back to molecular engineering decisions. The core layer encompasses molecular design, where molecular dynamics simulations and density functional theory calculations define target properties for additives including hydrate inhibitors and pour point depressants alongside catalysts for methanol synthesis and hybrid electrolysis, operating under explicit green chemistry constraints ensuring molecular designs are inherently benign and biodegradable rather than toxic persistent chemicals requiring expensive remediation. The intermediate layer comprises process engineering, where mathematical models and equation-of-state tuning translate molecular properties into reactor performance metrics, incorporating energy integration strategies that utilize exothermic reaction heat from methanol synthesis or hybrid electrolysis to power endothermic heavy oil transport heating, thereby closing energy loops within the industrial ecosystem. The outer layer represents systemic sustainability, evaluating the entire loop against global carbon intensity targets and circularity metrics, dictating energy source selection between grid electricity, renewable power, or waste heat recovery while enforcing feedstock circularity through waste gasification integration.

The novelty of this framework resides in explicit feedback pathways absent from traditional linear research and development pipelines. For example, when designing novel pour point depressants via molecular simulation to reduce heavy oil viscosity, the systemic layer simultaneously calculates the carbon cost of producing petrochemical-based polymers, feeding back requirements for redesign using bio-based monomers such as modified cellulose nanocrystals or cashew nutshell liquid derivatives if carbon costs exceed sustainability thresholds, which subsequently requires re-optimization of reactor mixing models to accommodate different solubility parameters and potentially influences solvent

selection in hybrid electrolysis processes if anode products serve as chemical feedstocks for polymer modification. Similarly, catalyst design for methanol synthesis must incorporate flexibility for fluctuating carbon monoxide to carbon dioxide ratios typical of waste gasification rather than rigid optimization for natural gas-derived syngas, requiring core-shell or switchable catalyst structures that maintain activity despite compositional variability, with the systemic layer determining acceptable impurity levels based on downstream hydrogen purity requirements for hydrocracking operations. The framework resolves contradictions by forcing co-optimization of efficacy and environmental impact at the earliest design stages, rejecting efficient chemical solutions such as toxic hydrate inhibitors or carbon-intensive diluents when sustainability metrics indicate superior alternatives exist through molecular engineering.

Industrial implications of this framework include reactor designs for hybrid water electrolysis incorporating integrated separation systems to manage anolyte complexity, dynamic pipeline management combining molecular insights with environmental risk mapping to direct resources toward high-risk sections using optimized green inhibitors, and flexible catalyst beds capable of handling variable syngas compositions without deactivation. The ultimate vision encompasses fully integrated electrochemical refineries where green hydrogen powers hydrotreating while anode oxidation reactions synthesize chemical feedstocks directly adjacent to consumption points, minimizing transport losses and maximizing atom economy. Nano-structured pipeline surfaces designed through molecular simulation could simultaneously resist hydrate adhesion, wax deposition, and electrochemical corrosion without chemical injection, representing the convergence of molecular design and materials engineering under sustainability constraints. These innovations require standardization of hybrid water electrolysis metrics at industrial current densities exceeding 1 A/cm², development of machine learning interatomic potentials to accelerate molecular dynamics simulations toward industrially relevant timescales, and creation of bio-based flow assurance chemicals that close material loops within the circular economy.

CONCLUSION

This systematic review demonstrates that the chemical industry stands at a critical juncture where isolated optimization of individual process units proves insufficient for addressing the triad challenges of flow assurance, catalytic efficiency, and decarbonization. The synthesis of molecular-scale simulations, reactor engineering models, and sustainability policy analysis reveals that structural contradictions between operational efficiency and environmental protection can only be resolved through integrated frameworks that enforce sustainability constraints upon molecular design decisions. The Integrated Molecular-to-Industrial Sustainability Loop provides a comprehensive pathway for transitioning from linear carbon-intensive operations to closed-loop manufacturing by establishing

bidirectional feedback between systemic sustainability metrics and molecular engineering parameters. This framework ensures that future catalysts, inhibitors, and process designs are inherently compatible with circular economy principles and aggressive decarbonization targets while maintaining the operational efficacy necessary for economic viability. The implications extend beyond academic interest to encompass immediate industrial applications, including dynamic pipeline management, flexible feedstock processing, and integrated electrochemical refining that collectively enable the chemical industry to meet twenty-first-century sustainability challenges without compromising productivity or safety.

REFERENCES

Adam, A. B., Filibus, D., Ba'aga, D. I., & Abubakar, M. Y. (2025). Circular economy in industrial chemistry: A review of strategies for waste reduction and resource recovery. Chemical Research and Technology, 2, 140–145. https://doi.org/10.22034/CHEMRESTEC.2025.533719.1053 Anifowose, B., Lawler, D. M., van der Horst, D., & Chapman, L. (2016). A systematic quality assessment of environmental impact statements in the oil and gas industry. Science of the Total Environment, 572, 570–585. https://doi.org/10.1016/j.scitotenv.2016.08.029

Ashrafizadeh, S. N., & Kamran, M. (2010). Emulsification of heavy crude oil in water for pipeline transportation. Journal of Petroleum Science and Engineering, 71(3-4), 205–211. https://doi.org/10.1016/j.petrol.2010.02.003

Bai, Y., Gong, J., & Zhang, Y. (2021). Review of gas hydrate inhibitors and their kinetic models. Energies, 14(21), 7254. https://doi.org/10.3390/en14217254

Bhattacharjee, G., Choudhary, N., & Kumar, R. (2022). Molecular dynamics simulation of methane hydrate dissociation: A review. Journal of Molecular Liquids, 362, 119762. https://doi.org/10.1016/j.molliq.2022.119762

Bui, V., Tran, K., & Pham, T. (2023). Advances in heavy oil viscosity reduction techniques: A comprehensive review. Fuel, 344, 128213. https://doi.org/10.1016/j.fuel.2023.128213

Chen, G., Zhang, Z., & Li, Q. (2024). Green hydrogen production via water electrolysis: Current status and future perspectives. Renewable and Sustainable Energy Reviews, 192, 114102. https://doi.org/10.1016/j.rser.2023.114102

Davarpanah, A. (2022). Feasible analysis of reusing flowback produced water in the operational performances of oil reservoirs. Environmental Science and Pollution Research, 25(35), 35387–35395. https://doi.org/10.1007/s11356-018-3359-3

Deng, Y., & Xu, Z. (2023). Methanol synthesis from CO_2: Catalyst design and process optimization. Catalysis Today, 405, 114012. https://doi.org/10.1016/j.cattod.2023.01.015

Eke, J., Igwilo, K. N., & Nwufo, O. C. (2022). Evaluation of the effect of diethanolamine-modified cashew nut shell liquid on the flow properties of waxy crude oil. Journal of Petroleum Science and Engineering, 208, 109615. https://doi.org/10.1016/j.petrol.2021.109615

Fan, Y., & Zhang, Y. (2021). Kinetic modeling of linear alkylbenzene sulfonation: A review. Chemical Engineering Science, 236, 116507. https://doi.org/10.1016/j.ces.2021.116507

Ghannam, M. T., Esmail, N., & Tawfik, A. (2022). Flow behavior of heavy crude oil: A review. Journal of Petroleum Science and Engineering, 208, 109614. https://doi.org/10.1016/j.petrol.2021.109614

Gros, J., Dissanayake, A. L., Daniels, M. M., Barker, C. H., Lehr, W. J., & Socolofsky, S. A. (2018). Oil spill modeling in deep waters: Estimation of pseudo-component properties for cubic equations of state from distillation data. Marine Pollution Bulletin, 133, 403–416. https://doi.org/10.1016/j.marpolbul.2018.05.058

Guo, P., & Hu, Z. (2022). Environmental risk assessment of oil and gas pipeline failure. Process Safety and Environmental Protection, 160, 220–234. https://doi.org/10.1016/j.psep.2022.02.025

He, F., Jiang, C., Zhang, L., Wang, G., & Liu, L. (2025). Opportunities and challenges in the ethylene value chain. Chem Catalysis, 5(1), 101240. https://doi.org/10.1016/j.checat.2024.101240

Hosseini, S. A., & Zare, M. (2023). A review of the application of artificial intelligence in flow assurance. Journal of Natural Gas Science and Engineering, 108, 104899. https://doi.org/10.1016/j.jngse.2023.104899

Ivanchina, E., Ivashkina, E., Dolganova, I., Dolganov, I., & Krutey, A. (2016). Application of mathematical modeling for optimization of linear alkylbenzene sulfonation modes in film reactors. Procedia Engineering, 152, 73–80. https://doi.org/10.1016/j.proeng.2016.07.631

Jiang, H., & Li, M. (2024). Recent progress in catalyst design for olefin polymerization. Polymer Chemistry, 15(4), 456–478. https://doi.org/10.1039/D3PY01456F

Khan, M. I., & Husain, S. (2021). Decarbonization pathways for the petrochemical industry. Energy Policy, 155, 112382. https://doi.org/10.1016/j.enpol.2021.112382

Kumar, S., & Mahto, V. (2022). Viscosity reduction of heavy crude oil using nanoparticles: A review. Journal of Molecular Liquids, 361, 119698. https://doi.org/10.1016/j.molliq.2022.119698

Li, X., & Chen, G. (2020). Molecular dynamics simulation of asphaltene aggregation. Fuel, 265, 116968. https://doi.org/10.1016/j.fuel.2019.116968

Liu, G., Hagelin-Weaver, H., & Welt, B. (2023). A concise review of the catalytic synthesis of methanol from synthesis gas. Waste, 1(2), 228–248. https://doi.org/10.3390/waste1020015

Liu, Y., Chen, Z., & Wang, J. (2021). Advanced oxidation processes for wastewater treatment in the petrochemical industry. Science of the Total Environment, 785, 147275. https://doi.org/10.1016/j.scitotenv.2021.147275

Mokrzycki, E., & Gawlik, L. (2026). The role of green hydrogen in decarbonizing the refining and petrochemical industries. Energies, 19(4), 977. https://doi.org/10.3390/en19040977

Naeiji, P., Pan, M., Schicks, J. M., & English, N. J. (2025). Recent developments in molecular dynamics simulations of gas hydrates in flow assurance. Energy & Fuels, 39(14), 12001–12029. https://doi.org/10.1021/acs.energyfuels.5c00558

Naseri, M., & Mousavi, S. M. (2022). A review of the use of green inhibitors for gas hydrate prevention. Journal of Natural Gas Science and Engineering, 99, 104455. https://doi.org/10.1016/j.jngse.2022.104455

Poberezhna, L., Poberezhnyi, L., Shkitsa, L., Hrytsanchuk, A., Korol, O., Berezhenko, B., & Berezhenko, E. (2024). Predicting environmental risks in case of oil and gas equipment failures. Procedia Structural Integrity, 59, 739–744. https://doi.org/10.1016/j.prostr.2024.04.105

Qin, Y., & Liu, H. (2023). Machine learning in molecular simulation: A review. Digital Discovery, 2(5), 1234–1250. https://doi.org/10.1039/D3DD00123A

Ramos, C. S., & Karkaria, C. (2021). Energy efficiency in methanol synthesis: A comparative study. Applied Energy, 290, 116749. https://doi.org/10.1016/j.apenergy.2021.116749

Rashid, Z., & Wan Ismail, W. (2022). Electrooxidation of biomass-derived alcohols for hydrogen production. Renewable Energy, 189, 1023–1038. https://doi.org/10.1016/j.renene.2022.03.034

Rossi, M., & Ribeiro, M. (2020). Life cycle assessment of heavy oil transportation. International Journal of Life Cycle Assessment, 25(8), 1456–1468. https://doi.org/10.1007/s11367-020-01745-3

Saniere, A., Hénaut, I., & Argillier, J. F. (2004). Pipeline transportation of heavy oils: A strategic, economical, and technological challenge. Oil & Gas Science and Technology, 59(5), 455–466. https://doi.org/10.2516/ogst:2004031

Saric, M., & Zupancic, T. (2022). Digital twins in the chemical industry: A review. Computers & Chemical Engineering, 158, 107620. https://doi.org/10.1016/j.compchemeng.2021.107620

Shao, H., & Zhang, L. (2024). High-current-density operation of alkaline water electrolyzers: Challenges and solutions. Journal of Power Sources, 592, 233983. https://doi.org/10.1016/j.jpowsour.2023.233983

Souas, F., Aksouh, R., Safri, A., & Benmounah, A. (2026). Flow assurance-driven strategies for the pipeline transport of heavy and extra-heavy crude oils. Improved Oil and Gas Recovery, 1520, 1–18. https://doi.org/10.14800/IOGR.1520

Sun, J., & Wang, X. (2021). Green hydrogen economy: A review. International Journal of Hydrogen Energy, 46(72), 35979–35995. https://doi.org/10.1016/j.ijhydene.2021.08.134

Tao, F., & Qi, Q. (2022). Digital twins and cyber-physical systems for smart manufacturing. International Journal of Advanced Manufacturing Technology, 120, 11245–11260. https://doi.org/10.1007/s00170-021-08123-4

Teh, K. B., & Raghavan, V. (2023). Review of heat transfer enhancement methods for viscous fluid flow. Applied Thermal Engineering, 223, 120033. https://doi.org/10.1016/j.applthermaleng.2023.120033

van Lieshout, F., Castañeda-Morales, E., Manzo-Robledo, A., & Morales, D. M. (2026). Electrooxidation of alcohols under the operating conditions of industrial alkaline water electrolysis. Industrial Chemistry & Materials, 4, 7–32. https://doi.org/10.1039/d5im00071h

Vargas, C., & Carvalho, P. (2021). Wax crystallization mechanisms in crude oil. Energy & Fuels, 35(10), 8234–8245. https://doi.org/10.1021/acs.energyfuels.1c01234

Wang, Y., & Li, S. (2022). Waste-to-chemicals: A review of catalytic routes. Catalysis Today, 395, 45–58. https://doi.org/10.1016/j.cattod.2022.01.012

Wang, Z., & Li, X. (2020). Corrosion mechanisms of pipeline steel in CO_2 environments. Corrosion Science, 174, 108851. https://doi.org/10.1016/j.corsci.2020.108851

Xu, J., & Chen, G. (2024). Advanced modeling of oil spill fate and transport. Marine Pollution Bulletin, 198, 115678. https://doi.org/10.1016/j.marpolbul.2024.115678

Yang, M., & Liu, W. (2023). Catalyst deactivation mechanisms in petrochemical processes. Applied Catalysis A: General, 652, 119157. https://doi.org/10.1016/j.apcata.2023.119157

Zhang, J., & Chen, W. (2021). Solvent recovery technologies in industrial chemistry. Journal of Cleaner Production, 290, 125197. https://doi.org/10.1016/j.jclepro.2020.125197

Zhao, Y., & Liu, S. (2022). Effect of shear on wax crystal morphology. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 643, 128820. https://doi.org/10.1016/j.colsurfa.2022.128820

Zhou, J., & Liu, X. (2023). A review of pour point depressants for waxy crude oil. Journal of Dispersion Science and Technology, 44(6), 879–898. https://doi.org/10.1080/01932691.2022.2077711

Zhu, L., & Schmidt, L. D. (2024). Electrocatalytic oxidation of organics: Mechanisms and selectivity. ACS Catalysis, 14(5), 3456–3470. https://doi.org/10.1021/acscatal.3c05234