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Editorial

Advancements and future trends in chemical process optimization: Challenges, opportunities, and applications

The chemical process industries are undergoing a profound transformation. This transformation is driven not only by the pressures of global competition, but also by the urgent imperative to address climate change, accelerate the energy transition, manage scarce resources, embrace circular economy principles, and meet societal expectations for sustainable production. Within this complex landscape, process optimization has emerged as a central strategic enabler—capable of linking fundamental research with industrial innovation and real-world deployment.

Traditional methods of process design and operation, though effective in their time, are often insufficient for the multidimensional challenges of today. Modern solutions must go beyond efficiency and profitability, integrating sustainability metrics, lifecycle thinking, advanced control, and resilient supply chains. This requires harnessing the potential of digital transformation, leveraging advances in computational power, artificial intelligence, big data analytics, and hybrid optimization to address problems at scales ranging from a single unit operation to complex, interconnected global networks.

Process intensification has also gained prominence as a way to achieve step-change improvements in efficiency, safety, and environmental performance. By reimagining unit operations and system architectures, researchers are discovering ways to reduce energy consumption, minimize waste, and create cleaner, more adaptable production pathways. Simultaneously, data analytics, machine learning, and predictive modelling are enabling dynamic, self-adjusting processes that can operate optimally even under uncertainty.

This Special Issue, *"Advancements and Future Trends in Chemical Process Optimization: Challenges, Opportunities, and Applications"*, captures this evolving landscape. The contributions move progressively through the spectrum of process optimization—from the foundational challenge of sustainability and decarbonization, to the computational sophistication of hybrid optimization and control, the transformative potential of process intensification, the integration of optimization into product and supply chain design, and finally, the data-driven intelligence that is shaping the next generation of industrial decision-making.

The journey begins with sustainable processes and carbon capture, a domain where optimization directly supports global climate goals. In *"Biomass Fly-ash Derived Li_4SiO_4 Solid for Pilot-Scale CO_2 Capture, Part I: Modelling for a Waste-to-Capture CO_2 Process"*, waste-derived sorbents are evaluated for their potential in post-combustion CO_2 capture, turning industrial residues into valuable assets for emissions mitigation. Complementing this, *"Optimal Allocation of Carbon Capture Technologies in the Electric Industry under a Carbon Emissions Trading Program"* presents a rigorous optimization framework that integrates environmental objectives into market-based regulatory schemes, demonstrating how decarbonization can be reconciled with economic realities.

From here, the focus shifts to hybrid optimization, advanced simulation, and process control, where computational precision meets algorithmic adaptability. *"Integrating Metaheuristic Methods and Deterministic Strategies for Optimizing Supply Chain Equipment Design in Process Engineering"* merges deterministic rigor with the exploratory capabilities of metaheuristics, yielding more efficient designs. In *"Advanced Process Simulation and Control: Utilizing Directional Bat Algorithm for Improved Chemical Process Efficiency"*, a nature-inspired metaheuristic enhances process control, improving stability and adaptability. The review *"Control of Multi-unit Chemical Processes for Production Transitions"* then offers a broader perspective, mapping the landscape of control strategies and highlighting opportunities for more robust operational flexibility.

These computational advances set the stage for process intensification and unit operation design, where the objective is not merely to optimize existing systems but to reinvent them. *"Intensified Alternative for Sustainable Gamma-Valerolactone Production from Levulinic Acid"* outlines an energy-efficient route for a key biomass-derived chemical. *"New Hybrid Reactive-Extractive Distillation with Two Reactants for Separating Water-Free Ternary Azeotropic Mixtures"* integrates reaction and separation into a single intensified configuration, reducing complexity and energy demand. Similarly, *"Design and Optimization of Shell-and-Tube Heat Exchangers through ANN and H-ANN Models"* demonstrates how neural networks can rapidly design high-performance heat exchangers, accelerating innovation in thermal systems.

Once processes are intensified, the natural next step is to extend optimization principles to product engineering and supply chain optimization. *"Preliminary Computer-Aided Design of Powdered Soft Beverages Integrating Heuristic Knowledge"* shows how computational tools and expert insight can create products with precise functional attributes. In parallel, *"Optimizing the Supply Chain for 3D-Printed Medical Prostheses: Balancing Cost and Environmental Impact"* addresses a healthcare context, developing a logistics model that aligns affordability with environmental stewardship.

The final step in this journey leads to data analytics and energy demand forecasting, where the digital transformation of process industries is unlocking unprecedented capabilities for prediction and adaptation. *"Exploring Clustering Tools in Process Systems Engineering: Innovations, Applications, and Future Directions"* critically examines clustering methods, revealing their potential for process monitoring and fault detection. Finally, *"Prediction of Electricity Demand in Weakly Interconnected Power Systems Using an Ensemble Time Series Model with a Bayesian Optimization Approach"* integrates ensemble modelling with

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Bayesian optimization to produce more accurate forecasts in complex energy networks—a vital capability for balancing supply and demand in future energy systems.

Taken together, the works in this Special Issue form a coherent narrative of progress—beginning with sustainability imperatives, advancing through computational innovation, process reimagining, system-wide integration, and culminating in data-driven intelligence. They show that the future of chemical process optimization lies in convergence: convergence of sustainability goals, advanced algorithms, intensified designs, and digital technologies into holistic, interdisciplinary frameworks.

Importantly, these contributions remind us that optimization is no longer a purely technical exercise. The challenges are complex, interconnected, and often constrained by economic, environmental, and social factors. Addressing them effectively requires collaboration across disciplines, industries, and sectors, bridging the gap between technological capability and practical implementation.

Several forward-looking directions emerge from this collective body of work:

- Coupling optimization with lifecycle and circular economy frameworks to ensure that efficiency gains are aligned with long-term environmental objectives.
- Scaling up intensified processes to bridge the gap between laboratory innovation and industrial deployment.
- Expanding AI-driven process systems engineering with explainable and trustworthy algorithms suitable for safety-critical environments.
- Integrating process and supply chain optimization to improve resilience against global disruptions.

By building on the foundations presented here, the process systems engineering community is well-positioned to define the next generation of chemical process optimization. The path forward will require pushing the boundaries of existing methods, integrating real-time data analytics, predictive modelling, and hybrid optimization into seamless decision-making frameworks that span from molecular design to global supply chains. Optimization must increasingly operate as the unifying discipline that connects sustainability objectives, advanced process configurations, and economic performance, ensuring that improvements are not isolated gains but systemic transformations.

Ultimately, the challenge is to transition from optimizing individual operations to optimizing entire interconnected systems—systems that can adapt dynamically, self-correct under uncertainty, and deliver consistent performance across technical, environmental, and economic dimensions. The contributions in this Special Issue bring us closer to that vision, demonstrating that chemical process optimization is not only a powerful tool for improving current operations, but also the strategic foundation for designing the sustainable, efficient, and resilient industrial systems of the future.

The Guest Editors would like to express their sincere gratitude to Chemical Engineering Research and Design for providing the opportunity to curate this Special Issue, and to all the authors who contributed their work. The articles presented here reflect cutting-edge and innovative research, offering valuable insights into the current trajectory of chemical process optimization. Collectively, they not only capture the state-of-the-art in the field but also illuminate the emerging trends that will shape its future.

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