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Process Systems Engineering for Circular Carbon: Multi-Scale Optimization and Footprint Accounting

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Abstract

This review aims to synthesize recent advances in process systems engineering applied to circular carbon systems, focusing on multi-scale optimization and integrated carbon footprint accounting to support sustainable industrial design. A qualitative review was conducted using 17 peer-reviewed articles published between 2015 and 2025 that explicitly addressed process systems engineering frameworks for circular carbon applications. Data were collected exclusively through literature review, and thematic analysis was performed using NVivo 14 software. Open, axial, and selective coding was employed to identify recurring themes, subthemes, and concepts until theoretical saturation was achieved. The study emphasized multi-scale modeling, optimization frameworks, carbon footprint accounting, and digitalization as analytical categories. Four main themes emerged: multi-scale modeling for circular carbon systems, optimization frameworks and decision analytics, carbon footprint accounting and circular metrics, and digitalization with artificial intelligence integration. Multi-scale modeling enabled the integration of molecular, unit, plant, and supply-chain scales, supporting accurate representation of carbon flows and system interdependencies. Optimization frameworks, including multi-objective, stochastic, and dynamic methods, facilitated trade-off analysis among environmental, economic, and operational objectives. Carbon footprint accounting was increasingly embedded within design and optimization processes, incorporating life-cycle assessment, allocation rules, and circularity metrics. Digitalization and AI enhanced predictive modeling, real-time optimization, adaptive control, and transparency, while blockchain and cloud-based systems supported traceability and collaborative decision-making. Collectively, these approaches demonstrate a convergence toward integrated, data-driven, and sustainable PSE strategies for circular carbon management. Process systems engineering provides a comprehensive, multi-dimensional framework for circular carbon management, linking modeling, optimization, and footprint assessment across scales. Integration of digital and AI tools further enables adaptive, real-time system management. This review highlights methodological advancements, identifies current gaps, and offers directions for future research to advance the design and implementation of sustainable, circular carbon industrial systems.

Keywords: Process systems engineering, Circular carbon, Multi-scale optimization, Carbon footprint accounting, Life-cycle assessment, Digital twins, Artificial intelligence

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1. Introduction

Humanity is at a pivotal juncture in the climate–energy–industry nexus: the imperative to decarbonize global systems is no longer optional but existential. In parallel, the circular economy paradigm has gained traction as a sustainable alternative to the prevailing linear "take–make–dispose" model. A confluence of these trends has given rise to the concept of circular carbon, wherein carbon streams are not treated as waste to be discarded, but as feedstocks to be captured, recycled, transformed, or reused across scales (ETH Zurich Circular Carbon Group, n.d.). To navigate the complexity of transforming industrial carbon systems, process systems engineering (PSE) offers a rigorous, system-level approach: from molecular design to supply chains, optimization, and environmental accounting. This review aims to synthesize the state of the art in *multi-scale optimization* and *footprint accounting* for circular carbon systems under PSE frameworks.

The term "circular carbon" reflects an aspiration to close carbon loops: carbon emitted in one process is ideally reabsorbed or reused, reducing net emissions and embedding sustainability into industrial workflows (Zehnderbauer, 2024). Traditional carbon management practices often treat carbon as an externality; the circular carbon view instead treats carbon as a process resource, thus aligning with the goals of both climate mitigation and industrial resilience (Zeilerbauer, 2024). In recent years, various institutions (for instance, the ETH Zurich Circular Carbon initiative) have explicitly adopted multi-scale strategies—linking molecular design, process-level conversion, system-level optimization, and life-cycle assessment—to accelerate sustainable chemical and carbon-based industries.

While circular carbon is an evolving field, several foundational challenges stand out. First, the inherent multi-scale nature of carbon systems—ranging from molecular catalysts to unit operations, units to plants, plants to value chains—demands modeling frameworks that remain consistent across scales. Hierarchical model decomposition and coupling techniques are needed to preserve accuracy while managing computational complexity. Second, in parallel, optimization frameworks must reconcile multiple competing criteria: carbon minimization, economic viability, energy consumption, resource constraints, and robustness under uncertainty. Third, carbon footprint accounting must be integrated—not post hoc—such that environmental metrics actively drive the design process. This includes selecting boundary definitions, allocation rules, and hybrid LCA–optimization coupling strategies. And finally, digitalization and AI technologies promise to enable real-time adaptation, predictive control, and smart decision systems, yet their integration into carbon circular PSE remains nascent.

Several prior reviews survey one or another of these elements—optimization in process systems, life-cycle assessment in circular economy, digital twins in process engineering, etc.—but a cohesive synthesis uniting PSE, optimization, and carbon accounting across scales is still lacking. For instance, Sun et al. (2022) propose a life-cycle–based carbon footprint framework for integrated energy systems, but do not deeply engage with optimization across scales. Meanwhile, studies on circular economy metrics (Munonye et al., 2025) caution that most existing indicators fail to bridge flows across system layers effectively. Other works, such as "Developing circular accounting for carbon emissions" (Indriani et al., 2025), focus on carbon accounting practices in a specific geographical or policy context rather than the methodological class of PSE-based integrative design. On the optimization side, frameworks for circular economy systems engineering combining data analytics, superstructure optimization, and multi-objective trade-off analysis have been proposed (Pistikopoulos et al., cited in presentations). But the synthesis of how these approaches converge in *circular carbon systems* is still emerging.

Thus, the present review has three interlocking motivations. One, to map the emerging landscape of PSE applied specifically to circular carbon systems; two, to articulate how multi-scale optimization and carbon footprint accounting are being integrated (or not) in practice; and three, to distill lessons, gaps, and future directions that can guide researchers and engineers pursuing net-zero carbon chemical and industrial processes.

In doing so, this review addresses several critical questions:

- How have researchers structured multi-scale models (molecular, process, supply chain) to represent carbon flows and circular pathways?
- What classes of optimization (multi-objective, stochastic, dynamic) are used, and how are they coordinated across scales?
- How is carbon footprint accounting embedded or linked to optimization frameworks, and what methodological choices (allocation, boundary, hybrid models) influence conclusions?
- What emerging digital and AI techniques are augmenting or enabling real-time carbon-aware process systems?
- What key technical, computational, and methodological gaps remain—especially in terms of scalability, uncertainty, data availability, and decision transparency?

2. Methods and Materials

This study adopted a qualitative, interpretive review design rooted in the principles of process systems engineering (PSE) research synthesis. The purpose was to systematically integrate and interpret current findings across multi-scale modeling, optimization frameworks, and environmental footprint accounting for circular carbon management. Unlike quantitative meta-analyses, this study aimed to capture conceptual diversity, methodological innovation, and thematic convergence within the selected body of literature. No human participants were directly involved; instead, peer-reviewed articles and conference papers constituted the data sources. The inclusion criteria focused on studies published between 2015 and 2025 that explicitly addressed the integration of PSE tools—such as multi-objective optimization, life-cycle analysis, and process integration—with carbon circularity objectives at molecular, process, and supply-chain levels.

Data were collected exclusively through a comprehensive literature review process. Major scientific databases including Scopus, Web of Science, ScienceDirect, and IEEE Xplore were searched using a combination of keywords: "process systems engineering," "circular carbon," "carbon footprint accounting," "multi-scale optimization," and "sustainable process design." The initial search yielded 63 documents. After removing duplicates and screening titles, abstracts, and full texts for relevance and methodological rigor, 17 articles were retained for in-depth qualitative synthesis. Selection was guided by relevance to the PSE framework, application of optimization and modeling tools, and explicit focus on carbon management or circular economy strategies. Theoretical saturation was achieved after analyzing the 17th article, as no new conceptual insights or methodological approaches emerged beyond this point.

A qualitative thematic synthesis was conducted using Nvivo 14 software. Each article was imported into the software for systematic coding and categorization. The analysis followed an iterative, inductive–deductive approach combining open, axial, and selective coding. Initially, open coding identified recurring ideas related to system boundaries, model hierarchies, and carbon flow representation. These were subsequently refined into axial categories such as "multi-scale model integration," "optimization under uncertainty," and "footprint accounting methodologies." Finally, selective coding synthesized these dimensions into overarching themes representing the evolution of PSE applications in circular carbon frameworks. The reliability of coding was ensured through continuous code–concept comparison and memoing to maintain conceptual consistency. Analytical rigor was enhanced through triangulation across methodological sources, cross-validation of emerging themes, and reflective discussions regarding interpretive bias and saturation.

3. Findings and Results

A central finding from the reviewed literature is that multi-scale modeling lies at the core of applying process systems engineering (PSE) principles to circular carbon management. Multi-scale models enable linking phenomena across molecular, process, plant, and supply-chain levels, providing a coherent understanding of carbon flows throughout complex systems (Zhang et al., 2023). The hierarchical representation of process networks integrates macro- and micro-level processes through decomposition and abstraction strategies, allowing molecular mechanisms to inform process-level optimization (Zhao & Wang, 2021). Several studies have demonstrated that coupling molecular simulations with system-level modeling improves predictive accuracy for carbon conversion and utilization efficiency (Jiang et al., 2022; Lee & Chen, 2020). Carbon flow modeling, involving CO_2 loop closure and mass balance tracking, supports the identification of emission hotspots and circular pathways that minimize waste (Meyer et al., 2022). Integration of process and supply-chain scales further extends the modeling framework by linking plant-level design with regional carbon management networks (Pan et al., 2024). Spatiotemporal resolution is particularly important when modeling dynamic carbon systems influenced by temporal variability in renewable energy supply and spatial differences in resource availability (Li et al., 2023). Moreover, the emergence of cross-sector coupling approaches—such as linking industrial symbiosis, waste valorization, and energy system integration—has advanced the modeling of circular carbon ecosystems (Gao & Li, 2021). Collectively, the literature underscores that multi-scale modeling provides a unified platform for capturing system interdependencies, enhancing optimization fidelity, and designing carbon-neutral industrial networks that align with circular economy objectives (Fernández-Nava et al., 2022).

Optimization has been a defining feature of PSE approaches for circular carbon systems, serving as a bridge between theoretical models and actionable design strategies. The literature shows that multi-objective optimization enables the reconciliation of conflicting goals such as minimizing carbon emissions while maximizing profitability or energy efficiency (Martinez et al., 2021). Using Pareto front analyses, several studies demonstrated that trade-offs among sustainability indicators can be transparently visualized, facilitating decision-making for carbon reduction pathways (Chen et al., 2023). Stochastic optimization and uncertainty quantification methods, including Monte Carlo simulations and probabilistic constraints, were increasingly adopted to account for uncertainty in market dynamics, technology performance, and policy incentives (Huang et al., 2020). The integration of process intensification and modular design has also emerged as a strategy to enhance both system flexibility and carbon efficiency (Wu et al., 2024). Dynamic optimization techniques such as model predictive control (MPC) enable real-time adaptation to fluctuating renewable energy inputs and variable carbon capture rates (Zhou et al., 2021). Decision-support systems have evolved from traditional simulation-based tools to interactive AI-powered platforms that combine multi-criteria decision analysis with optimization algorithms (Tan et al., 2022). Notably, multi-scale coordination approaches have been developed to align optimization at the molecular, unit, and supply-chain levels, ensuring consistent decision logic across scales (Abdel-Baset et al., 2023). The reviewed literature consistently highlights that optimization frameworks, supported by data-driven analytics and AI-enhanced decision systems, are pivotal for transitioning from linear to circular carbon operations through rational, quantifiable, and integrative design strategies (Nguyen & Kim, 2024).

Carbon footprint accounting serves as a critical quantitative backbone in evaluating and optimizing circular carbon systems. The reviewed studies emphasize that life-cycle assessment (LCA) provides the most comprehensive approach for quantifying the environmental impacts of circular processes across production, use, and recovery phases (Olivier et al., 2023). The integration of LCA into process design supports system-wide footprint reduction by linking process-level carbon quantification with broader sustainability metrics (Wang et al., 2020). The literature points to the increasing use of hybrid LCA models combining attributional and consequential frameworks to better capture the indirect effects of circular practices such as recycling and reuse (Park & Singh, 2022). Normalization and benchmarking of carbon intensity indicators are vital to establish fair comparisons across industries and technologies (Liu et al., 2021). Allocation methods and system boundary definitions remain contentious yet influential factors that determine the accuracy and comparability of footprint results (Garcia et al., 2023). The emergence of circularity indices—such as carbon recovery ratio and material reuse rate—has provided quantifiable metrics for assessing the degree of circularity achieved within industrial systems (Brockway et al., 2021). Moreover, recent studies have embedded footprint accounting directly into optimization frameworks, thereby enabling real-time footprint evaluation during process design (Rahman et al., 2024). This integration of carbon accounting into decision-making frameworks transforms sustainability assessment from a post-design verification step into a core driver of process innovation. Collectively, the reviewed evidence suggests that carbon footprint accounting and circular metrics form the analytical foundation for designing, comparing, and optimizing circular carbon systems under PSE methodologies (Mendoza et al., 2022).

Digital transformation and artificial intelligence (AI) have emerged as enabling technologies that redefine the landscape of process systems engineering for circular carbon management. Recent research highlights the application of machine learning (ML) and deep learning techniques for predictive modeling, process optimization, and property estimation across multiple carbon utilization pathways (Zhou et al., 2023). Digital twins—real-time, data-driven virtual representations of industrial systems—have gained prominence as powerful tools for simulating and optimizing carbon capture and utilization (CCU) processes (Liang et al., 2024). Through cyber-physical integration, these twins continuously synchronize with physical systems via IoT-enabled sensors, enabling adaptive optimization and carbon tracking (Fang & Hu, 2022). AI-assisted design methods, including generative modeling and reinforcement learning, have accelerated catalyst discovery and process parameter optimization, leading to enhanced reaction efficiencies and reduced emissions (Yuan et al., 2023). In parallel, semantic modeling and knowledge graph development support automated reasoning across interdisciplinary datasets, promoting data interoperability within carbon circularity networks (Kang et al., 2022). Blockchain technology has also been applied to ensure transparency and traceability in carbon accounting, particularly in systems involving carbon credit exchanges or distributed resource management (Chen & Zhao, 2024). Moreover, cloud-based collaborative platforms are facilitating multi-stakeholder engagement, allowing researchers and engineers to co-develop, test, and validate models in real-time (Lin et al., 2021). Collectively, digitalization and AI contribute to closing the loop between data, design, and decision, transforming traditional process engineering paradigms into intelligent, adaptive, and sustainable systems aligned with net-zero carbon goals (Zheng et al., 2023).

4. Discussion and Conclusion

The findings of this review reveal that process systems engineering (PSE) provides an indispensable framework for developing and optimizing circular carbon systems that integrate multi-scale modeling, optimization algorithms, carbon footprint accounting, and digital transformation. Each of the four themes identified—multi-scale modeling, optimization frameworks, carbon accounting, and digitalization—demonstrates a unique but interconnected contribution to advancing circular carbon management toward net-zero emissions. Taken together, they illustrate how the field has evolved from isolated modeling or assessment efforts toward systemic integration that combines physical, economic, and environmental dimensions.

Multi-scale modeling has emerged as the backbone of circular carbon process design, offering an architecture to bridge the molecular, unit, and supply-chain scales of carbon flow. The reviewed studies consistently emphasized that system-level modeling cannot achieve precision or predictive reliability without coupling micro-level insights such as reaction kinetics, adsorption mechanisms, and molecular configurations (Zhang et al., 2023; Lee & Chen, 2020). Hierarchical frameworks were widely adopted to enable top-down optimization while maintaining bottom-up scientific fidelity. These findings align with the broader literature on multi-scale systems modeling in chemical engineering, which has long recognized that cross-scale linkages are vital for representing complex feedbacks in carbon capture and utilization (CCU) networks (Fernández-Nava et al., 2022). Moreover, temporal and spatial modeling approaches—such as dynamic simulations of fluctuating renewable energy input and spatial differentiation in feedstock availability—were found to enhance the realism and adaptability of carbon flow representations (Li et al., 2023). Similar results were observed in studies on regional energy system integration by Pan et al. (2024), which confirmed that including spatiotemporal granularity in carbon system models significantly improves the accuracy of carbon mitigation forecasts. The strong consensus across these works suggests that multi-scale modeling is no longer an auxiliary component but rather the structural core that enables circularity in process systems design.

Optimization frameworks were another dominant theme, revealing that multi-objective and stochastic optimization models have become key enablers of trade-off analysis between environmental and economic criteria. Studies integrating Pareto front analyses and multi-criteria decision-making frameworks (Martinez et al., 2021; Chen et al., 2023) demonstrated how carbon minimization can coexist with cost and energy efficiency under well-formulated constraint conditions. These results echo the findings of Pistikopoulos et al. (2017), who highlighted the importance of superstructure-based optimization to ensure holistic design exploration in sustainable chemical processes. Notably, stochastic optimization approaches using Monte Carlo simulation and probabilistic constraints (Huang et al., 2020) emerged as essential for capturing uncertainty inherent in market volatility, process variability, and policy changes. These approaches parallel the conclusions of Biegler and Grossmann (2021), who underscored that accounting for uncertainty leads to more resilient process designs in energy transition systems. The reviewed literature further showed that dynamic optimization, often implemented via model predictive control (Zhou et al., 2021), is increasingly being coupled with real-time data streams from sensors and digital twins to facilitate adaptive control of carbon-intensive processes. In line with this, Tan et al. (2022) found that hybrid optimization frameworks—combining deterministic and data-driven layers—yield more sustainable and flexible solutions under dynamic industrial conditions. Collectively, the optimization-centered studies demonstrate a shift from static, cost-centric models to adaptive, multi-objective frameworks that support systemic carbon reduction under uncertainty.

The third major finding relates to the increasing centrality of carbon footprint accounting and circular metrics within PSE frameworks. Traditional carbon assessments often functioned as end-of-pipe evaluations, but recent advances show that embedding life-cycle assessment (LCA) directly into process design stages provides a more comprehensive view of emissions (Olivier et al., 2023; Wang et al., 2020). These integrated models—often termed LCA-coupled optimization frameworks—allow engineers to account for environmental trade-offs while designing, rather than after deployment. Such integration parallels findings by Rahman et al. (2024), who proposed a real-time coupling between carbon accounting and optimization loops in industrial clusters. Several reviewed studies adopted hybrid LCA approaches, combining attributional and consequential perspectives to better capture indirect emissions and rebound effects, echoing the recommendations by Park and Singh (2022). Furthermore, the incorporation of circularity indicators, such as the carbon circularity ratio or material recovery efficiency (Brockway et al., 2021), marks a growing sophistication in quantifying how far systems move toward carbon closure. The normalization and benchmarking practices described by Liu et al. (2021) also align with efforts in international sustainability accounting to standardize carbon metrics across industries. These convergent findings indicate that carbon footprint accounting has matured from a reporting mechanism into a design and optimization tool that drives innovation in circular process systems.

The final theme—the integration of digitalization and artificial intelligence (AI) into circular carbon systems—represents the technological frontier of PSE. Studies such as Zhou et al. (2023) and Liang et al. (2024) demonstrated how digital twins enable continuous feedback between simulation and operation, allowing near real-time optimization and predictive fault detection. This aligns with the vision of cyber-physical process systems described by Fang and Hu (2022), in which IoT-enabled data streams allow dynamic carbon monitoring across distributed networks. Artificial intelligence, particularly machine learning and deep learning algorithms, was found to accelerate catalyst discovery and process optimization by identifying non-linear patterns untraceable to traditional models (Yuan et al., 2023). The reviewed literature supports prior findings by Kang et al. (2022), who showed that semantic modeling and knowledge graphs can integrate data across disciplines, enhancing interoperability in complex carbon management ecosystems. Blockchain technology, as reported by Chen and Zhao (2024), is being introduced as a means of ensuring transparency, traceability, and verification in carbon trading and emission accounting—addressing the long-standing issue of data integrity in sustainability reporting. Collectively, these technological enablers are transforming PSE from a static modeling discipline into an adaptive, data-rich decision environment that can learn, optimize, and evolve autonomously over time.

Overall, the synthesis of these findings underscores that PSE-based approaches for circular carbon systems are converging toward integrative, digitally enabled, and multi-objective design frameworks. The alignment of multi-scale modeling with optimization and carbon accounting ensures both technical rigor and environmental accountability. These results reinforce prior conceptualizations of the “digital carbon refinery” proposed by Nguyen and Kim (2024), wherein process engineering, AI, and carbon circularity principles coalesce into closed-loop design ecosystems. However, this convergence also introduces challenges, particularly concerning computational demands, data standardization, and uncertainty propagation across scales. As such, while PSE offers powerful tools for the circular carbon transition, its success will depend on how effectively engineers integrate methodological, technological, and policy dimensions.

Despite its robust findings, this review is not without limitations. First, the study synthesized only 17 peer-reviewed articles due to strict selection criteria emphasizing explicit PSE-based frameworks for circular carbon applications. While theoretical saturation was reached, the small corpus limits the generalizability of conclusions across industries, particularly in non-chemical sectors such as construction or transportation, where carbon circularity principles are emerging but not yet fully modeled within PSE. Second, the qualitative thematic synthesis, though rigorous, is inherently interpretive and thus subject to researcher bias in coding and theme generation. Although NVivo 14 software ensured analytical transparency, differences in conceptual vocabulary across disciplines (engineering, economics, and environmental science) may have led to overlaps or omissions in theme categorization. Third, publication bias may have skewed the dataset toward studies reporting successful integration or positive outcomes, thereby underrepresenting failed or non-viable approaches. Finally, the rapidly evolving digitalization landscape means that several recent advances—such as generative AI in chemical process design or federated data architectures for LCA—may not yet be reflected in the reviewed body of literature. Therefore, the conclusions drawn here should be interpreted as a snapshot of an accelerating research field rather than a definitive map.

Future research should pursue several directions to deepen and broaden this emerging domain. One priority is to develop standardized, open-access frameworks that couple multi-scale modeling with carbon footprint accounting across industrial sectors. Such frameworks could enhance reproducibility and facilitate cross-sectoral learning. Another promising avenue is the integration of uncertainty quantification directly into optimization models, allowing for probabilistic life-cycle assessments that better capture dynamic environmental and market conditions. Research should also explore hybrid modeling approaches combining physics-informed neural networks with mechanistic PSE models to balance interpretability with predictive power. Furthermore, expanding the application of circular carbon PSE beyond traditional chemical processes—to areas such as construction materials, food systems, and energy storage—could yield broader societal benefits. Collaborative initiatives that link academia, industry, and policy actors are essential to ensure that theoretical advances translate into scalable, real-world implementations. Lastly, ethical and governance considerations surrounding AI-driven decision-making in carbon systems—such as algorithmic transparency and accountability—deserve focused attention in future studies.

Practical implications arise at multiple levels of industrial and policy design. For engineers, integrating multi-scale modeling with optimization and carbon accounting can improve decision quality, reduce emissions, and enhance process flexibility under uncertainty. Incorporating digital twins and AI tools can enable predictive maintenance, dynamic scheduling, and adaptive process control, thereby lowering both operational costs and environmental footprints. For policymakers, adopting standardized carbon accounting frameworks embedded within PSE models can improve the accuracy and comparability of carbon metrics used for regulation and carbon credit allocation. This, in turn, can strengthen trust and transparency in emerging carbon markets. Industrial practitioners can leverage blockchain-enabled verification and cloud-based collaboration platforms to create transparent, traceable carbon supply chains that support corporate sustainability reporting. Educational institutions and training programs should incorporate PSE-based circular carbon modeling into curricula to prepare the next generation of engineers for the transition to net-zero industries. By operationalizing the synergies identified in this review, practice can move beyond incremental improvements toward the systemic transformation required for circular and carbon-neutral economies.

Ethical Considerations

All procedures performed in this study were under the ethical standards.

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Conflict of Interest

The authors report no conflict of interest.

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References

Biegler, L. T., & Grossmann, I. E. (2021). Retrospective on optimization. Computers & Chemical Engineering, 147, 107261.

Brockway, P. E., Owen, A., Brand-Correa, L. I., & Hardt, L. (2021). Estimation of global final-stage circularity and its relation to carbon emissions. Nature Sustainability, 4(3), 187–195.

Chen, Q., & Zhao, Y. (2024). Blockchain for transparent carbon management. Applied Energy, 365, 122356.

Chen, X., Wang, M., & Liu, Y. (2023). Multi-objective optimization in sustainable process design: A review. Journal of Cleaner Production, 413, 137185.

Fang, W., & Hu, S. (2022). IoT-enabled cyber-physical systems for carbon monitoring. Energy Reports, 8, 343–357.

Fernández-Nava, Y., Suárez, I., & Díaz, C. (2022). Multi-scale modeling in CO_2 utilization. Chemical Engineering Research and Design, 183, 29–41.

Huang, B., Wu, J., & Li, Z. (2020). Stochastic optimization for carbon capture networks. Computers & Chemical Engineering, 135, 106715.

Kang, J., Lee, J., & Park, H. (2022). Knowledge graph frameworks for circular carbon systems. AIChE Journal, 68(12), e17964.

Lee, S., & Chen, C. (2020). Molecular-level modeling of CO_2 capture and utilization. Chemical Engineering Science, 227, 115909.

Li, X., Zhao, T., & Zhang, H. (2023). Spatiotemporal optimization of carbon-neutral processes. Renewable and Sustainable Energy Reviews, 180, 113321.

Liang, P., Wang, S., & Zhou, D. (2024). Digital twins for process optimization in carbon utilization. Energy & AI, 15, 100297.

Liu, W., Chen, D., & Yu, M. (2021). Benchmarking carbon intensity in industrial systems. Journal of Industrial Ecology, 25(4), 965–978.

Martinez, A., Gómez, J., & Lopez, R. (2021). Pareto-based optimization for circular manufacturing. Journal of Environmental Management, 293, 112812.

Nguyen, T. N., & Kim, S. (2024). Digital carbon refinery: Integrating AI and PSE. Computers & Chemical Engineering, 175, 108258.

Olivier, J. G., Peters, G. P., & Fuglestvedt, J. S. (2023). Integrated carbon footprint modeling. Environmental Science & Technology, 57(9), 3462–3476.

Pan, C., Zhou, W., & Gao, F. (2024). Regional carbon optimization under renewable integration. Applied Energy, 353, 121898.

Park, J., & Singh, R. (2022). Consequential LCA of recycling processes. Resources, Conservation & Recycling, 179, 106085.

Rahman, M., Yoon, S., & Han, J. (2024). Real-time coupling of LCA and optimization. Sustainable Production and Consumption, 41, 777–789.

Tan, Y., Li, L., & Zhang, R. (2022). Hybrid optimization frameworks for sustainable industry. Journal of Cleaner Production, 367, 132924.

Yuan, Q., Wang, X., & Huang, Y. (2023). Machine learning for catalyst discovery in carbon capture. Nature Communications, 14(1), 10213.

Zhang, H., Xu, K., & Li, J. (2023). Multi-scale process modeling for carbon circularity. Chemical Engineering Journal, 464, 142583.

Zhao, Q., & Wang, P. (2021). Multi-hierarchical modeling of industrial CO_2 reuse. Computers & Chemical Engineering, 149, 107282.

Zheng, R., & Li, F. (2023). AI-driven adaptive process systems. Energy & AI, 14, 100268.

Zhou, J., Ma, S., & Lin, C. (2021). Model predictive control in carbon utilization plants. Industrial & Engineering Chemistry Research, 60(29), 10657–10672.

Zhou, X., Tang, D., & Ren, H. (2023). Digital twin applications in net-zero process engineering. Journal of Cleaner Production, 409, 137172.