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Modeling Strategies for Decarbonization in the Chemical Industry: Pathways Toward Carbon Neutrality

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Abstract

The chemical industry is actively pursuing decarbonization through a range of emerging technologies and strategic approaches in response to escalating environmental regulations and increasing societal demand for sustainability. Understanding the environmental, economic, and emissions-related implications of these efforts is essential to shaping a more sustainable industrial future. Key areas of focus include carbon capture, utilization, and storage (CCUS), biomass-based feedstocks, electrification, circular economy practices, and renewable energy integration such as wind and solar. These measures aim to lower the sector's substantial carbon footprint and support global sustainability goals. Chemical companies are increasingly integrating advanced technologies, optimizing processes, and transitioning to sustainable raw materials. Advanced systems analysis models—such as process analysis, material flow analysis, life cycle assessment, techno-economic analysis, and machine learning—play a crucial role in evaluating and optimizing these decarbonization pathways. These models are applied across various analytical scales (micro, meso, and macro) to assess both current performance and future potential. Incorporating forward-looking, data-driven methodologies enables more informed decision-making and enhances the resilience of complex industrial systems. Although modeling frameworks rooted in industrial ecology, economics, and planetary boundaries have improved systems-level assessments, further efforts are needed to address ecosystem impacts comprehensively.

Keywords: Carbon Neutrality, Renewable Energy Integration, Process Optimization, Decarbonization, Circular Economy