Accelerating net-zero future *via* fluid dynamics and chemical kinetics

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The transition toward net-zero emissions requires a fundamental transformation of chemically reacting flow systems across energy generation, transportation, and industrial sectors. Conventional fossil-fuel combustion has supported global industrialization for more than a century. However, its associated greenhouse gas emissions, pollutant formation, and resources depletion have intensified the urgency for sustainable alternatives. This roadmap presents an integrated perspective on the role of fluid dynamics, combustion chemistry, advanced diagnostics, and intelligent modeling in enabling the low-carbon energy transition. Particular emphasis is placed on hydrogen, ammonia and sustainable aviation fuels as emerging energy carriers capable of supporting deep decarbonization pathways. It further discusses how high-fidelity simulations, laser diagnostics, and machine learning are revolutionizing the knowledge and control of reactive flow under realistic operational circumstances. In contrast to these, scalable industrial decarbonization solutions like carbon capture, chemical looping combustion, and oxygen-carrier technologies are also discussed for the reduction of emissions from hard-to-abate sectors. A comprehensive path connecting basic kinetics, multiscale transport phenomena, digital intelligence and industrial implementation from 2025 to 2050 was proposed. The net-zero future will not only depend on alternate clean fuels, but also on developments in turbulence-chemistry interaction, reaction mechanism development, reactor design, and integrated system optimization. The study presented is consistent with the net-zero objective and indicates key research priorities essential to achieve dependable, economically viable, and ecologically sustainable reacting-flow systems.

INTRODUCTION

Global energy systems are undergoing a rapid transition driven *via* climate mitigation targets, increasing energy demand, and international commitments toward carbon neutrality. Fossil fuels continue to dominate worldwide energy consumption due to their high energy density, established infrastructure, and economic accessibility. Nevertheless, combustion of coal, oil, and natural gas remains the primary contributor to anthropogenic carbon dioxide emissions, particulate matter, sulfur oxides, and nitrogen oxides, resulting in environmental and health consequences. Decarbonization is not just a matter of replacing fuels. The modern energy systems are intricate interactions of chemical kinetics, turbulence, heat transfer, fluid dynamics and multiphase transport.[1] Chemical reaction fluxes are therefore at the heart of the global net-zero transition. Future low-carbon technologies should concurrently achieve combustion stability, high thermal efficiency, fuel flexibility and ultra-low pollutant emission. The so-called energy trilemma is one of the big obstacles in the energy transition. The energy trilemma is the balance between energy security, energy justice and environmental sustainability. Many industrial sectors, including aviation, shipping, heavy transportation, and high temperature manufacturing, remain strongly dependent on combustion-based systems despite the tremendous growth in renewable power production. Carbon-free and low-carbon fuels such as hydrogen, ammonia and sustainable aviation fuels are emerging as key avenues to profound decarbonization.

Recent breakthroughs in computational fluid dynamics, laser diagnostics, artificial intelligence and kinetic modeling are providing unparalleled comprehension of responding flows under actual operation settings. At the same time, industrial carbon mitigation solutions, such as chemical looping combustion and carbon capture technologies, are maturing for large-scale application.[2] This roadmap outlines a comprehensive framework that connects fundamental reacting-flow physics with practical low-carbon energy applications. The debate blends breakthroughs in alternative fuels, sophisticated diagnostics, intelligent modeling and industrial decarbonization techniques while highlighting future research paths essential to expedite global net-zero ambitions.

ZERO-CARBON FUEL FRONTIERS

Research frontiers in zero-carbon fuels include the development and implementation of carbon-free energy carriers for broad-based decarbonization of the power production, transportation and industrial sectors. Various frontiers were Hydrogen, ammonia, synthetic electrofuels and improved bio-derived fuels. Research is being carried out on clean production methods, combustion characteristics, storage and transportation concerns, emission reduction, and integration with renewable energy systems to produce sustainable and ultra-low emission energy conversion. Hydrogen combustion is one of the most promising approaches for carbon-neutral energy conversion, with the release of water vapor generated without direct carbon emissions.[3] Hydrogen may be produced *via* renewable-powered electrolysis, thermochemical cycles of biomass conversion and photocatalytic water splitting. Among them, photocatalytic hydrogen generation has gained increased attention, due to its capabilities of concomitantly converting solar energy and purifying wastewater streams. Notwithstanding the environmental benefits of hydrogen combustion, significant problems are related with its physicochemical features. Hydrogen has very fast laminar flame speeds, very wide flammability limits, low ignition and great diffusivity. These properties greatly raise the dangers of flashback, thermoacoustic instabilities and uncontrolled heat release in actual combustion systems. Future hydrogen-based turbines, engines, and rocket propulsion systems require enhanced flame stabilization tactics, adaptive fuel injection systems and precise chemical kinetic mechanisms that describe turbulence-chemistry interactions at increased pressures and temperatures. Moreover, significant research efforts are necessary to enhance materials durability in hydrogen-rich combustion conditions, notably in high-temperature gas turbines and rocket propulsion systems. To mitigate flashback risks, advanced technologies such as micro-mix burners and porous media combustion are being developed. Micro-mix burners utilize very small-scale mixing to prevent flame propagation into the nozzle, while porous media provide high thermal inertia and flame stabilization through internal heat recirculation. Furthermore, lean-premixed combustion and exhaust gas recirculation (EGR) are progressively utilized to lower flame temperatures, mitigate thermal NOx production, and improve combustion stability in hydrogen-rich environments.

Ammonia has become an appealing carbon-free energy carrier since its existing infrastructure worldwide for storage and delivery, as well as its high volumetric energy density.[4] Compared to hydrogen, ammonia may be liquefied at relatively mild circumstances, making it excellent for long-distance energy transfer and seasonal storage purposes. Ammonia combustion, however, has several obstacles, such as limited reactivity, narrow flammability limits, and high ignition temperature. In addition, burning of ammonia can result in significant nitrogen oxide emissions, as nitrogen atoms are intrinsic in the fuel structure. Recent research has shown that ammonia mixed with hydrocarbon fuels or hydrogen can increase flame stability and combustion intensity while emitting less carbon. Experimental and computational studies of ammonia-doped methane, ethane, and propane flames show dramatic changes in flame structure, distribution of heat release, radical chemistry and routes for NO production. The results demonstrate the use of ammonia as a fuel but also as a combustion modifier capable of influencing reacting-flow

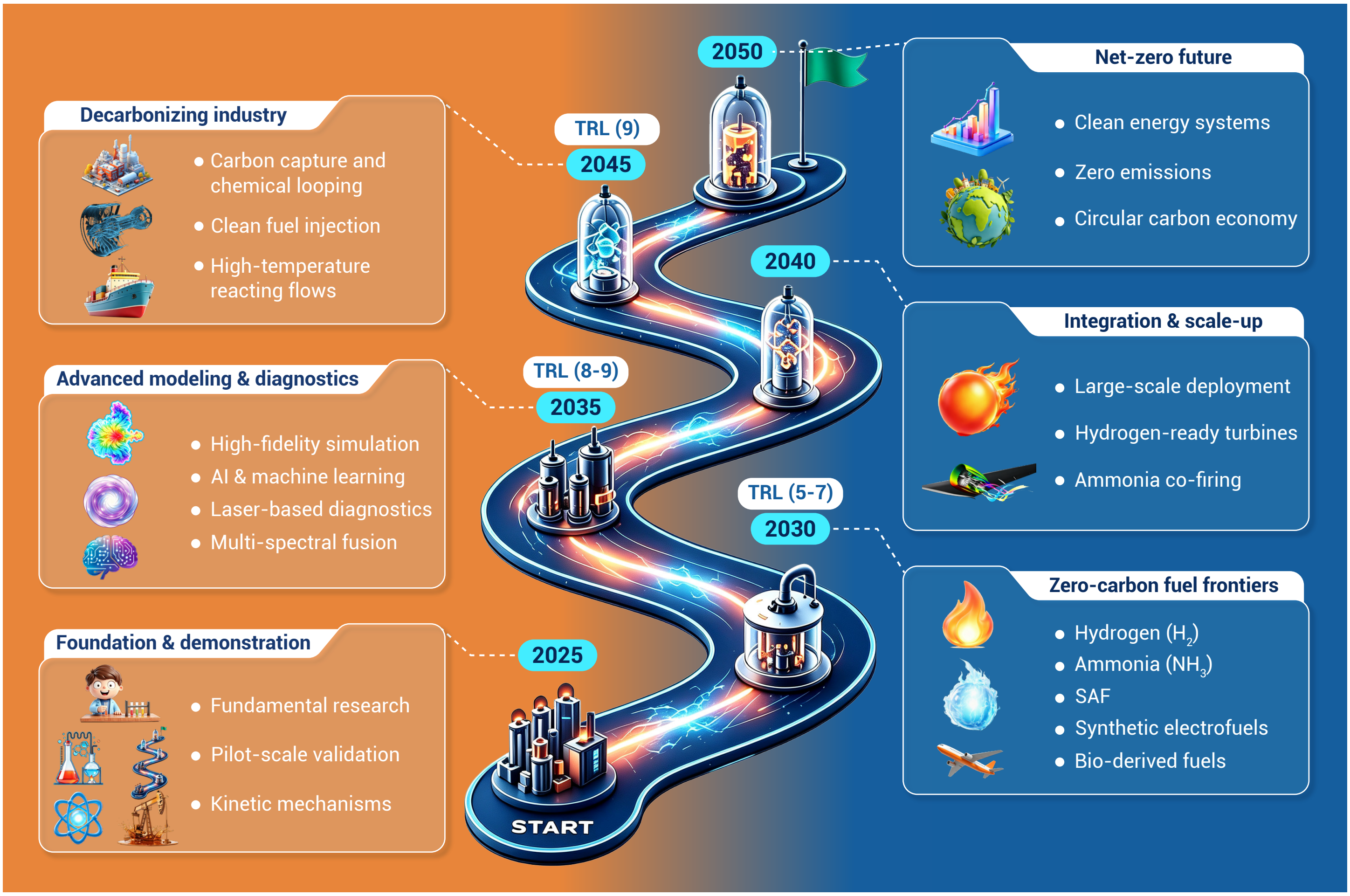

Figure 1. Roadmap to accelerate net-zero emissions with fluid dynamics, chemical kinetics, and intelligent reacting-flow technologies, 2025–2050 The transition from fundamental research and pilot validation to advanced modelling, zero carbon fuel deployment, industrial decarbonization and large-scale integration of hydrogen, ammonia, sustainable aviation fuels, synthetic electrofuels, bio-derived fuels, artificial intelligence and carbon capture technologies is mapped out in the roadmap. In tandem, these phases demonstrate the development of low-carbon reacting-flow systems towards an integrated net-zero future with clean energy systems, zero emissions, and a circular carbon economy. Representative technology milestones include (Technology Readiness Levels) 2025–2030 (TRL 5–7; pilot demonstrations and fuel blending <20%), 2030–2040 (TRL 8–9; commercial deployment with fuel-dependent sustainable fuel utilization of approximately 50–80% and PINN-enabled predictive combustion control), and 2040–2050 (TRL 9; large-scale integrated net-zero energy systems, widespread deployment of carbon-neutral fuels, autonomous AI-driven optimization, and application-specific thermal efficiencies exceeding 45%).

dynamics. Cutting-edge strategies like stratified combustion and catalytic combustion are emerging to address these challenges. Stratified combustion allows for optimized reactivity and NOx control by creating localized equivalence ratio gradients, while catalytic combustion enhances low-temperature stability and reduces the ignition temperature of ammonia-rich mixtures. Emerging approaches including catalytic ammonia cracking and plasma-assisted combustion are also being explored to improve flame stability while minimizing NOx emissions. Future research directions include the development of low-NOx combustion techniques, pressure-dependent kinetic processes, and predictive multiphase models for ammonia cracking and co-firing systems.

The deployment of zero-carbon fuels is also governed by economic factors. Green hydrogen production costs are projected to decline to \$1.5–2.0/kg by 2030, driven by policy subsidies such as the US Inflation Reduction Act and the EU Hydrogen Bank. Furthermore, carbon tax thresholds of \$50–100/tCO_2 are expected to be the tipping point for the wide-scale adoption of ammonia and hydrogen in industrial sectors. Together, declining fuel costs and supportive policy instruments are expected to accelerate technology progression from pilot demonstrations (TRL 5–7) toward commercial deployment (TRL 8–9). The utilization of ammonia in industrial furnaces, marine engines and gas turbines will depend greatly on progress in turbulence-resolved models and real-time combustion diagnostics.

The aviation sector represents one of the most difficult industries to decarbonize because of stringent energy-density requirements and long infrastructure lifetime. Sustainable aviation fuels (SAFs) therefore serve as a critical transitional solution for reducing greenhouse gas emissions over their lifecycle while maintaining compatibility with existing aircraft engines and fueling systems. SAFs can be produced *via* multiple conversion pathways including alcohol-to-jet, gas-to-jet, oil-to-jet, and sugar-to-jet technologies.[5] Depending on the availability of regional resources, sustainable fuel production may employ biomass-derived feedstocks, waste oils, agricultural wastes and syngas streams. SAF combustion does generate carbon dioxide while it's operating, but lifetime emissions can be cut by up to 80% because the carbon comes from sustainable biomass sources. However, the scalability of SAF production is still limited by feedstock supply, catalyst deactivation, process costs, and fuel certification requirements. Future advancement in sustainable aircraft will involve the combination of chemical kinetics with supply-chain optimization, carbon lifecycle analysis, and sophisticated reactor engineering. Research also must address trends for soot generation, aromatic-content requirements, and fuel atomization characteristics under aviation-relevant operating circumstances.

ADVANCED MODELING AND DIAGNOSTICS

High-fidelity computational approaches are becoming critical tools to study reacting flows in low carbon combustion systems. Direct numerical simulation (DNS) without turbulence modeling assumptions allows extensive research of turbulence-chemistry interactions, giving information about flame structure, radical transport and ignition dynamics. On the other hand, large eddy simulation (LES) provides a feasible predictive capacity for industrial scale systems by resolving huge turbulent structures and simulating subgridscale processes. LES is progressively being applied to gas turbines, hydrogen combustors, ammonia burners, chemical looping reactors. Modern reacting-flow modeling combines accurate chemical kinetics with multiscale transport models, radiation heat transfer and multiphase interactions. Such techniques are critical for the prediction of ignition delay durations, pollutant production paths and combustion instabilities under actual settings. Recent kinetic investigations of surrogate aviation fuels and cyclic carbonate pyrolysis have shown the ability of reaction pathway analysis and rate-of-production estimations to identify prominent elementary processes governing oxidation behavior. These discoveries are important for mechanism reduction and combustion optimization.[6]

Experimental diagnostics remain critical for validating numerical simulation and understanding transient combustion phenomena. Laser-based techniques such as planar laser-induced fluorescence (PLIF), particle image velocimetry (PIV) and Raman scattering enable nonintrusive measurements of temperature fields, velocity distribution, and reactive species concentrations. Recent investigations of magnetically confined methane flames revealed that external magnetic fields can substantially influence flame shape, stability, and oxygen transport behavior. The enhanced combustion efficiency under magnetic confinement increased oxygen diffusion while decreasing flame distortion and instability. Moreover, multi-spectral fusion approaches based on infrared, ultraviolet, visible-spectrum, and laser-based diagnostics have shown tremendous potential to enhance flame characterization, combustion instability detection, and pollutant monitoring in complicated reactive flow systems. Laser diagnostic also provide essential data for validating kinetic mechanisms and turbulence models in hydrogen and ammonia combustion systems. Future low-carbon combustors will increasingly depend on real time optical monitoring systems integrated with adaptive control strategies capable of responding dynamically to combustion fluctuations.

Artificial intelligence (AI) and machine learning (ML) are revolutionizing the responding flow research rapidly.[7] Data-driven models are being implemented now for combustion optimization, fuel characterization, kinetic mechanism reduction, predictive maintenance and emissions forecasting. ML algorithms for combustion optimization assess multidimensional operational factors including equivalency ratio, temperature, pressure, turbulence intensity, and fuel composition to discover ideal combustion conditions for maximizing thermal efficiency while reducing pollutant generation. AI-assisted techniques are being explored for kinetic mechanism reduction. The goal is to find the dominant species and reaction pathways in a complicated reaction network to reduce computational complexity and therefore enable faster simulations of large-scale reacting flows without significant loss of prediction accuracy. Machine learning techniques have exhibited great accuracy in flame categorization, spectrum analysis and combustion-state prediction based on laser induced breakdown spectroscopy datasets. Neural networks and support vector machine models can predict the combustion properties with an accuracy of >99% when the circumstances are controlled. The addition of ML methods in biofuel production systems is expanding for catalyst selection, feedstock optimization, reactor design, and process-scale prediction. These strategies drastically cut computing cost, while speeding up screening procedures in experiments. The future of intelligent combustion systems will likely include hybrid frameworks that combine physics-based simulations and data-driven learning algorithms. Such technologies might allow for autonomous combustion control to minimize emissions while optimizing efficiency under varying operational settings. Physics-Informed Neural Networks (PINNs) represent a key advancement in this area, where Navier-Stokes equations and chemical kinetic rate laws are embedded directly into the neural network's loss function. In addition to momentum conservation, PINNs enforce species transport, energy conservation, and reaction-rate constraints, enabling thermodynamically consistent reacting-flow predictions. This ensures that the AI-driven predictions remain physically consistent, even when training data is sparse or noisy, thereby providing a robust framework for simulating complex reacting flows.

DECARBONIZING INDUSTRY

Industrial sectors including cement, steel, petrochemicals, and refining contribute substantially to global greenhouse gas emissions because of their dependence on high-temperature combustion processes.[8] Achieving net-zero targets in these sectors therefore requires advanced carbon mitigation technologies integrated directly into industrial reacting-flow systems. Carbon capture and storage (CCS) technologies are becoming increasingly important for reducing industrial emissions while maintaining operational continuity in existing infrastructure.[9] Among emerging CCS approaches, chemical looping combustion has attracted major attention because it inherently separates carbon dioxide without requiring energy-intensive gas separation processes. In chemical looping systems, oxygen is transferred from air reactors to fuel reactors *via* oxygen carriers, usually metal oxides. This indirect combustion route avoids direct air-fuel interaction and hence produces concentrated streams of carbon dioxide for sequestration. Recent investigations of flame-synthesized $LaMnO_3$ oxygen carriers revealed good performance for methane conversion and improved oxygen transport capacity. Density functional theory simulations showed that multi-center electron transport processes greatly contribute to methane activation and prevent the generation of unwanted by-products.[10] Further work requires attention on the durability of oxygen carriers, cyclic stability, sintering resistance, and hydrodynamics at the reactor scale under industrial standard conditions.

Hydrogen injection into industrial combustion systems represents a near-term strategy for reducing carbon emissions without complete infrastructure replacement. Co-firing hydrogen with natural gas can lower carbon intensity wile maintaining combustion reliability. However, hydrogen blending alters flame speed, ignition delay, and heat release dynamics. Industrial furnaces and gas turbines therefore require redesign of fuel injectors, burner geometries, and control systems to safely accommodate hydrogen-enriched fuels. Hybrid combustion systems employing hydrogen, ammonia and bio-fuels may provide the best flexibility for future industrial energy systems. Such systems will demand integrated multiphysics modeling frameworks that are capable of capturing linked fluid dynamic and chemical kinetic processes.

CONCLUSION AND FUTURE OUTLOOK

Chemically reacting flows will remain central to global energy systems throughout the twenty-first century, even as the world transitions toward net-zero future. The challenges are no longer limited to replacing fossil fuels; instead, it involves redesigning combustion systems capable of operating efficiently, flexibly, and sustainably using carbon-free and low-carbon energy carriers. Hydrogen, ammonia, and sustainable aviation fuels each offer unique opportunities and challenges requiring advances in chemical kinetics, turbulence modeling, diagnostics, and reactor engineering, Simultaneously, industrial decarbonization depends heavily on scalable carbon capture technologies, oxygen-carrier systems, and intelligent combustion optimization. Recent progress in laser diagnostics, high-fidelity simulation, and artificial intelligence is rapidly accelerating the understanding of low-carbon reacting flows. Nevertheless, major scientific barriers remain in fuel flexibility, combustion stability, emission reduction, and large-scale economic deployment. This roadmap highlights that the pathway to net-zero emissions will involve an amalgamation of combustion science, fluid dynamics, materials engineering, computational modeling, and machine intelligence. Continued collaboration between academia, industry, and policymakers will be critical for translating laboratory breakthroughs into commercially viable low-carbon energy systems that can underpin a sustainable future.

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