ENERGETICS

Ammin/Dumarey - The Future Fuel Trilemma: Hydrogen, Methanol, or Ammonia for Decarbonizing Heavy-Duty Engines

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Context of the research activity

In the context of global efforts to decarbonize the transport sector, the search for alternative fuels to replace conventional fossil-based energy carriers has gained significant momentum. While battery electrification is progressing rapidly in the passenger vehicle segment, it remains a limited option for long-haul and high-load applications due to energy density and infrastructure constraints. For these sectors, hydrogen, methanol, and ammonia are emerging as viable and scalable alternatives capable of enabling significant reductions in greenhouse gas emissions.
Each of these fuels offers unique advantages: hydrogen is carbon-free and features high reactivity, methanol is liquid at ambient conditions and easily integrated into existing infrastructure, and ammonia combines carbon-free combustion with relatively simple storage and transport. However, their fundamental differences in chemical composition, ignition characteristics, flame behavior, and pollutant formation mechanisms result in complex combustion phenomena that must be carefully understood and controlled in order to unlock their potential in internal combustion engines.
Accurate numerical modeling of combustion processes is essential to guide engine design and fuel selection. In particular, advanced Computational Fluid Dynamics (CFD) models, capable of capturing fuel-specific kinetics and turbulent combustion phenomena, are powerful tools for evaluating and optimizing the performance, efficiency, and environmental impact of alternative fuels. Despite recent progress, a comprehensive and comparative modeling framework for hydrogen, methanol, and ammonia combustion under engine-relevant conditions is still lacking.

The primary goal of this PhD research is to develop and validate detailed CFD combustion models for hydrogen, methanol, and ammonia, aimed at supporting the clean and efficient use of these fuels in heavy-duty internal combustion engines. Specific objectives include:
• Selection of fuel-specific reaction mechanisms for hydrogen, methanol, and ammonia, with particular focus on ignition behavior and pollutant (e.g., NO¿, unburned fuel).

Objectives	• Implementation and validation of detailed and reduced kinetic schemes within a high-fidelity CFD framework (e.g., CONVERGE,or equivalent). • Simulation of engine-relevant combustion scenarios, covering a range of operating conditions typical of large bore engines, including lean and ultra lean mixtures, different injection strategies (PFI/DI), and pressure/temperature variations. • Comparative assessment of combustion efficiency, emissions, and abnormal combustion phenomena, such as knock, misfire, pre-ignition. • Support to engine design and optimization, by providing insights into the trade-offs between fuel reactivity, combustion stability, and emissions, contributing to the definition of tailored combustion strategies for each fuel. This research will contribute to a technology-neutral assessment of next-generation fuels for sustainable transport, enabling informed decisions in fuel and engine development for the heavy-duty sector.

Skills and competencies for the development of the activity	• Excellent knowledge of fluid-dynamics and engine thermodynamics • Knowledge of 1D/3D CFD simulation codes (such as GT-SUITE, CONVERGE CFD)