In search of an optimal combustion strategy for mitigating secondary organic aerosol in combustion engines

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The heightened prevalence of respiratory ailments linked to the generation of secondary organic aerosols (SOA) underscores the need for combustion engines characterized by reduced emissions of volatile organic compound (VOC) precursors [1, 2]. The combustion process quality significantly influences the production of emitted VOCs from vehicles, thereby impacting the concentration of SOA in the atmosphere [3]. The study aims to control the aerosolization process of n-Heptane droplets in a premixed air-methane-contained RCCI engine by adjusting the injection pattern to identify the most efficient pattern from both thermodynamic (energy, exergy, and efficiency) and environmental (NOx, CO, CO2, and VOC emissions, as well as SOA concentration) perspectives. The intricate process of SOA formation resulting from engine combustion is modelled by integrating computational fluid dynamics (CFD) with combustion chemistry and atmospheric chemistry and physics. First, crucial in-engine aerosol phenomena, including spraying, break-up, atomization, turbulent dispersion, collision and coalescence, and vaporization of fuel droplets, combustion flame dynamics, and the generation of combustion products are modelled. Then, extending beyond the engine, another model considers the atmospheric chemistry of the emitted products and the subsequent nucleation, condensation, evaporation, deposition, and transport of species and particles across different atmospheric layers. Moreover, the simulation delves into aerosol particle chemistry, addressing phenomena such as dissolution, dissociation, and heterogeneous reactions of VOCs within the particles. The findings reveal that unlike expecting better combustion for the strategy of right triangle injection due to better atomization, smaller fuel droplet generation, faster gasification, and higher temperature, it yields the highest HC and outdoor particles and accounts for the lowest Gross Indicated and combustion efficiencies among its counterparts. On the other hand, the strategy of right double-boot fuel injection has the highest Gross Indicated and combustion efficiencies with 39.86% and 94.88%, implying a 0.3% and 0.5% improvement compared to the base (parabolic) injection strategy, respectively.

[1] Huang, Hao, et al. "Characteristics of volatile organic compounds from vehicle emissions through on–road test in Wuhan, China." Environmental Research 188 (**2020**): 109802.
[2] Hong-Li, Wang, et al. "Volatile organic compounds (VOCs) source profiles of on-road vehicle emissions in China." Science of the Total Environment 607 (**2017**): 253-261.
[3] Costagliola, M. A., et al. "Combustion efficiency and engine out emissions of a SI engine fueled with alcohol/gasoline blends." Applied energy 111 (**2013**): 1162-1171.