International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

CFD Framework for Mechanism Validation in the Advanced Fuel Ignition Delay Analyzer (AFIDA)

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Accurate validation of chemical kinetic mechanisms is critical for reliable fuel combustion simulations. Traditional platforms—such as shock tubes and rapid compression machines (RCMs)—are widely used but time-consuming and resource-intensive, requiring large fuel volumes and complex setups. The Advanced Fuel Ignition Delay Analyzer (AFIDA), a constant-volume combustion chamber (CVCC), offers a more efficient alternative. It enables high-throughput ignition delay time (IDT) measurements using only 40 mL of fuel, with each test completed in under 20 minutes. AFIDA is particularly suited for low-volatility fuels, such as those used in aviation and diesel applications, which challenge conventional IDT devices. Despite its advantages, AFIDA's use for kinetic model development has been limited. One barrier is the lack of publicly available, validated CFD models. Another is the presence of physical processes—such as spray atomization and mixing—that introduce non-chemical ignition delays, which zero-dimensional simulations cannot capture.

We present an open-source CFD model of the AFIDA device implemented in CONVERGE CFD software [1]. The model incorporates detailed spray physics, including Kelvin-Helmholtz and Rayleigh-Taylor droplet breakup, dynamic drag, evaporation via the Frossling model, and RNG k-ε turbulence with adaptive mesh refinement (AMR) based on velocity and temperature gradients. Autoignition is simulated using the SAGE detailed chemistry solver under constant-volume conditions, demonstrated with the C3Mech mechanism [2] for n-heptane. Validation conditions replicate AFIDA test environments (e.g., 600–850 K, 10–20 bar). The CVCC's cylindrical symmetry is exploited by simulating a 1/7 radial section with a single injector delivering 8.5 mg of n-heptane over a 2 ms pulse. Unlike previous CFD studies requiring over 10,000 core-hours per case [3], our optimized setup achieves accurate IDT prediction in under 4,200 core-hours. To further improve accessibility and reproducibility, we provide a lightweight Python interface that generates all required CONVERGE input files from simple user inputs—fuel species, initial conditions, and injection parameters—eliminating the need for manual configuration in CONVERGE Studio.

This framework enables rapid, automated validation of reduced chemical kinetic models against AFIDA data, offering a practical alternative to zero-dimensional reactors that overlook key physical effects. By combining high-fidelity physics, open accessibility, and ease of use, our tool supports faster development of fuel-specific kinetic models, particularly for sustainable aviation fuels and other emerging candidates.

References

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