

Computational and Data-Driven Modeling of Combustion in Reciprocating Engines or Gas Turbines, Volume II

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1. Introduction

Climate change and the progressive depletion of fossil fuel reserves have prompted research into alternative energy sources that can meet the requirements of efficiency and sustainability in all sectors [1–3]. Nevertheless, such a transition faces significant technical, economic, environmental, and social challenges in implementing and constructing infrastructures [4].

For this reason, well-established energy systems, i.e., reciprocating engines and gas turbines, remain essential in the short and medium terms to meet the constantly increasing demand for energy, despite being characterized by combustion processes.

Apart from a more rational usage and management of the system [5], researchers have been focusing on utilizing alternative fuels [6,7] and implementing innovative strategies [8,9]. Traditional experimental approaches remain indispensable but are no longer sufficient on their own to address the complex phenomena governing modern combustion systems [10]. In this context, computational and data-driven modeling has become not just a complementary tool but a central pillar of scientific progress.

In modern scientific literature, experimental tests and numerical simulations are commonly presented together [11,12], comprehensively illustrating the various aspects that characterize the object of investigation [13,14].

This Special Issue collects several studies that exemplify how computational methods and experimental validation reinforce one another. Moreover, the ten published articles span a broad spectrum of applications in which reciprocating ignition engines (ICEs) and gas turbines (GTs) are employed, examining the combustion process and its effects from different points of view. Every study investigates advanced technology or introduces a novel methodology to deepen the understanding of combustion behavior and enable cleaner, more adaptable, and more efficient energy systems.

Notably, numerical modeling offers multiple approaches: lumped-parameter models and machine learning analyze overall system behavior, generally providing performance information, whereas computational fluid dynamics (CFD) focuses on the intricate details of reactive fluid dynamics. This Editorial explores the contributions of each article and frames them to highlight the broader trends currently shaping the future of propulsion and power generation.

2. 0D/1D Approaches

0D/1D approaches are widely used to simulate physical systems focusing on global behavior, albeit at a reduced level of detail. For example, D'Antuono et al. [15] used a 1D predictive model to evaluate the performance of a light-duty spark-ignition (SI) engine fueled with a blend of ammonia and hydrogen, 85% and 15% in volume, respectively.



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In ref. [16], ethanol vaporization was assessed in a six-cylinder SI using single-point injection (SPI). Gaitanis et al. [17] examined waste heat recovery in an advanced humidified micro-GT cycle. Also, as presented by Farrokhi et al. [18], it is possible to predict the thermochemical outcomes of oxidation processes by solving the basic mass and energy conservation equation.

Moreover, this approach couples multiple subsystems. Perrone et al. (Contribution 1) presented a combined heat-and-power production plant based on an ICE fueled with the syngas produced by a gasifier embedded in the system. Three users characterized by different thermal and electric loads were hypothesized: a health center, a hotel, and a residential building.

Szwaja et al. (Contribution 2) introduced a thermodynamic approach for evaluating the in-cylinder heat release and the mean combustion temperature in a hydrogen-fueled SI engine. In particular, a novel method for calculating the specific heat ratio accounting for molar contraction—that is, the reduction in the number of moles typical during hydrogen combustion—is proposed.

Matijošius et al. (Contribution 3) investigated the effects of cylinder group deactivation on fuel consumption and pollutant emissions in ICEs.

3. Machine Learning

The rapid maturation of machine learning models explains their wide utilization in the current scientific literature. Algorithms can be calibrated based on data collected from a test bench [19], or based on outcomes of 0D/1D models [20], further establishing the synergistic contribution of every approach.

Brusa et al. (Contribution 4) developed a hybrid method for combustion and knocking prediction based on the superimposition of physical models and artificial neural networks. This method leverages the superior robustness inherent in physical models and combines it with the adaptability and learning capabilities of neural networks, thereby enhancing overall predictive accuracy.

Such an approach can also be applied for exhaust temperature estimation; therefore, in the following article (Contribution 5), the same authors used this information to extend the focus to the turbine placed downstream of the engine for turbocharging. Indeed, the temperature levels across this component significantly affect the engine performance and the aftertreatment systems.

4. CFD

While the previous approaches are useful for fast simulations, high-fidelity CFD remains at the heart of combustion research. Several contributions to this Special Issue demonstrate how CFD continues to push boundaries in both predictive accuracy and practical impact.

Cecere et al. (Contribution 6) studied the combined effects of fuel composition and injection angle on the combustion of an $\text{NH}_3/\text{H}_2/\text{N}_2$ jet in an air crossflow using LES. Four distinct fuel mixtures, with hydrogen concentrations ranging from 15% to 60% by volume, are injected into the air at two different angles (90° and 75°), considering operating conditions frequently encountered in micro-GTs. Based on the results obtained in a previous work [21], where the authors thoroughly analyzed the turbulent structure of the flame using DNS, this study highlighted that the lowest H_2 content leads to the highest temperatures and NO production.

The current interest in hydrogen as an alternative fuel is widespread, owing to its carbon-free nature. Nevertheless, its tendency to abnormal combustion generally demands the redesign of some components [22,23]. Di Nardo et al. (Contribution 7) developed a

novel burner for GT applications capable of operating with hydrogen-enriched natural gas (NG) over a wide range of hydrogen content while maintaining low NO_x emissions. To this end, a multidisciplinary methodology consisting of CFD simulations to determine geometry, a mechanical prototype design, and experimental tests to evaluate the effective capacity of the burner to work with hydrogen, was employed.

Blending hydrogen with natural gas was also investigated in Contribution 8, with a dual-fuel marine engine application. Starting from a baseline configuration in which methane is the primary fuel, increasing fractions of methane, 10%, 30%, 50%, 60%, and up to 100%, are gradually replaced with hydrogen. To obtain more accurate ignition timing predictions, a kinetic mechanism from the literature, which accounts for low-temperature reactions, was coupled into the CFD framework code. The results demonstrated that both hydrogen percentage and mixture density influence the ignition timing, as these parameters affect the vaporization of the fuel responsible for initiating the ignition. Furthermore, the complete substitution of methane with hydrogen reduces CO₂ emissions by up to 54%, accompanied by significantly increased NO_x emissions of approximately 76%.

Beyond hydrogen, other fuels have been investigated as alternative solutions; in particular, alcohols, which can be produced from renewable feedstocks, are gaining momentum due to their similar physical and chemical properties to those of gasoline. The possibility of storing them in a liquid state is a significant benefit, but their high latent heat of vaporization, on the other hand, poses several challenges in the injection phases [24]. In Contribution 9, the effects of uneven fuel distribution among the cylinders of an SI engine converted to operate on ethanol are presented. The engine, as presented in ref. [16], features an SPI system; the different cylinder phasing and the aforementioned difficulties associated with vaporization lead to variations in the equivalence ratios among the cylinders. In a subsequent work [25], the same authors tested multipoint injection strategies, ultimately overcoming fuel delivery issues. However, the inefficient vaporization process forms a wall film in the intake duct, involving nearly 10% of the injected fuel.

Finally, in Contribution 10, the development processes of a multi-platform selective catalytic reduction (SCR) system for mobile applications are described. Indeed, SCR system performance directly depends on the upstream combustion, especially in terms of temperature and chemical composition.

Conflicts of Interest: The authors declare no conflicts of interest.

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