Editorial

Numerical Investigations ofCombustion—An Overview

Mohsen Ayoobi 1, Pedro R. Resende 2,3 and Alexandre M. Afonso 3,*

1 Division of Engineering Technology, Wayne State University, Detroit, MI 48201, USA; mohsen.ayoobi@wayne.edu
2 proMetheus, School of Technology and Management (ESTG), Polytechnic Institute of Viana do Castelo (IPVC), Praça Gen. Barbosa 44, 4900-347 Viana do Castelo, Portugal; pedroresende@estg.ipvc.pt
3 Centro de Estudos de Fenômenos de Transporte, Departamento de Engenharia Mecânica, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal
* Correspondence: aafonso@fe.up.pt

With the recent advancements in computational capacities and the widespread applications of machine learning in engineering problems, the role of numerical methods has been becoming more and more important to improve existing models or develop new models that can help researchers to better understand the underlying physics of combustion, their interaction with other physical phenomena such as turbulence, and their impacts on the performance of the related applications at both fundamental and practical levels. This Special Issue aims to highlight the most recent advances in the development and application of such numerical methods. This editorial presents an overview of the articles published under this Special Issue is presented.

Resende et al. [1] conducted a numerical investigation to analyze the combustion characteristics of a H2 and air mixture in a complex geometry of an undulate microchannel. The findings from this article help to understand and verify whether the flammability at microscales can be improved by designing non-straight microchannels as an alternative to the burner with recirculation of reaction products. In particular, the authors of this article evaluate the effect of the geometry on the combustion characteristics over a range of different inlet velocities while keeping other boundary conditions, including the equivalence ratio and external heat flux losses, the same.

Using both experimentally and numerically obtained data, Mitu et al. [2] examined the influence of hydrogen on the laminar burning velocity for different methane/hydrogen and natural gas/hydrogen mixtures with air at ambient initial conditions. In particular, this paper reports laminar burning velocities (LBV) of hydrogen-blended methane–air and natural gas–air mixtures, using mixtures at ambient initial pressure and temperature (p0 = 0.97–1.04 bar, T0 = 22–25 °C). The mixtures of interest in this work consist of single fuel–air (CH4–air) and multifuel–air mixtures, where the multifuel was CH4 blended with H2, or natural gas blended with H2, both under various amounts of added hydrogen, in the range of 0 to 50 mol% (with respect to the initial fuel amount). With this study, they showed that hydrogen addition increased LBV for all the examined binary flammable mixtures. The fraction of added hydrogen affects LBV linearly at moderate hydrogen fractions. However, this impact becomes stronger at higher hydrogen fractions. This study shows that hydrogen addition can significantly change the thermal diffusivity of flammable CH4–air or natural gas/air mixtures, the rate of heat release, and the concentration of active radical species in the flame front, thus contributing to LBV variation. The findings from this work contribute to the existing data pool for flame propagation in hydrogen-blended CH4/air and natural gas/air mixtures.

Considering the fact that the multiple-injection strategy could potentially be the solution to reduce engine exhaust gas emissions, Seol et al. [3] investigated the combustion process and emission characteristics inside the cylinder of a two-stroke marine main engine equipped on a university’s training ship. In this work, the authors used the simulation
software ANSYS Fluent 2019R2 to perform 3D simulations and capture the combustion process and emission formation inside the engine cylinder. In these simulations, they considered two operating modes of the engine—single-injection mode and double-injection mode—and analyzed the in-cylinder pressure, temperature, and emission characteristics. The results from this work showed that using double-injection mode reduces the in-cylinder pressure and temperature peaks by 6.42% and 12.76%. NO and soot emissions were also reduced up to 24.16% and 68%, respectively, in the double-injection mode in comparison with the single-injection mode. However, CO$_2$ emission and ISFOC were increased by 7.58% and 23.55%, respectively, in the double-injection mode. Both positive and negative effects of the double-injection strategy on the engine should be taken into consideration by the operators.

Białecki et al. [4] verified a reactivity model to compare the combustion process of different alternative fuels in turbine engines. For this research, they used synthetic blending components from alcohol to jet and hydro-processed esters and fatty-acid technologies and their blends with conventional jet fuel. Using laboratory tests (bench tests were carried out on a test rig with a miniature turbojet engine) to understand the differences between the properties of the tested fuels and record the carbon oxide concentrations in the exhaust gas, they were able to form empirical power functions and describe the relations between carbon oxide concentration and fuel mass flow rate. These formulations suggested that that the combustion mechanism of the fuel with the blend of Jet A-1 and hydro-processed esters and fatty acids is different from that of the fuel that contains an alcohol or jet synthetic component.

Payri et al. [5] conducted research towards modeling the fuel injection process to characterize the in-cylinder mixture formation and subsequent combustion process in modern direct-injection gasoline engines. In particular, these modeling efforts are important to understand flash boiling, which usually occurs when the fuel is injected into an ambient pressure below the saturation pressure of the liquid and is characterized by fast breakup and evaporation rates. Flash boiling could potentially lead to undesired behaviors such as spray collapse and affect the mixture preparation negatively. In particular, the work by Payri et al. developed a comprehensive spray model that was validated for the Spray G baseline condition (G1) and extended to cold flash-boiling conditions. First, this model was implemented for iso-octane and then extended to n-hexane, n-heptane, and n-pentane. The extension of the model to different fuels was a novel approach and enabled the assessment of fuel properties on spray morphology under flash-boiling conditions.

Mitu et al. [6] conducted rigorous experimental measurements in a spherical combustion bomb to investigate the combustion characteristics of N$_2$-diluted CH$_4$-N$_2$O mixtures with a stoichiometric equivalence ratio at several initial pressures (0.5–1.75 bar) and initial ambient temperatures. The methodology employed in this study is based on the cubic law of the pressure rise during the early (incipient) period of flame propagation. Their results include the burnt mass fractions and flame radii at various moments of flame propagation in the course of the incipient stage, while reporting the cubic law coefficients and corresponding laminar burning velocities of the selected time interval. The findings from this work contribute to safety enhancement in industrial facilities that handle and store nitrous oxide while expanding the combustion database for fuel-N$_2$O flames. Furthermore, such investigations of hydrocarbon-nitrous oxide combustion can provide valuable information on the fundamental chemical kinetics relevant to complex oxidation systems involving nitrogen and help address prediction-, prevention-, and protection-related concerns.

To address the increasing demand for clean and green energy, researchers have been investigating potential fuels with low emissions, such as synthetic gas (syngas), especially at microscales. Combustion in microscale systems presents even more complexity, and it is important to describe syngas combustion and comprehend its properties at such scales. In this direction, Pokharel et al. [7] studied premixed syngas combustion in a two-dimensional channel, with a length of 20 mm and a half-width of 1 mm, using computational approaches. They used a fixed temperature gradient at the upper wall to account for the conjugate
heat transfer through the walls. Using the San Diego mechanism involving 46 species and 235 reactions, stoichiometric premixed syngas combustion with various compositions of carbon monoxide, methane, and hydrogen, over a range of inlet velocities was simulated. Simulation results were used to define different metrics and analyze various combustion phenomena, such as ignition, flame stabilization, and flames with repeated extinction and ignition. The flame stability and ignition time were found to correlate with the inlet velocity for a given syngas mixture composition. Similarly, for a given inlet velocity, the correlation of the flame properties with respect to the syngas composition was further scrutinized. Since syngas is generated from a variety of different sources and methodologies, it can consist of different species of a wide range of concentrations. Therefore, the findings of this work are critically important in selecting the appropriate composition of syngas depending on the application.

Grimm et al. [8] investigated an atmospheric prototype burner, designed for operation in a hybrid power plant, both numerically and experimentally, to examine its capabilities. With the help of a solid oxide fuel cell (SOFC) mounted upstream of the burner in the gas turbine system, a potentially large operational flexibility and efficiency can be achieved. Operating the burner with the SOFC off-gas, heat-loss mechanisms are in the order of magnitude of the thermal power output. Therefore, the combustor requires careful design considerations, which can be addressed using the multiple computational fluid dynamics (CFD) modeling strategies utilized in this study. The findings from this work show that the presented combustor system enables low-calorific combustion over a large range of operation conditions, despite major heat-loss effects, and results in low NOx emissions.

Quintino et al. [9] conducted one-dimensional numerical simulations for three base biogas blends (BG100, BG90, and BG80) with different equivalence ratios (0.8 to 1.0) and hydrogen contents in the fuel mixture (up to 50% in volume). The results from these simulations were used to study the impact of H2 enrichment on the laminar flame speed (SL) of lean biogas/air flames and develop an analytical correlation to model SL to extend the application range of the existing equations in the literature. Analyzing the impacts of thermal diffusive, dilution, and chemical effects of CO2 and H2 on SL at ambient pressure and temperature, they proposed a correlation that was in good agreement with the data from the literature and simulations. By isolating the contributions of CO2 and H2 in independent variables, the proposed equation in this work can be directly used to estimate SL without the need for a priori adaptations of fit parameters.

Jadidi et al. [10] proposed a novel approach to predict soot emissions at low computational costs using artificial neural networks (ANN). While soot formation in combustion systems is a major concern due to its adverse environmental and health effects, most industrial device simulations still neglect or simply approximate soot formation to avoid the complexity of this phenomenon and/or reduce computational costs (processing hardware and time). It is therefore essential to develop accurate, easy-to-use, and computationally inexpensive methodologies to accurately estimate soot concentrations. The authors of this article built and trained an ANN using data from the CoFlame code [11]. This ANN can work as a post-processing tool to estimate the soot volume fraction numerically with a low computational cost at various conditions, while it only needs properties from the gas-phase conservation equations (mass, momentum, energy, and species mass fractions) as inputs. It is noted that the authors have addressed the issues of dimensionality that were observed previously in the library-based soot-estimator models, which can potentially extend the concept of the soot estimator to transient and turbulent flames. The accuracy of the proposed methodology can be improved by using more accurate CFD simulations to generate more quality data and better train the network and minimize the error propagation effect. This work is one the first attempts (if not the first) to train artificial neural networks based on detailed modeling of soot formation.

The article published by Adebiyi et al. [12] revolves around the flame behavior and its propagation regimes. Specifically, they quantified the morphology and dynamics of a premixed flame propagating through a comb-shaped array of obstacles in open channels of
various blockage ratios with fuel mixtures of various thermal-expansion ratios. This work was conducted using computational simulations of the reacting flow described by transport properties, a fully compressible hydrodynamics, and Arrhenius chemical kinetics. They observed that in relatively wider channels, it is more likely for the flame to experience more than one propagation regime. Post-processing the simulation results, the authors identified three main stages of flame propagation in a fully open obstructed pipe, namely: (i) quasi-steady propagation, (ii) exponential flame acceleration, and (iii) saturation of the burning velocity. The accelerating phase was found to be exponential in nature and consistent of the theoretical prediction from the literature. The quasi-steady propagation stage fits the regime of flame oscillations for the low-Reynolds-number flames. In the stage of saturation burning velocity, the growing flame velocity saturates when approaching the speed of sound. The authors determined that the blockage ratio is the main parameter that influences the final saturated flame tip velocity. The authors also employed machine learning with the logistic regression algorithm to characterize and differentiate the parametric domains of accelerating and non-accelerating flames.

Hu et al. [13] conducted a numerical investigation to help determine the required quality of inert gas agents in fire suppression systems. This work is significantly important regarding health and safety concerns associated with active chemicals because inert gas agents have the potential to be widely used in fire suppression systems. In this study, the authors developed the general expressions between oxygen concentration, the discharge rate of inert gas agents, and the ventilation rate of the air–agent mixture. These expressions can help to minimize the hypoxic effects in an occupied area when accurately controlling the discharge quantity of inert gas agents to dilute the oxygen concentration. They then used the Fire Dynamic Simulator to model the dilution and fire-extinguishing efficiencies of inert gas agents when discharging inert gas agents into an enclosure was modeled. Using simulation results, they showed that the average oxygen mass fraction approximately reaches the design level at the end of the discharge period. The findings from this work indicate that the ventilation systems not only play an important role in mitigating the risk of over-pressurizing the released inert gas agents but also help to reduce the required quantity of inert gas agents.

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