energies

Editorial

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

Maria Cristina Cameretti and Roberta De Robbio *

Department of Industrial Engineering, University of Naples Federico II, Via Claudio 21, 80125 Naples, Italy
* Correspondence: roberta.derobbio@unina.it

1. Introduction

The targets set by the Paris Agreement to limit greenhouse gas emissions and global warming aim to significantly reduce the levels of pollutants emitted in the atmosphere from all sectors, including transportation and land use energy production [1].

To this aim, new technologies are progressively entering the market as represented by electrification [2,3] or solutions to avoid the enhancement of climate-altering species, like carbon capture and storage [4,5].

Nevertheless, the well-established internal combustion energy systems, i.e., reciprocating engines and gas turbines, still represent a key in the short and medium term; hence, reducing all kinds of emissions and optimizing their operation is mandatory [6–9]. As a matter of fact, having a deep knowledge of the several processes occurring in the reactive domain or predicting the performance of the overall system can help to prevent the formation of harmful species [10], to study the feasibility of alternative primary energy sources and to optimize their combustion development [11].

To this aim, computational modeling represents a powerful tool, making it possible to investigate a wide range of operating conditions, even the extreme ones, avoiding risk of damage and reducing general costs, i.e., facility setup, maintenance, and supplies. Numerical modeling includes several approaches that can study the same problem on different levels. For example, one-dimensional and machine learning can analyze and predict the entire system performance [12,13], while CFD focuses in detail on the processes occurring inside a fluid domain [14]. Of course, the models must be validated before considering them reliable. Experimental investigations can provide the data to understand the behavior of the thermal energy system and, thus, provide the base for the building of the model itself. On the other hand, it is known that experimental activities and numerical computations are strictly linked.

The present Special Issue includes nine research articles and a review on the role of micro gas turbines (MGTs) in the distributed energy production. The nine articles' applications cover reciprocating internal combustion engines (ICEs) and gas turbines (GTs), making use of all the above-mentioned different modeling approaches, demonstrating a complete contribution to each field of the topic.

2. Modeling of Reciprocating Internal Combustion Engines

Clean mobility is surely the most urgent topic. ICEs still represent the predominant energy conversion system for all sizes and kinds of land [15,16] and sea applications [17,18].

Diesel engines have been progressively banned in several countries due to the high emissions of particulate matter (PM) and nitrogen oxides (NO_x). However, it is well known that they feature levels of power, weight, efficiency, and reliability that are compatible with off-road and marine applications. For this reason, researchers are continuing to study new methodologies and strategies to reduce the above-mentioned pollutants in this type of engine.

Citation: Cameretti, M.C.; De Robbio, R. Computational and Data-Driven Modeling of Combustion in Reciprocating Engines or Gas Turbines. *Energies* **2024**, *17*, 3863. https://doi.org/10.3390/en17163863

Received: 27 May 2024
Accepted: 12 June 2024
Published: 6 August 2024

To this aim, the Dual Fuel (DF) combustion concept is a promising solution. It consists of the partial substitution of diesel fuel with a cleaner fuel, such as natural gas. However, the high emissions of unburned hydrocarbons (UHCs) have led to attempts to improve the combustion characteristics with the addition of hydrogen [19,20].

Cameretti et al. (Contribution 1) examined the overall combustion development in a single-cylinder research engine compression ignition engine via CFD simulations of hydrogen/methane blends as primary fuels. Starting from experimental measurements to validate the full methane and full hydrogen cases, a progressive enhancement of hydrogen energy share is numerically analyzed. The results demonstrated that the presence of hydrogen leads not only to reduced emissions of carbon-based species but also to a strong increase in temperature and consequently NO_x.

Abdelhameed and Tashima (Contribution 2) studied two important techniques for a reduction in NO_x in marine engines: exhaust gas recirculation (EGR) and water-in-fuel emulsion. Both cause a decrease in thermal efficiency. Therefore, their combination is modeled with a synergetic approach that involved CFD and 0D/1D tools on the basis of experimental results to minimize NO_x while maintaining an adequate level of thermal efficiency.

Falai and Misul (Contribution 3) used machine learning to develop virtual sensors for monitoring NO_x emissions in diesel engines. The virtual sensor is calibrated via the Extreme Gradient Boosting (XGBoost) algorithm on the basis of collected data from a test bench at steady-state conditions, claiming a prediction accuracy of almost 98%. Instead, the accuracy reduces to 85% in dynamic conditions as demonstrated in an on-road driving mission.

Doppalapudi et al. (Contribution 4) numerically investigated the effects of the shape of the combustion chamber on injection profiles and in-cylinder distributions of temperature, velocity, and turbulent motions (swirl and tumble ratio), with the aim to assess the most improved configuration in terms of combustion characteristics. They evaluated five chamber shapes and suggested avoiding wide bowls that may induce uneven combustion across the cylinder. Instead, better results can be obtained with split bowls.

Spark ignition (SI) engines, as leading powertrain technologies, are being investigated and improved as well. As widely discussed by Sforza et al. (Contribution 5), a possible solution to minimize thermal losses, while reducing to zero soot particles and drastically reducing NO_x, is to operate the engine with homogeneous ultra-lean premixed mixtures (CH_4-air). Nevertheless, the progressive shift towards increasingly high values of the air-to-fuel ratios raises doubts in the applicability of the most commonly used numerical models for SI engines. To this aim, the authors of the paper evaluated two different flamelet-based models, typically used for premixed mixtures: the Coherent Flame Model and the Flame Area Model. The results were compared with experiments carried out on a Darmstadt TSF burner. They observed that, near the burner exit, the flamelet assumption is still valid and the models accurately predict the combustion behavior. In contrast, in the typical conditions of homogeneous ultra-lean mixtures, the models are no more capable of providing reliable results. Thus, the authors suggested modifications and extensions to the flamelet-based models to improve CFD simulations.

Following the path of using carbon-free fuel in order to drastically reduce CO_2 emissions, the paper by D'Antuono et al. (Contribution 6) concerned the study of an ammonia/hydrogen blend, 85% and 15%, respectively, by volume, in a light-duty SI engine using a 1D predictive model. Ammonia features low combustion characteristics that limit its operating capacity as pure fuel; however, with respect to hydrogen, it is easier to store on vehicles. To overcome such an issue, the authors demonstrated that the addition of H_2 to the air–fuel mixture allows us to improve the flammability of NH_3, extending the range of operation of the engine.

3. Modeling of Gas Turbines

Since gas turbines of all sizes are employed in the aviation industry and power generation, researchers are committed to reducing the emissions from this type of internal combustion engine, which is also the object of this Special Issue, as well as complying with the regulations set for these sectors [21,22].

Castiglione et al. (Contribution 7) evidenced that the most viable option to achieve a low-emission aero-propulsion system is the utilization of alternative bio and synthetic fuels, the so-called sustainable aviation fuels (SAFs), instead of fossil fuels. When supplied with new fuels, the engine might undergo architectural modifications; consequently, advanced control systems are mandatory to ensure a safe and efficient operation. Therefore, the authors developed linear models for direct fuel control of a turboshaft aircraft engine obtained using two approaches: Small Perturbation and System Identification. Moreover, the linear models included the component degradation, demonstrating a reliable link with performance, especially when the Small Perturbation technique is adopted.

Clean bioenergy generation in gas turbines is the focus of the paper by Lu at al. (Contribution 8). The authors proposed an optimized methodology for the developed pressurized Chemical Looping Combustors via a zero-dimensional model validated by experimental data. Through such technology, combustion occurs in two separated reactors (air and fuel). The modeling of the air reactor can be found in a previous paper [23], while in the present Special Issue, a metal oxide is reduced in the fuel reactor, providing the oxygen for the oxidation of the fuel, and then regenerated in the air reactor. At the fuel reactor outlet, pure carbon dioxide can be obtained by condensing water vapor. In this way, the CO_2 can be easily compressed and stored.

As already observed for ICEs, hydrogen and ammonia are interesting alternative fuels for gas turbines as well, as demonstrated by Giacomazzi et al. (Contribution 9). However, to use such alternative fuels and simultaneously reduce NO_x emissions, it is necessary to operate a reassessment of the combustor. Indeed, the flame structure of NH_3 could favor NO formation. Thus, the authors investigated the micro-mixing combustion system of a non-premixed jet flame of $NH_3/H_2/N_2$ blend in air crossflow via Direct Numerical Simulation (DNS). Such a simple configuration provided evidence of the turbulent mixing and its effects on the flame structure.

Finally, this Special Issue includes a wide and detailed review on the use of micro gas turbines [24]. MGTs are gaining more attention in the current energy production scenario because it is shifting from a centralized structure to a distributed one with the necessity to exploit local renewable resources. In this regard, MGTs are compact and highly flexible, being able to operate with different fuels and at different load levels [25]. The review illustrates in detail the combustion of several liquid and gaseous fuels, also obtained from biomasses considered to emit net zero CO_2. In addition, due to the reduced size and the typical high temperature at the exhaust of gas turbines, this particular power plant can be perfectly integrated with other energy systems with a low environmental impact, for example, solar fields, ORC, and fuel cells, and it can be utilized in CHP and CCHP assets.

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

List of Contributions:

1. Cameretti, M.C.; De Robbio, R.; Mancaruso, E.; Palomba, M. CFD Study of Dual Fuel Combustion in a Research Diesel Engine Fueled by Hydrogen. *Energies* **2022**, *15*, 5521. https://doi.org/10.3390/en15155521.
2. Abdelhameed, E.; Tashima, H. EGR and Emulsified Fuel Combination Effects on the Combustion, Performance, and NOx Emissions in Marine Diesel Engines. *Energies* **2022**, *16*, 336. https://doi.org/10.3390/en16010336.
3. Falai, A.; Misul, D.A. Data-Driven Model for Real-Time Estimation of NOx in a Heavy-Duty Diesel Engine. *Energies* **2023**, *16*, 2125. https://doi.org/10.3390/en16052125.
4. Doppalapudi, A.T.; Azad, A.K.; Khan, M.M.K. Analysis of Improved In-Cylinder Combustion Characteristics with Chamber Modifications of the Diesel Engine. *Energies* **2023**, *16*, 2586. https://doi.org/10.3390/en16062586.
5. Sforza, L.; Abdelwahid, S.; Lucchini, T.; Onorati, A. Ultra-Lean Premixed Turbulent Combustion: Challenges of RANS Modelling. *Energies* **2022**, *15*, 5947. https://doi.org/10.3390/en15165947.

6. D'Antuono, G.; Lanni, D.; Galloni, E.; Fontana, G. Numerical Modeling and Simulation of a Spark-Ignition Engine Fueled with Ammonia-Hydrogen Blends. *Energies* **2023**, *16*, 2543. https://doi.org/10.3390/en16062543.
7. Castiglione, T.; Perrone, D.; Strafella, L.; Ficarella, A.; Bova, S. Linear Model of a Turboshaft Aero-Engine Including Components Degradation for Control-Oriented Applications. *Energies* **2023**, *16*, 2634. https://doi.org/10.3390/en16062634.
8. Lu, W.; Bartocci, P.; Abad, A.; Bischi, A.; Yang, H.; Cabello, A.; de Las Obras Loscertales, M.; Zampilli, M.; Fantozzi, F. Dimensioning Air Reactor and Fuel Reactor of a Pressurized CLC Plant to Be Coupled to a Gas Turbine: Part 2, the Fuel Reactor. *Energies* **2023**, *16*, 3850. https://doi.org/10.3390/en16093850.
9. Giacomazzi, E.; Cecere, D.; Cimini, M.; Carpenella, S. Direct Numerical Simulation of a Reacting Turbulent Hydrogen/Ammonia/Nitrogen Jet in an Air Crossflow at 5 Bar. *Energies* **2023**, *16*, 7704. https://doi.org/10.3390/en16237704.

References

1. Paris Agreement to the United Nations Framework Convention on Climate Change, December 12, 2015, T.I.A.S. No. 16-1104. Available online: https://www.state.gov/16-1104/ (accessed on 11 May 2024).
2. Yildiz, A.F.; Sahinler, R.; Ozturk, C. Data-Driven Modelling of a Plug-In Hybrid Electric Vehicle. In Proceedings of the 2023 14th International Conference on Electrical and Electronics Engineering (ELECO), Bursa, Turkiye, 30 November–2 December 2023; pp. 1–5. [CrossRef]
3. Camacho, M.d.l.N.; Jurburg, D.; Tanco, M. Hydrogen Fuel Cell Heavy-Duty Trucks: Review of Main Research Topics. *Int. J. Hydrog. Energy* **2022**, *47*, 29505–29525. [CrossRef]
4. Li, X.; Zhou, R.; Yang, H.; Liang, Z.; Yao, Y.; Yu, Z.; Du, M.; Lou, D.; Li, K. Properties of Carbonic Anhydrase-Containing Active Coatings for CO_2 Capture. *Processes* **2024**, *12*, 810. [CrossRef]
5. Shervani, S.; Tansug, L.P.; Tezel, F.H. Microporous Adsorbent-Based Mixed Matrix Membranes for CO_2/N_2 Separation. *Energies* **2024**, *17*, 1927. [CrossRef]
6. Godiño, J.A.V.; García, M.T.; Aguilar, F.J.J.-E. Experimental Investigation and Modelling of Biodiesel Combustion in Engines with Late Direct Injection Strategy. *Energy Rep.* **2022**, *8*, 7476–7487. [CrossRef]
7. Napolitano, P.; Di Domenico, D.; Di Maio, D.; Guido, C.; Golini, S. Ultra-Fine Particle Emissions Characterization and Reduction Technologies in a NG Heavy Duty Engine. *Atmosphere* **2022**, *13*, 1919. [CrossRef]
8. Zucareli de Souza, T.A.; Frez, G.V.; Pinto, G.; Costa, R.; Roque, L.F.A.; Coronado, C.J.R.; Vidigal, L.P.V. *CFD Analysis of Different Biogas Upgrading Levels for Dual-Fuel Operation in Diesel Engines*; SAE Technical Paper 2023-24-0055; SAE International: Capri, Naples, Italy, 2023. [CrossRef]
9. Barone, G.; Buonomano, A.; Del Papa, G.; Maka, R.; Palombo, A. How to Achieve Energy Efficiency and Sustainability of Large Ships: A New Tool to Optimize the Operation of on-Board Diesel Generators. *Energy* **2023**, *282*, 128288. [CrossRef]
10. Breer, B.; Rajagopalan, H.; Godbold, C.; Johnson, H.; Emerson, B.; Acharya, V.; Sun, W.; Noble, D.; Lieuwen, T. Numerical Investigation of NOx Production from Premixed Hydrogen/Methane Fuel Blends. *Combust. Flame* **2023**, *255*, 112920. [CrossRef]
11. Zhu, J.; Wang, Z.; Li, R.; Liu, S.; Hua, Y. Experimental Study and Prediction Model of Combustion Stability and Combustion Mode Variation of Burning Methanol/Biodiesel Blends for Diesel Engines. *Fuel* **2023**, *335*, 127038. [CrossRef]
12. Galloni, E.; Lanni, D.; Fontana, G.; D'Antuono, G.; Stabile, S. Performance Estimation of a Downsized SI Engine Running with Hydrogen. *Energies* **2022**, *15*, 4744. [CrossRef]
13. Shetty, S.; Shetty, R.P.; Shrinivasa Rao, B.R. Experimental Investigation and Artificial Neural Network Modelling of Combustion Pressure Parameters of Dual Spark Plug SI Engine. *Mater. Today Proc.* **2023**, *92*, 189–201. [CrossRef]
14. Füzesi, D.; Wang, S.; Józsa, V.; Chong, C.T. Ammonia-Methane Combustion in a Swirl Burner: Experimental Analysis and Numerical Modeling with Flamelet Generated Manifold Model. *Fuel* **2023**, *341*, 127403. [CrossRef]
15. Perrone, D.; Castiglione, T.; Falbo, L.; Bova, S.; D'Epiro, C. *1-D Numerical Model of a Spark Ignition Engine Fueled with Methanol for Off-Grid Charging Stations*; SAE Technical Paper 2023-24-0098; SAE International: Capri, Naples, Italy, 2023. [CrossRef]
16. Ramognino, F.; Sforza, L.; D'Errico, G.; Gomez-Soriano, J.; Onorati, A.; Novella, R. *CFD Modelling of Hydrogen-Fueled SI Engines for Light-Duty Applications*; SAE Technical Paper 2023-24-0017; SAE International: Capri, Naples, Italy, 2023. [CrossRef]
17. Ichikawa, Y.; Niki, Y.; Takasaki, K.; Kobayashi, H.; Miyanagi, A. Experimental Study of Combustion Process of NH3 Stratified Spray Using Imaging Methods for NH3 Fueled Large Two-Stroke Marine Engine. *Appl. Energy Combust. Sci.* **2023**, *13*, 100119. [CrossRef]
18. Nyongesa, A.J.; Kim, J.K.; Lee, W.-J. Investigation on the Combustion of Ammonia Using Direct High/Medium-Pressure-Otto Injection Approach in a Diesel Two-Stroke Marine Slow Speed Engine. *J. Energy Inst.* **2024**, *114*, 101641. [CrossRef]
19. Sehili, Y.; Loubar, K.; Tarabet, L.; Cerdoun, M.; Lacroix, C. Development of Predictive Model for Hydrogen-Natural Gas/Diesel Dual Fuel Engine. *Energies* **2023**, *16*, 6943. [CrossRef]
20. De Robbio, R.; Cameretti, M.C.; Mancaruso, E.; Tuccillo, R.; Vaglieco, B.M. *CFD Analysis of Different Methane/Hydrogen Blends in a CI Engine Operating in Dual Fuel Mode*; SAE Technical Paper 2022-01-1056; SAE International: Krakow, Poland, 2022. [CrossRef]

21. Inoue, C.; Higaki, S.; Fujii, H.; Ishikawa, N.; Ueda, Y. On-Site Direct Imaging of Carbon Dioxide Emissions from Aircraft during Landing and Take-off Cycle. *Environ. Adv.* **2023**, *13*, 100432. [CrossRef]
22. Carusotto, S.; Goel, P.; Baratta, M.; Misul, D.A.; Salvadori, S.; Cardile, F.; Forno, L.; Toppino, M.; Valsania, M. Combustion Characterization in a Diffusive Gas Turbine Burner for Hydrogen-Compliant Applications. *Energies* **2022**, *15*, 4117. [CrossRef]
23. Bartocci, P.; Abad, A.; Bischi, A.; Wang, L.; Cabello, A.; de Las Obras Loscertales, M.; Zampilli, M.; Yang, H.; Fantozzi, F. Dimensioning Air Reactor and Fuel Reactor of a Pressurized Chemical Looping Combustor to Be Coupled to a Gas Turbine: Part 1, the Air Reactor. *Energies* **2023**, *16*, 2102. [CrossRef]
24. De Robbio, R. Micro Gas Turbine Role in Distributed Generation with Renewable Energy Sources. *Energies* **2023**, *16*, 704. [CrossRef]
25. Di Nardo, A.; Bo, A.; Calchetti, G.; Giacomazzi, E.; Messina, G. Study on the Fuel Flexibility of a Microgas Turbine Combustor Burning Different Mixtures of H_2, CH_4, and CO_2. *J. Eng. Gas Turbine Power* **2020**, *142*, 061001. [CrossRef]