

Editorial Special Issue on Modelling, Simulation and Control in Combustion Processes of Renewable Fuels

Ján Pitel' ^{1,*}, Jan Hrdlička ² and Ivan Pavlenko ³

- ¹ Department of Industrial Engineering and Informatics, Faculty of Manufacturing Technologies, Technical University of Košice, Bayerova 1, 080 01 Prešov, Slovakia
- ² Department of Energy Engineering, Faculty of Mechanical Engineering, Czech Technical University in Prague, Technická 1902/2, 166 07 Prague, Czech Republic
- ³ Department of Computational Mechanics Named after V. Martsynkovskyy, Faculty of Technical Systems and Energy Efficient Technologies, Sumy State University, 2, Rymskogo-Korsakova St., 40007 Sumy, Ukraine
- * Correspondence: jan.pitel@tuke.sk

The modeling and simulation of combustion processes is still a challenging field. It requires integrating heat and mass transfers, flow conditions, and reaction chemistries. The available tools for such modeling methods are very different and are usually problemspecific. One particular field of interest is the fluidized bed combustion of solid fuels, which additionally encounters fluidized bed hydrodynamics and particle interactions. Recent trends in the field focus on a more detailed description and understanding of the burn-out mechanism of solid fuel particles, which is essential for modeling in order to produce reasonable outputs. From a control point of view, for example, the dynamic models of combustion processes are essential in model-based control algorithms. Due to their complexity, dynamic modeling based on partial differential equations and parameter identification for the corresponding transient models is a topical problem that can be solved using a comprehensive approach based on experimental data, numerical simulation, regression modeling, and artificial intelligence methods. One common challenge is validating the models in an actual process, which requires in-depth and precise measurements that are typically complicated by limited access to the combustion process zone. This information is also essential for controlling and monitoring combustion processes.

The most topical problems consider the combustion processes of renewable fuels and possible solutions; up-to-date tools for reaction chemistry modeling and flow, heat, and mass transfer simulations during combustion processes; the numerical simulation of transient combustion processes; parameter identification for models of combustion processes; advanced control algorithms of combustion processes; and sensors for monitoring and controlling combustion processes have been presented and solved in the Special Issue on Modelling, Simulation and Control in Combustion Processes of Renewable Fuels (https://www.mdpi.com/journal/processes/special_issues/combustion_processes_ renewable_fuel).

Pour et al. [1] mainly numerically investigated a particular type of portable incinerator. Their application in municipal solid waste management is growing due to the ability of such instruments to produce energy and, more specifically, reduce waste volumes. The article proposed a numerical simulation of the combustion process using computational fluid dynamics. As a result, the most critical parameters were investigated for a reliable design of a domestic portable incinerator. A previous design of simple incinerators was also used to apply natural gas as one of the fossil fuels. The main parameters of the designs were also investigated. Validation was performed for the mesh quality test and the occurrence of chemical reactions near the burner of the incinerator. The results showed that by moving the primary burner into the secondary chamber of the incinerator, the temperature and the heating ability could be affected dramatically. Finally, it was found that by increasing the flow rate of the cooling air inside the incinerator to some extent, the combustion process is



Citation: Pitel', J.; Hrdlička, J.; Pavlenko, I. Special Issue on Modelling, Simulation and Control in Combustion Processes of Renewable Fuels. *Processes* 2022, *10*, 2530. https://doi.org/10.3390/ pr10122530

Received: 31 October 2022 Accepted: 21 November 2022 Published: 29 November 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). improved. On the other hand, by introducing more cooling air, the evacuation of hazardous gases from the exhaust also improved.

Guo et al. [2] conducted a numerical investigation on De-NO_x technology and abnormal combustion control for a hydrogen engine using an exhaust gas recirculation (EGR) system. This is a topical problem because abnormal combustion and high NO_x emissions limit the applications of hydrogen-fueled engines. Nowadays, hydrogen engines use exhaust gas recirculation technology to control the intensity of premixed combustion and reduce NO_x emissions. Therefore, the research aimed to improve abnormal combustion. The results indicated that the peak in-cylinder pressure continuously increased with the increase in the ignition advance angle and was closer to the top dead center. Additionally, the mixture burned violently near the theoretical air-fuel ratio, and the combustion duration was shortened. Moreover, NO_x emissions, the average pressure, and the in-cylinder temperature decreased as the EGR ratio increased. Furthermore, increasing the EGR ratio led to an increase in combustion duration and a decrease in the peak heat release rate. The EGR system could delay the spontaneous combustion reaction of the end gas and reduce the probability of knocking. The pressure rise rate was controlled, and the in-cylinder hot spots were reduced by the EGR system, which could suppress the occurrence of the pre-ignition in the hydrogen engine.

Guo et al. also provided a numerical study on the pilot injection conditions of a marine two-stroke lean-burn dual-fuel engine [3]. In this regard, notably, the global demand for clean fuels is increasing in order to meet the requirements of the International Maritime Organization of 0.5% global Sulphur cap and Tier III emission limits. Moreover, natural gas has begun to be popularized on liquefied natural gas ships because of its low cost and environmentally friendly. In large-bore marine engines, ignition with pilot fuel in the chamber is a proper way to reduce combustion variability and extend the lean-burn limit. However, the occurrence of knock limits the increase in power. Therefore, this paper investigated the effect of pilot fuel injection conditions on the performance and engine knocking of a marine two-stroke low-pressure dual-fuel engine. Engine simulations were performed under different pilot fuel parameters. The results showed that the average incylinder temperature, the average in-cylinder pressure, and the NO_x emissions gradually decreased with the delay of the pilot injection timing. Furthermore, the combustion situation gradually deteriorated as the pilot injection duration increased. A shorter pilot injection duration was beneficial for reducing NO_x pollutant emissions. Moreover, the number of pilot injector orifices affected the ignition of pilot fuel and the flame propagation speed inside the combustion chamber.

Liaposhchenko et al. [4] modeled the technological processes for a rectification plant in second-generation bioethanol production. Since fuels obtained from crude oil (as a non-renewable source) increase the amount of carbon dioxide in the atmosphere when burned, alternative energy sources are used worldwide. Therefore, the research aimed to study various technological modes at the rectification unit to produce fuel bioethanol from lignocellulosic biomass. The main goal was to solve the applied scientific problems of rational designs and technological optimizations to obtain boundaries of energy consumption to ensure that the quality of bioethanol is sufficient for a consumer. For this purpose, recent approaches for numerical simulation of chemical technological processes were applied to study the operating processes and to optimize technological parameters. The plant model was designed from various modules that allow us to simulate technological processes efficiently and accurately for all the primary units of the rectification equipment. The methodology based on the phase equilibrium was applied. As a result, a mixture with 74% of bioethanol and 9% of impurities was obtained in the brew column. Moreover, in the epuration column, a mixture of 46% bioethanol and 2.2% impurities was obtained in the bottoms. Finally, in the alcohol column, the mass fractions of distillate of 96.9% and impurities of 2.7% were reached. The obtained results allowed solving applied scientific problems with respect to technological optimization and rational designs to evaluate energy

consumption in bioethanol production. As a result, a range of heating steam consumption was evaluated to provide the heat and mass transfer processes of bioethanol concentration.

A comparison of ethanol, methanol, and butanol blending with gasoline and its effect on engine performance and emissions using engine simulation was provided by Iliev [5]. The problem is also topical because air pollution is associated with serious problems both with respect to people's health and the environment. In this regard, over the past few years, there has been particularly intense demands for alternatives to fossil fuels because of the effects that have resulted when these fuels are burned. Additionally, with respect to the smoke from fuels burned for heating and harmful emissions that industrial installations release, exhaust emissions from vehicles create a large share of fossil fuel pollution. Alternative fuels are derived from resources other than fossil fuels. Because alcoholic fuels have several physical and propellant properties that are similar to gasoline, they can be alternative fuels. Therefore, the study aimed to develop a gasoline engine model to predict the influence of different alcohol-blended fuels on performance and emissions. For this study, the particular software was used to analyze the characteristics of the gasoline engine when operating with different mixtures of ethanol, methanol, butanol, and gasoline. The obtained results from different fuel blends showed that when alcohol blends were used, brake power decreased, brake-specific fuel consumption increased compared to gasoline use, and CO and HC concentrations decreased as the fuel blend's percentage increased.

A very important renewable fuel is wood biomass, which has been used for energy since the earliest cavemen made wood fires for cooking or for generating heat. Biomass is the only renewable carbon-based fuel. Combustion is currently the most common way to obtain energy from biomass. For this purpose, wood pulp is used, particularly as a piece of wood or in the form of wood chips. However, several factors affect the biomass combustion process. Vitázek et al. studied the thermal decomposition of wood chips from an apple tree in a static air atmosphere under isothermal conditions [6]. The results of the study have shown that this process can be described by the rate of the first-order chemical reaction, but the designed reaction model is valid only for a temperature range of 250–290 °C mainly due to lignin decompositions. Nevertheless, the obtained kinetic parameters could be used for the optimization of the combustion process of wood chips in small-scale biomass boilers.

The formation of particulate matter and gaseous emissions during biomass combustion is influenced by many aspects. One of these aspects is how much combustion air needs to be supplied to the heat source during combustion and how to redistribute it. Therefore, the performance and emission parameters determined using different distributions of the amount of combustion air of the wood stove with beech wood as a fuel have been studied by Holubčík et al. [7]. Eighteen different settings with primary, secondary, and tertiary air supplies were realized. Heat output, efficiency, particulate matter, carbon monoxide, and nitrogen oxides were measured or determined. Based on the analysis of gaseous emissions (CO and NO_x), it was found that using the setting with a ratio of 25/50/25(primary/secondary/tertiary) air supplies could be the best in terms of achieving suitable efficiency and heat power. However, the PM concentration using this setting reached a higher value.

Combustion processes are complex and, from a control point of view, strongly nonlinear. Their measurements generate complex data that require proper analyses for further designing prediction and control systems. A novel feature extraction and validation technique for the data-driven prediction of oxy-fuel combustion emissions in a bubbling fluidized bed experimental facility was studied by Marzova and Bukovsky [8]. The experimental data were analyzed and preprocessed to minimize the size of the data set while preserving patterns and variances and to find an optimal configuration of the feature vector. The Boruta Feature Selection Algorithm (BFSA) was used for mapping between available measurements (features) and emissions (outputs), and it found the feature vector's configuration. The Multiscale False Neighbours Analysis (MSFNA) has been newly extended and proposed to validate the BFSA's design for emission prediction to assure minimal uncertainty in mapping between feature vectors and corresponding outputs. The combination of conventional BFSA with MSFNA appeared to be capable of clearly validating and proposing a proper sampling period that is computationally difficult with a standalone BFSA.

Advanced control strategies for biomass combustion systems can guarantee good combustion conditions using controlled variables such as feed temperature and the residual oxygen content of the flue gas. In addition, online fuel characterization as a part of process control could help optimize combustion processes, increase fuel flexibility, and reduce emissions. A concept of a new sensor module for identifying fuel properties using the principle of hot air convective drying was presented by Meiller et al. [9]. The idea is to pass warm air with 90 °C through a bulk of fuel such as wood chips and to measure different characteristics such as moisture, temperatures, and pressure drop over the bulk material as a function over time. These functions form the basis for drawing conclusions and for estimating relevant fuel properties, which would allow the biomass combustion control system to adjust the speed of the fuel input, the amount of combustion air, or the speed of grate motion in such a way that optimized operation of the biomass boiler is possible. This will contribute to the better utilization of the existing potential in the field of biogenic solid fuels. The concept is also interesting for other processes, such as gasification or pyrolysis, or could be part of the fuel quality's management process.

The possibility of the efficient control of small- and medium-scale biomass-fired boilers by implementing low-cost sensors to sense the trend of carbon monoxide emissions when controlling biomass combustion processes was studied by Mižáková et al. [10]. Based on the theoretical analysis, a block diagram of the principles of the process control system was designed to provide the near-optimal control of biomass combustion regardless of its quality parameters. A cost-effective hardware solution to obtain the dependence of CO emissions on O₂ concentration in flue gas during combustion and new control algorithms have been implemented into the process control and monitoring system of the biomassfired boilers to test them in real operations. The designed and tested control algorithms use information about the trend of CO emissions in the flue gas to continuously evaluate the dependence of these emissions on the O_2 concentration. In this manner, the proposed and verified control of the biomass combustion process with the aim of keeping the O_2 concentration as low as possible (to reach low flue gas energy losses) successfully ensured an important condition for the quality of the combustion process that CO emissions do not exceed the permitted values for small and medium biomass-fired boilers. This was achieved for the parameters of wood chips: moisture content at 35–45% and size of 35–40 mm. The implemented control system and algorithms have even been able to ensure the required combustion quality of wood chips with a moisture content of up to 50% and for different types of wood: fir, beech, and oak.

Overall, novel approaches have been developed in computational modeling and advanced control to address longstanding challenges in increasing energy efficiency and decreasing environmental pollution arising from renewable fuel combustion.

Author Contributions: Conceptualization, J.P. and I.P.; methodology, J.H.; validation, J.P., J.H. and I.P.; formal analysis J.H.; investigation, J.P. and I.P.; resources, J.H.; writing—original draft preparation, I.P.; writing—review and editing, J.P.; supervision, J.H.; project administration, J.H. and I.P; funding acquisition, J.P. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the Slovak Research and Development Agency under the contract No. APVV-15-0602; by the Ministry of Education, Youth and Sports under OP RDE grant number CZ.02.1.01/0.0/0.0/16-019/0000753 "Research centre for low-carbon energy technologies"; and by the project VEGA 1/0704/22 granted by the Ministry of Education, Science, Research and Sport of the Slovak Republic.

Data Availability Statement: Not applicable.

Acknowledgments: The scientific results have been partially obtained within the research project "Creation of new granular materials for nuclear fuel and catalysts in the active hydrodynamic environment" (state reg. no. 0120U102036), ordered by the Ministry of Education and Science of Ukraine.

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

References

- 1. Saffari Pour, M.; Hakkaki-Fard, A.; Firoozabadi, B. Numerical Investigation of a Portable Incinerator: A Parametric Study. *Processes* **2020**, *8*, 923. [CrossRef]
- 2. Guo, H.; Zhou, S.; Zou, J.; Shreka, M. A Numerical Investigation on De-NOx Technology and Abnormal Combustion Control for a Hydrogen Engine with EGR System. *Processes* 2020, *8*, 1178. [CrossRef]
- Guo, H.; Zhou, S.; Zou, J.; Shreka, M. A Numerical Study on the Pilot Injection Conditions of a Marine 2-Stroke Lean-Burn Dual Fuel Engine. *Processes* 2020, *8*, 1396. [CrossRef]
- Liaposhchenko, O.; Marenok, V.; Skydanenko, M.; Pavlenko, I.; Ochowiak, M.; Mižáková, J.; Pitel', J.; Storozhenko, V.; Smyrnov, V.; Shmatenko, V. Modeling of Technological Processes for a Rectification Plant in Second-Generation Bioethanol Production. *Processes* 2021, 9, 944. [CrossRef]
- 5. Iliev, S. A Comparison of Ethanol, Methanol, and Butanol Blending with Gasoline and Its Effect on Engine Performance and Emissions Using Engine Simulation. *Processes* **2021**, *9*, 1322. [CrossRef]
- Vitázek, I.; Šotnar, M.; Hrehová, S.; Darnadyová, K.; Mareček, J. Isothermal Kinetic Analysis of the Thermal Decomposition of Wood Chips from an Apple Tree. *Processes* 2021, 9, 195. [CrossRef]
- Holubčík, M.; Čajová Kantová, N.; Jandačka, J.; Čaja, A. The Performance and Emission Parameters Based on the Redistribution of the Amount of Combustion Air of the Wood Stove. Processes 2022, 10, 1570. [CrossRef]
- Marzova, K.; Bukovsky, I. Feature Selection and Uncertainty Analysis for Bubbling Fluidized Bed Oxy-Fuel Combustion Data. Processes 2021, 9, 1757. [CrossRef]
- 9. Meiller, M.; Oischinger, J.; Daschner, R.; Hornung, A. Development of a New Sensor Module for an Enhanced Fuel Flexible Operation of Biomass Boilers. *Processes* **2021**, *9*, 661. [CrossRef]
- Mižáková, J.; Pitel', J.; Hošovský, A.; Pavlenko, I.; Ochowiak, M.; Khovanskyi, S. Biomass Combustion Control in Small and Medium-Scale Boilers Based on Low Cost Sensing the Trend of Carbon Monoxide Emissions. *Processes* 2021, 9, 2030. [CrossRef]