

Article

Combustion of Fuel Surrogates: an application to gas turbine engines

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Abstract: The previously developed models for fuel droplet heating and evaporation processes, mainly the Discrete Multi Component Model (DMCM), and Multi-Dimensional Quasi-Discrete Model (MDQDM) are investigated for the aerodynamic combustion simulation. The models have been recently improved, and generalised for a broad range of bio-fossil fuel blends so that the application areas are broadened with increased accuracy. The main distinctive features of these models are that they consider the impacts of species thermal conductivities and diffusivities within the droplets to account for the temperature gradient, transient diffusion of species and recirculation. A formulation of fuel surrogates is made, using the recently introduced model, referred to as “Complex Fuel Surrogate Model (CFSM)” and analysing their heating, evaporation, and combustion characteristics. The CFSM is aimed to reduce the full composition of fuel to a much smaller number of components based on their mass fractions, and to formulate fuel surrogates. Such approach has provided a proof of concept with the implementation of the developed model into a commercial CFD code ANSYS-Fluent. A case study is made for the CFD modelling of gas-turbine engine using kerosene fuel surrogate. The surrogate is proposed using the CFSM. The model is implemented into ANSYS-Fluent via a user-defined function to provide the first full simulation of the combustion process. Detailed chemical mechanism is also implemented into ANSYS Chemkin for the combustion study.

Keywords: Kerosene; CFD; Combustion; Fuel; Gas-turbine; Numerical analysis

1. Introduction

The energy demand is sharply increasing along with the increase in worldwide population and global fossil fuel consumption. This demand is expected to grow at an average annual growth rate of around 1% [1]. Currently, more than 99% of the transport sector is powered by combustion engines, which contribute to around 14% of Greenhouse Gas Emissions (GGE) [1,2]. Due to the depletion of fossil fuels, governments and industries are aiming to shift from the dependency on fossil fuels to renewable energy sources (e.g., biofuels) [3–5]. The use of mixture of biofuels (e.g., biodiesel and ethanol) with fossil fuels in standard propulsion systems can reduce GGE and lead to complete combustion [6]. According to the US environment protection agency, all gasoline engine vehicles can use a blend of gasoline fuel with up to 10% volume fraction of ethanol without the need for engine modification [7]. The reduction in CO₂ emissions without loss of engine performance is noticeable for this mixture [8]. According to the European Renewable Ethanol Association, replacing the European gasoline with a mixture of 10% ethanol and 90% gasoline (known as E10) would reduce the GGE by 6% [9]. Mixtures with up to 15% of ethanol

and 85% of gasoline fuel have been approved for use in 2001 and newer vehicles, under the U.S. federal standards for renewable fuel [10]. Unsurprisingly, this increase in the ethanol content in the baseline fuel would reduce the GGE even further. For diesel fuel, it is known that mixtures with up to 85% diesel and 15% ethanol are used in standard diesel engines without significant impacts on these engines [11]. Also, it has been reported in [12] that ethanol can be blended with diesel fuel at up to 20% ethanol.

Based on scientific ground of the applicability of bio-fossil fuel blends in conventional gasoline and diesel engines [13], governments set targets for the use of biofuels by increasing their fractions in the baseline fuel (gasoline and diesel). According to the UK Department for Transport, the British Government has legislated a new policy for increasing the percentage of bio/fossil fuel blends from 4.75% in 2018 to 9.75% in 2020 and to 12.4% in 2032 to achieve its obligations regarding reducing the GGE by 6% by the end of 2020 [14]. Recently, the US administration gave approval for the compulsory use of E15 [15].

The importance of the multi-component fuel droplets heating and evaporation processes has been highlighted in literature [13,16,17]. These processes precede the onset of ignition, and play an essential role in the performance of engines due to their very short time before the ignition of the air/fuel mixture [18]. Incomplete combustion and high levels of pollutant are expected when the fuel is not well mixed with air and completely evaporated. As such, understanding these processes is crucial to the design and optimum operation of engine. Different models were developed for the simulation of multi-component fuel droplet heating and evaporation [19–22]. In most cases, the modelling of heating and evaporation of multi-component droplets were represented by single components, for instance gasoline was represented by iso-octane [23] and diesel was represented by n-dodecane [24,25]. These approaches were based on two assumptions: 1) the effect of species diffusion inside droplets during the evaporation process and 2) the effect of finite thermal conductivity with droplets could be ignored. Most of these studies (e.g. [26,27]) relied on these assumptions to reduce the model complexity and the computational cost (CPU time).

The importance of considering the effect of species diffusion inside droplets and finite thermal conductivity was highlighted in many studies and they were modelled using the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) models [28–30]. The importance of the latter models was represented by the fact that they considered the recirculation, temperature gradient and species diffusion inside droplets. Recent models were developed to consider ETC/ED models including the Discrete Multi-Component Model (DMCM), Quasi-Discrete Model (QDM) and Multi-Dimensional Quasi-Discrete Model (MDQDM). The combustion studies were always based on the approximation of the composition of a fuel by certain number of components to match the real combustion characteristics of the fuel [31,32]. These approximations, commonly known as fuel surrogates, were mainly used due to the unavailability of the chemical mechanisms of many components and the lack of the computational resources. Although fuel surrogates were good representatives of the real fuel composition in terms of their chemical behaviour, these surrogates might not be able to match the physical characteristics of that fuel.

2. Fuel composition

In this analysis, kerosene fuel surrogate is inferred from [33], and formulated using the complex fuel surrogate model in [34]. The formulated surrogate is then compared with the kerosene surrogate provided in the commercial CFD software tool ANSYS-Fluent. The suggested surrogate is examined in terms of heating and evaporation using the implemented CFSM into ANSYS-Fluent via the User-Defined Function (UDF). Finally, the ignition time delay of the suggested surrogate is predicted and compared to those of the fuel composition of kerosene and ANSYS kerosene suggested surrogate. The Complex Fuel Surrogate Model (CFSM), which has been discussed and presented in detail in earlier

studies (e.g., [34,35]), was used for the formulation of kerosene surrogate. The composition of the full kerosene is shown in Table 1.

Table 1. Molar fractions of kerosene fuel, inferred from [36].

Carbon no	n-alkanes	iso-alkanes	cycloalkanes/olefins	alkylbenzenes	naphtobenzenes	diaromatics
C7	0.19	0.23	0.17	0.09	-	-
C8	0.19	0.39	0.63	0.61	-	-
C9	0.49	1.72	2.38	1.56	0.22	-
C10	0.70	4.09	5.83	2.72	1.06	0.09
C11	0.75	5.33	6.93	2.19	1.81	0.25
C12	1.15	6.67	7.40	3.00	3.48	0.3
C13	0.87	5.06	4.49	2.91	0.9	0.06
C14	0.89	5.14	3.78	1.74	0.24	-
C15	0.57	5.63	1.67	0.35	-	-
C16	0.05	2.11	0.74	-	-	-
C17	-	-	0.48	-	-	-
Total %	5.84	36.09	34.52	15.16	7.70	0.7

The composition shown in Table 1 was investigated in terms of heating and evaporation using the DMCM. The CFSM was then used to generate a surrogate for the kerosene fuel. The CFSM was limited for 2 Approximate-Discrete Components (ADC) (i.e. the generated surrogate consisted of two components only). This limit in the number of components was because the generated surrogate was later used for combustion studies using detailed chemical mechanisms. The two generated ADC were iso-decane ($C_{10}H_{22}$) and cyclododecane ($C_{12}H_{24}$), with fractions of 0.534 and 0.466, respectively. These two components with their fractions represent the suggested surrogate for kerosene. The evolutions of droplet diameter for the suggested surrogate, using the CFSM, were compared with the predictions of the Multi-Dimensional Quasi-Discrete Model (MDQDM) and DMCM (Figure 1). For this comparison, a single droplet was considered using some typical gas turbine conditions. The initial droplet diameter and temperature were 100 μm and 375 K, respectively. The ambient gas temperature and pressure were 800 K and 4 bar respectively.

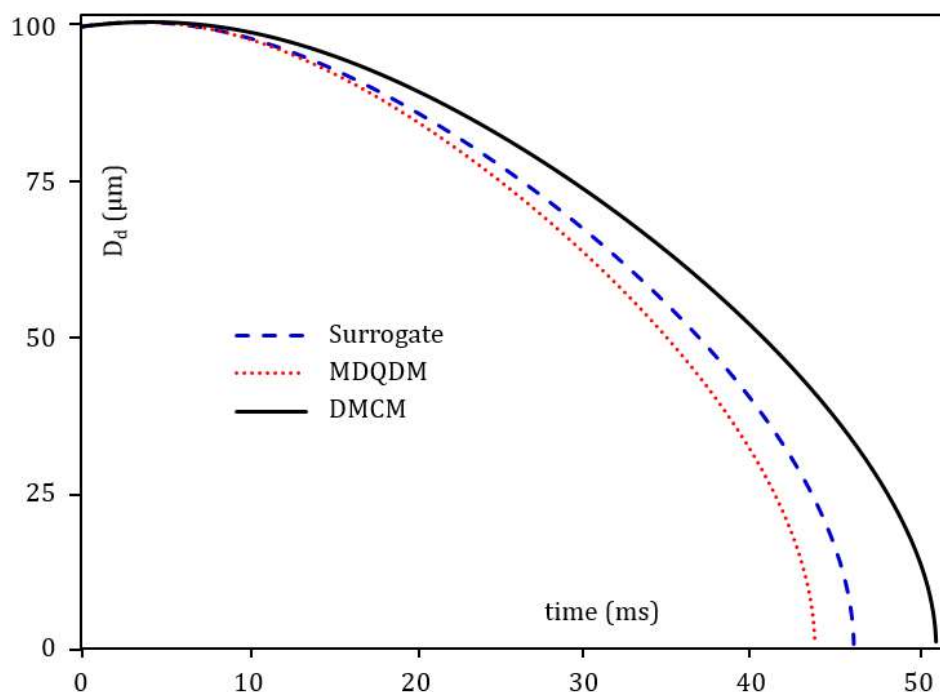


Figure 1. The droplet evaporation versus time for kerosene using the DMCM, MDQDM and surrogate (CFSM).

Compared to the full composition, the suggested surrogate shows 7.6% deviation. This deviation can be well reduced if only one extra component was considered for the surrogate. For the implementation and combustions studies, however, this deviation is acceptable in order to maintain no more than two components.

The Materials and Methods should be described with sufficient details to allow others to replicate and build on the published results. Please note that the publication of your manuscript implicates that you must make all materials, data, computer code, and protocols associated with the publication available to readers. Please disclose at the submission stage any restrictions on the availability of materials or information. New methods and protocols should be described in detail while well-established methods can be briefly described and appropriately cited.

3. Combustion analysis

The main reason behind the implementation of the DMCM model into ANSYS-Fluent is due to the fact that the latter software tool does not take into account several factors for the droplet heating and evaporation, e.g. temperature gradient, diffusion of species, and internal recirculation inside moving droplets. Instead, it is based on the assumption that all these factors can be ignored. The reasons behind these simplifications were discussed in Chapter 2. The work presented in [37] was the first work that investigated the implementation of a model for droplet heating and evaporation by accounting for the temperature gradient inside the droplet. The work of [37] was for mono-component. This work was then generalised in [38] to the case of binary-components in which the diffusion of species were also considered, combined with the temperature gradient inside the droplet. The latter work, however, was conducted for cooling evaporation in which the droplet was left in the ambient for evaporation. Furthermore, no full evaporation was observed.

In this proof-of-concept work, the thesis finding of CFSM was implemented into a commercial CFD code with an attempt to simulate the gas turbine combustion processes. A detailed analysis of the heating and evaporation of the generated kerosene fuel surrogate was implemented into the 3D CFD model. The implemented heating and evaporation model takes into account the temperature gradient, species diffusion and recirculation inside droplets. Such an approach is the first of its kind for any former literature work. This

was done via the implementation of the DMCM into ANSYS-Fluent using the UDF. The heating and evaporation were assumed to take place in a can type combustor. The computational domain and polyhedral mesh used for the hydrodynamic model are shown in Figure 2.

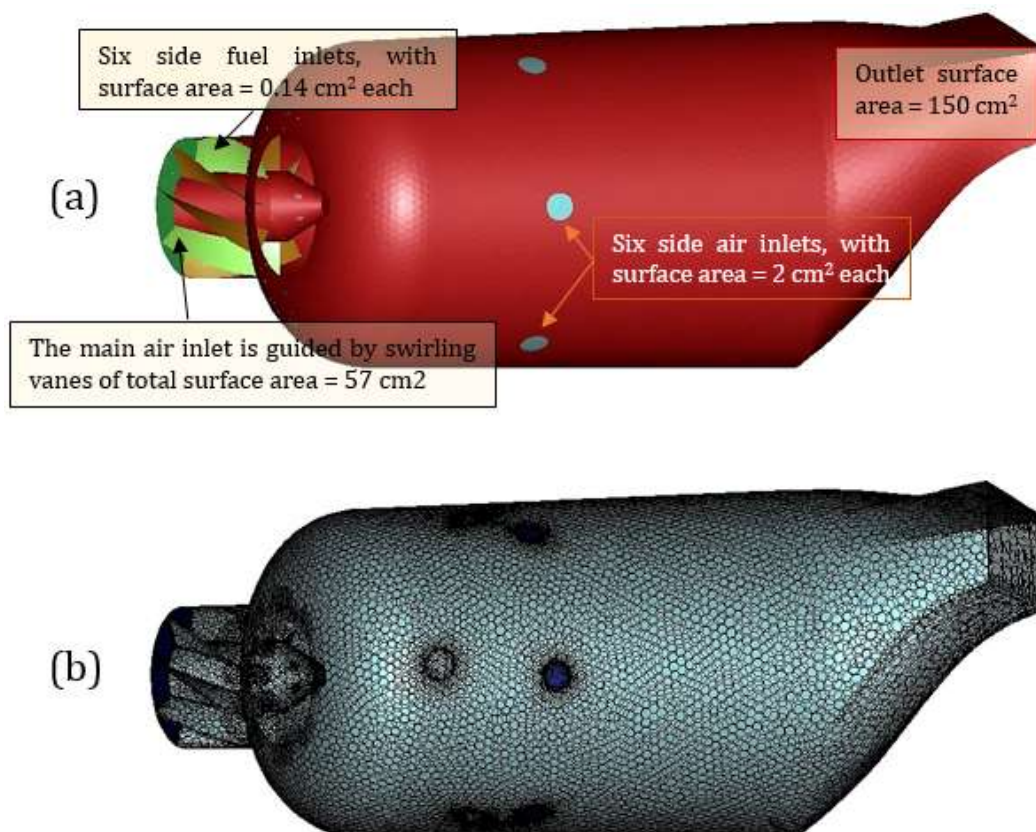


Figure 2. The can combustor geometry, showing (a) the internal walls of the system, and (b) the polyhedral mesh, used in the CFD simulation. The cell volume range is 0.0057647 – 470 mm³, the face cell area range is 0.014 – 8 mm², and the total number of cells is 262,255.

The droplet lifetime predicted by the new ANSYS CFD model was assessed in comparison to the original in-house code for a 100 μm diameter droplet moving into stationary air at $U_d = 1 \text{ m} \cdot \text{s}^{-1}$. The initial fuel temperature was $T_o = 375 \text{ K}$ under the ambient air temperature and pressure of $T_g = 800 \text{ K}$ and $p_g = 4 \text{ bar}$, respectively. In Figure 71, the evolution of droplet diameter with time is presented using three approaches: 1) the results predicted by standard ANSYS-Fluent software using constant properties; 2) the results predicted by ANSYS-Fluent and transient properties of fuel components using the UDF, but without the CFM; and 3) ANSYS-Fluent results with full implementation of the CFM and transient thermodynamic and transport properties.

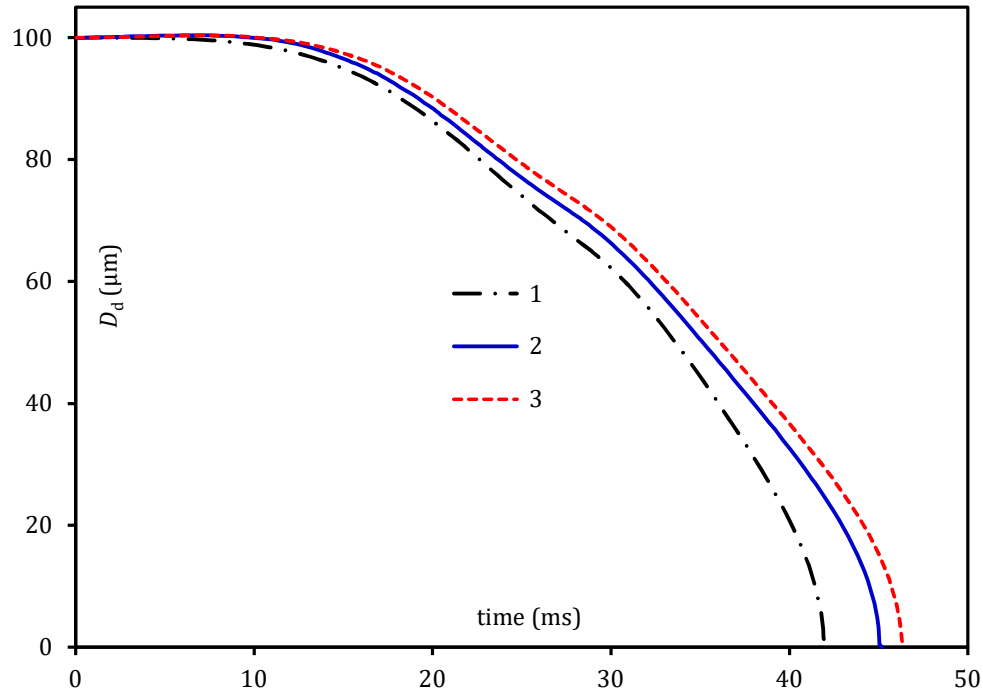


Figure 3. The evolutions of droplet diameter using the three modelling approaches: 1 refers to Standard ANSYS-Fluent results, with constant properties, 2 refers to ANSYS-Fluent results, with in-house properties using UDF, and 3 refers to ANSYS-fluent results incorporating the CFM using UDF.

As follows from Figure 3, the incorporation of the DMCM into ANSYS-Fluent leads to prediction of up to 10.4% longer evaporation times compared to the case when the standard ANSYS-Fluent model is used. A contour of the droplet evaporation inside the can combustor is shown in Figure 4. As can be seen from that figure, all droplets are injected at a diameter of 100 μm , and all these droplets are evaporated at around a distance of 40% of the injection point. The results validating ANSYS-Fluent simulation that incorporated the new model is presented in Figure 5. The validation was done by comparing the computed results with experimental data reported in the literature [39]. This was based on a kerosene droplet with initial diameter 1.8 mm and initial temperature 298 K. The droplet was exposed to an air flow rate of 20 L/min at 0.1 MPa ambient pressure. As can be seen from Figure 5, there is a general agreement between the numerical results and experimental data. In CFM analyses, the effect of thermal swelling on droplet heating and evaporation was taken into account.

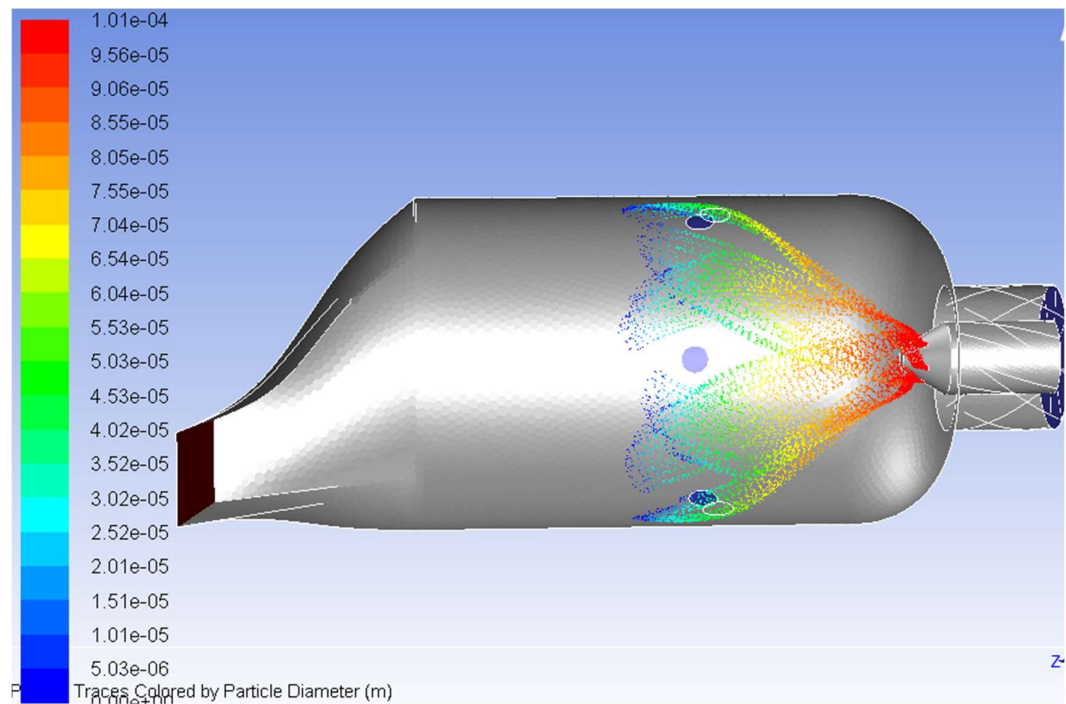


Figure 4. Profile of droplet diameter starting from the injection until the full evaporation.

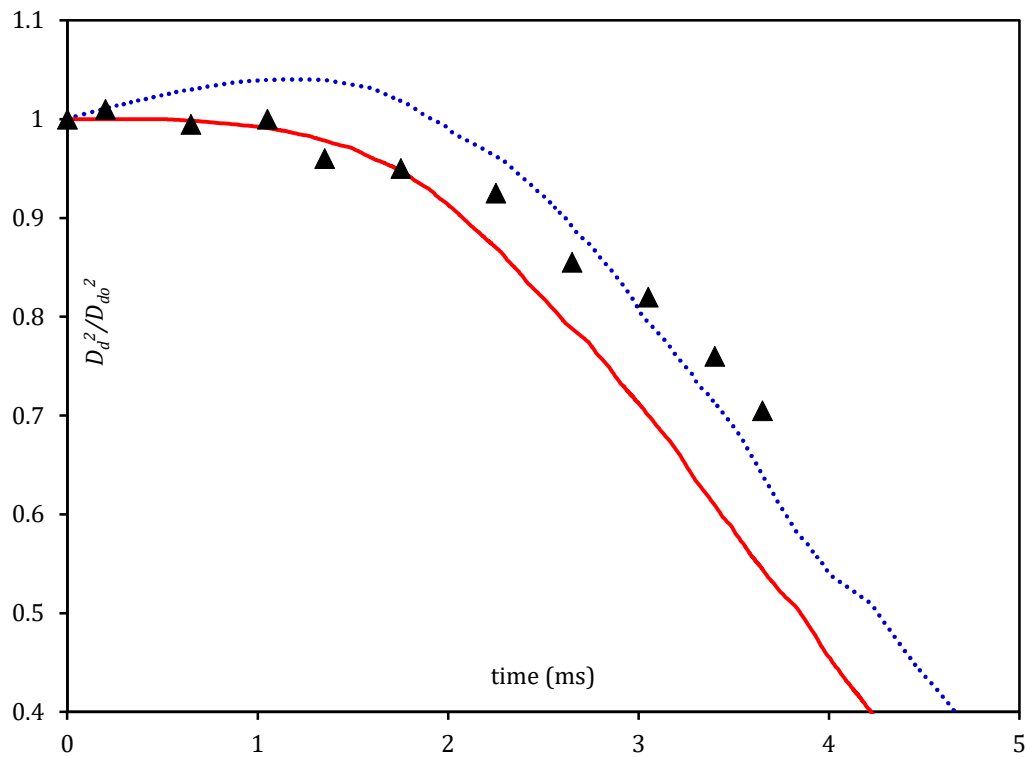


Figure 5. The validation of the models for the normalised squared droplet diameters predicted by the standard ANSYS-Fluent (solid curve), and ANSYS-Fluent incorporating the CFM (dotted curve), using data reported in [39] (bold triangles) for kerosene fuel.

4. Pre-combustion Analysis

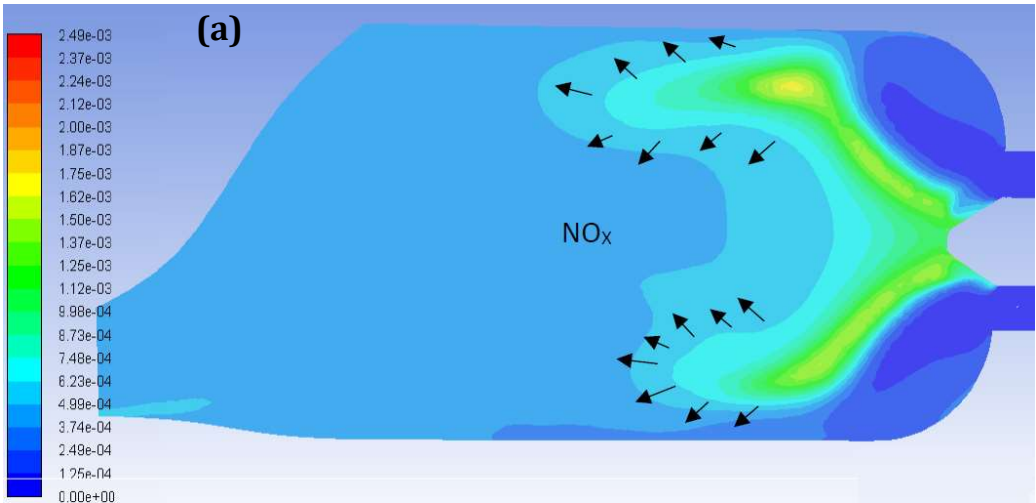
The combustion characteristics of the suggested surrogate (53.4% iso-decane and 46.6% cyclododecane) was also compared with the simulated results of a suggested kerosene surrogate in ANSYS. The latter surrogate consists of one hypothetical component (C₁₂H₂₃) which does not exist in real life. The combustion of the surrogates was investigated based on the partially premixed combustion model with FGM state relation for diffusion flamelet and a non-adiabatic system. A co-axial air-blast atomizer was used with primary and secondary air and fuel mass flowrates of 0.15, 0.025 and 0.003 kg/s, respectively. The main input parameters for the simulation are presented in Table 2.

Table 2. The input parameters used for the combustion simulation.

Parameter	Value	Unit
Primary injection air velocity	10	m/s
Secondary injection air velocity	6	m/s
Fuel mass flowrate	0.003	Kg/s
Ambient pressure	4	Bar
Air Temp	293	K
Fuel Temp	375	K
Oxidation Temp	800	K

A realizable $\kappa - \varepsilon$ turbulence model was used for the hydrodynamic region with enhanced wall treatment. The combustion mechanism of iso-decane and cyclododecane (components of the suggested surrogate) were imported from [40]. The chemical mechanism of iso-decane and cyclododecane were merged together using ANSYS Chemkin. The resulting chemical mechanism of the two components, included 194 species with 1459 reactions. The domain pressure and velocity were coupled in a quasi-transient manner. The chemical reaction model showed homogeneous combustion. As can be seen from Figure 74, the entrainment of air flow enhances the oxidation of the mixture (suggested surrogate and air) with charge from the dilution holes. The NO_x and CO₂ are at a relatively low level, indicating well diluted fuel leading to complete combustion.

Further illustrations of the combustion species formation inside the can combustor, and at various sections along its length are provided in Figure 7.



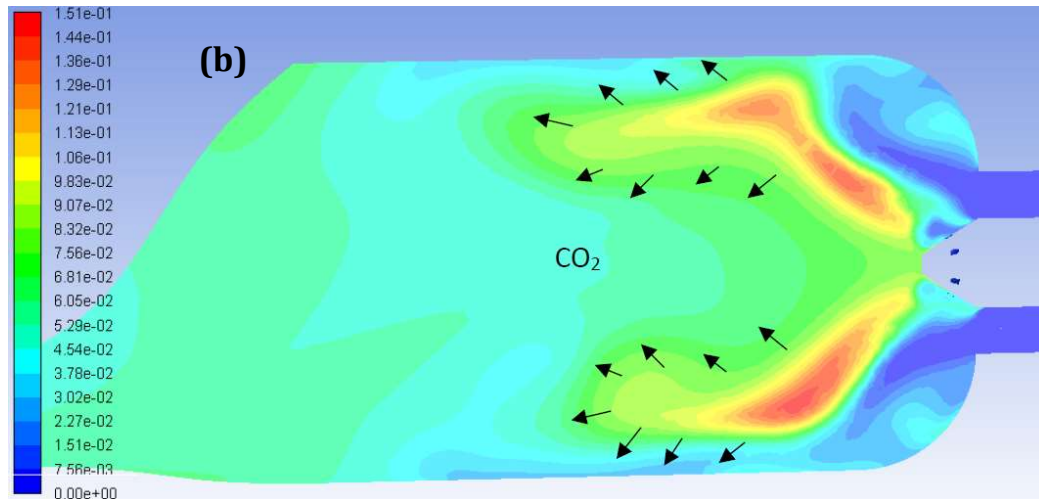
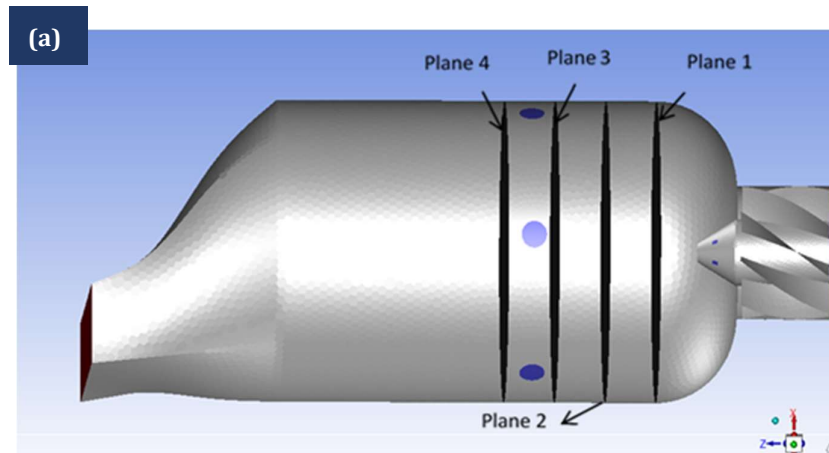


Figure 6. The species distribution, (a) NOX and (b) CO₂, at the symmetry plane of the combustion chamber using the suggested kerosene surrogate (53.4% iso-decane and 46.6% cyclododecane).

The above results were obtained for the suggested surrogate. The species distributions were also obtained for ANSYS kerosene surrogate. The distribution of NOX, and CO₂ are shown in Figure 8. Compared to Figure 7, it can be seen that the implementation of the detailed combustion chemistry of the suggested kerosene surrogate leads to lower NOX, and CO₂. This is because the combustion chemistry of the ANSYS kerosene surrogate does not include a detailed species generated because of the combustion process. Instead, it includes 20 species only (N₂, O₂, C₁₂H₂₃, CO, CO₂, H₂O, H₂, C, OH, CH₄, H, O, HO₂, H₂O₂, HCO, CHO, NO, HOCO, C₂H₆ and HCOOH). Hence, the mass fractions of NOX, and CO₂ are higher than those of the suggested surrogate (using the CFSM) with the detailed combustion chemistry.



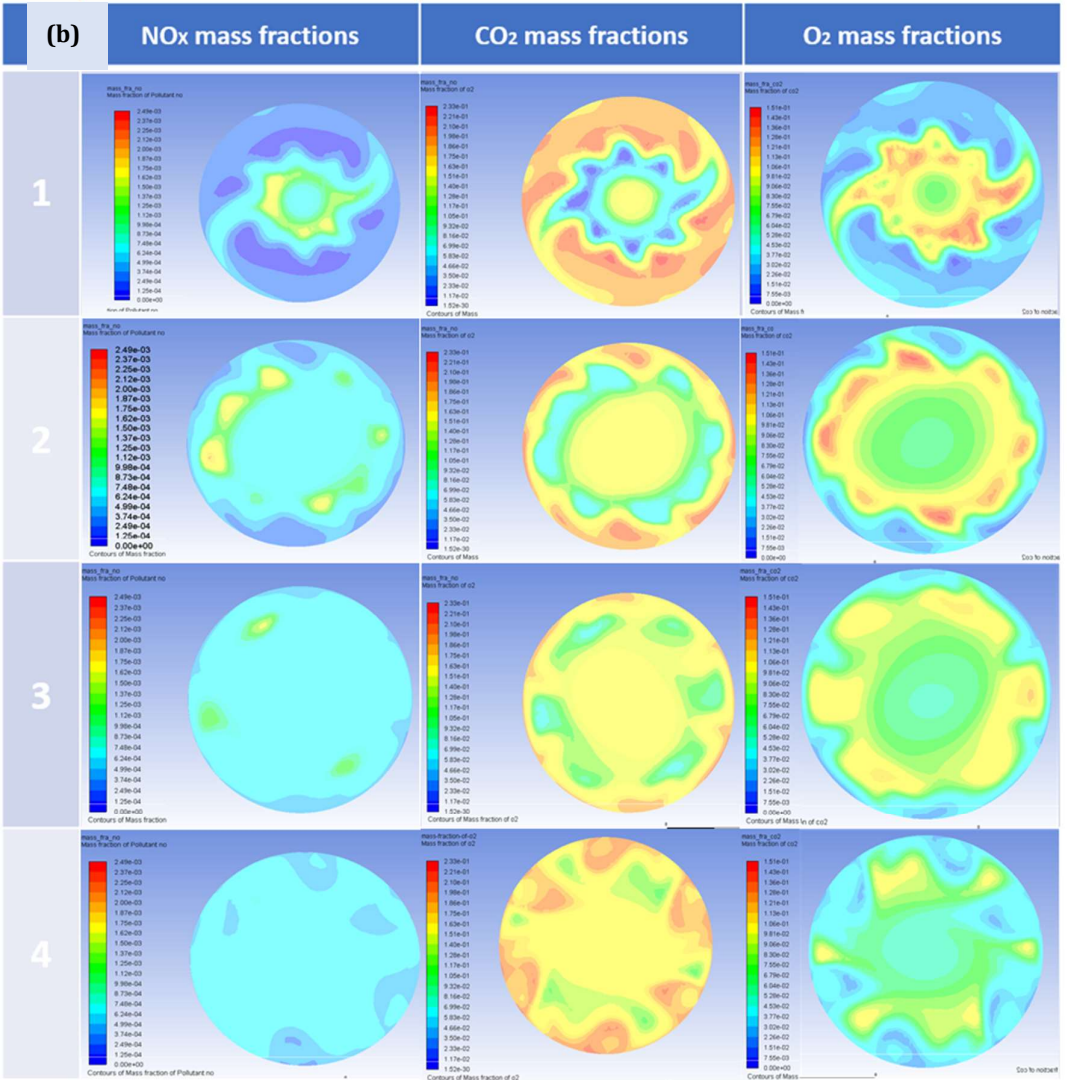
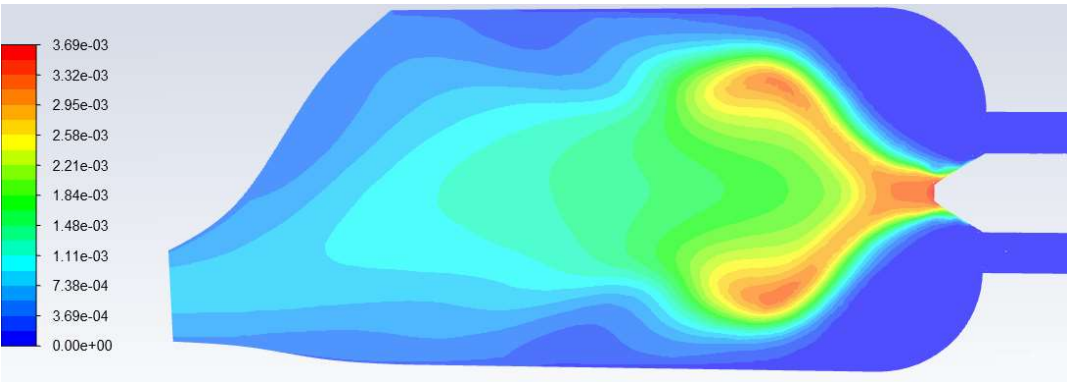


Figure 7. Species formation and distribution across the can combustor at four planes, showing (a) the four planes along the combustor, and (b) the profile contours for the four planes.



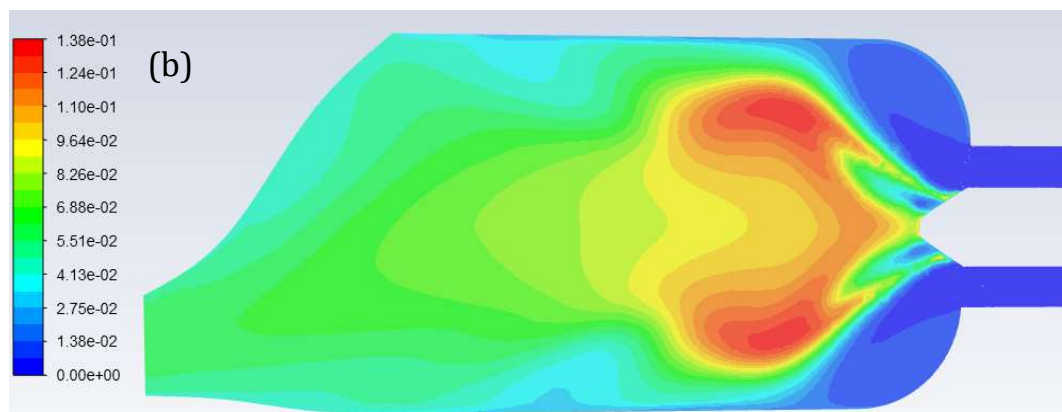


Figure 8. The species distribution, (a) NOX and (b) CO₂, at the symmetry plane of the combustion chamber using ANSYS kerosene surrogate (C₁₂H₂₃).

The Thermodynamic characteristics of the combustion process of the suggested surrogate and ANSYS surrogate are presented in Table 3. Noticeable difference between the two surrogates is observed. The thermodynamic characteristics of ANSYS surrogate are always higher because, in average, this surrogate is heavier than the suggested surrogate.

Table 3. Thermodynamic characteristics of the combustion process.

Parameter	ANSYS surrogate	Suggested surrogate
Total reaction heat (MJ/kg)	-4.99E+02	-4.03E+02
Internal Energy (MJ/kg)	3.11E+04	3.05E+04
Total enthalpy at the outlet (MJ/kg)	3.48E+02	3.41E+02
Evaporation enthalpy (MJ/kg)	-1.61	-1.473

The ignition time delays of kerosene surrogates were estimated at different combustion temperatures, pressures and equivalence ratios. The Arrhenius relationships of ignition time delay suggested in [41], for RP-3 kerosene, was used for the suggested surrogate (53.4% iso-decane and 46.6% cyclododecane) using the appropriate activation energy. The relationships can be expressed as [42]:

$$\tau_{\text{ign}} = 4.719 \times 10^{-3} P^{-0.72} \phi^{1.27} \exp\left(\frac{Ea}{RT}\right) \quad (1)$$

where P is the pressure in Pa, ϕ is the equivalence ratio (fuel/air ratio), Ea is the activation energy which is 134.68 kJ/mol, R is the universal gas constant in kJ/mol. K and T is the oxidation temperature in K. The ignition time delay of the suggested kerosene surrogate was compared to the full composition of kerosene fuel. The ignition time delay of the latter one was estimated based on a modified form of the Arrhenius relationships (using the appropriate activation energy), recommended for a multi-component kerosene of n-decane, n-dodecane, isocetane, methylcyclohexane and toluene with a molar fraction of 14%, 10%, 30%, 36%, 10%, respectively. Further details on this expression can be found in [42]:

$$\tau_{\text{ign}} = 6.824 \times 10^{-3} P^{-0.71} \phi^{1.59} \exp\left(\frac{Ea}{RT}\right) \quad (2)$$

The Ea for the kerosene fuel is 132.8 kJ/mole.

A comparison between the ignition time delay of the full composition of kerosene fuel and the two surrogates (suggested surrogate and ANSYS surrogate) is presented in Figure 9. The analysis is conducted at ambient pressure 4 bar, equivalence ratio 1 and oxidation temperature range 1000-1500 K. The prediction of the ignition time delays of the fuel and its suggested surrogate are very close at the high oxidation temperature. However, a significant difference is noticed at low oxidation temperature. To improve the predictions of the ignition time delay at low oxidation temperature, surrogate with higher number of components is possibly needed. The ignition time delay of the surrogate

suggested in ANSYS deviates significantly from that of the full composition of kerosene fuel. The main reason behind that deviation is that the activation energy of ANSYS surrogate is noticeably low (118 kJ/mole).

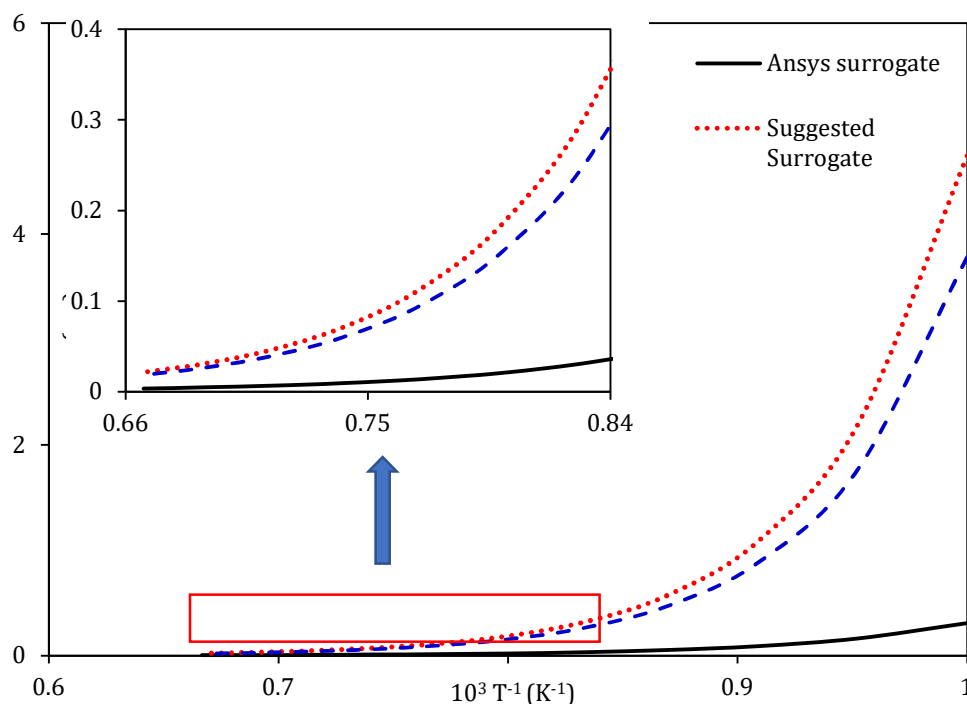


Figure 9. Ignition time delay of the full composition of kerosene fuel and its surrogates (suggested surrogate and Ansys surrogate) at pressure of 4 bar and equivalence ratio of 1.

Based on the results obtained above, one can say that formulated surrogates should include higher number of components (not only two as suggested) to improve the predictions accuracy. This vision can be true to a limited extent, since the chemical mechanisms are compatible for a wider range of components. If a certain fuel is represented by at least two components with reasonable component fraction, these two components can reproduce certain characteristics of that fuel with a negligible deviation. For example, representing kerosene fuel by n-hexadecane only will overpredict its evaporation time, while the evaporation time will be underpredicted if the kerosene fuel is represented by n-octane only. Therefore, using a mixture of the two components with appropriate distribution to their mass fractions may solve the problem. This will also reduce the computational cost significantly. Based on these justifications, the suggested surrogate, generated by the CFSM, consisted of two components in this chapter.

5. Conclusions

The Complex Fuel Surrogate Model (CFSM) was used to generate surrogate for kerosene fuel. A heating and evaporation model including the suggest surrogate was then implemented into ANSYS-Fluent for verification. The combustion of the suggested surrogate was also investigated based on partially premixed combustion model. The chemical mechanism of 194 species with 1459 reactions was implemented into the CFD code. The ignition time delay of the suggested surrogate was compared to those of the surrogate suggested by ANSYS and the full composition of kerosene fuel. Results proved that the customised version of ANSYS-Fluent including the implemented model showed close agreement with experimental data. This was attributed to the physics inside droplet that the implemented model considered which were the temperature gradient, recirculation and mainly species diffusion. The generated surrogate, using the CFSM, showed closer

predictions for the ignition time delay to the full composition of kerosene fuel than that of the surrogate suggested by ANSYS. It was demonstrated through simulations in this chapter that surrogate of at least two components can capture the actual characteristics of the real fuel if there was an appropriate distribution to the mass fraction of these two components. This will have substantial influence in terms of the computational efficiency.

Author Contributions: Conceptualization, M.A.Q.; methodology, M.A.Q.; software, M.A.Q.; validation, H.S.S.; formal analysis, M.A.Q.; investigation, M.A.Q.; writing—original draft preparation, M.A.Q.; writing—review and editing, H.S.S.; All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Acknowledgments: The authors acknowledge resourcing the data via the direct and indirect contributions of the following colleagues: Professor S.S. Sazhin (University of Brighton), Dr O. Rybdylova (University of Brighton), Dr N.A. Al-Esawi (University of Northampton), and Mr G. Wang (UCL)

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

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