

CFD Modelling of Heavy Fuel Oil Spray Combustion

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Abstract

Global shipping uses Heavy Fuel Oil (HFO) as the primary fuel. HFO is a mixture of oil refinery residue and cutter stock, hence it contains large numbers of hydrocarbons with a wide range of molecular weights and dissimilar structures. Conventional thermodynamics modelling techniques are inadequate for HFO vaporisation modelling. The present article summarises continuous thermodynamics vaporization models along with chemical kinetics models for decomposition and polymerisation, and soot burnout models employed to study the behaviour of HFO spray combustion. Models are implemented via subroutines in a diesel spray simulation in the CFD package StarCD. The simulation is applied to a constant volume spray combustion chamber. The present model accounts for the formation and burnout of liquid phase soot in diesel engines. This soot will be emitted as Black Carbon if unburnt. The models are examined for two representative fuel samples. Good qualitative agreement is shown between the simulations and published experimental data.

Introduction

Maritime transportation is reliable, economical and energy efficient, and emits fewer greenhouse gases per tonne-km of goods than other forms of transport [1]. It uses Heavy Fuel Oil (HFO), a blended mixture of high viscosity refinery residue and more volatile, less viscous cutter stock [2]. Although HFO is the principal marine fuel, to date very little work has been conducted on modelling its vaporisation and combustion behaviour due to its chemical complexity. Most of the work found in the literature on the vaporisation of multicomponent fuels is based on binary component mixtures or up to ten discrete components [3]. In discrete components modelling, each component requires a separate transport equation, which needs to be solved at every time step requiring considerable computation power. An alternative approach is needed for complex multicomponent fuels such as HFO, such as the continuous thermodynamics technique, which represents the fuel components as a series of multi distribution Probability Density Functions rather than a series of discrete components [4, 5].

The present work examines the vaporisation, pyrolysis and surface oxidation processes of HFO spray combustion in marine diesel engines. The model builds on the previous semi-empirical model developed by Goldsworthy [2] with the aim of describing vaporisation and pyrolysis processes from first principles. The developed model should give insight into the various mass transport, chemical transformation and heat transfer processes within a diesel spray context. Emphasis in the present article is also given to modelling the heterogeneous oxidation of coke or in other words the formation of cenospheres, which is one of the contributors to Black Carbon or Soot Carbon [6, 7]. Ramanathan & Carmichael [8] postulated that Black Carbon may be a significant contributor to rising global temperatures because it absorbs solar energy in the atmosphere and reduces the albedo of snow (reflectivity). This reduction of snow albedo may be important in the Arctic where rapid climate change is occurring [9], and shipping access to the area will increase due to retreating sea ice.

Fuel combustion is a combination of many individual processes. According to Ikegami et al.[10] combustion process of HFO comprises of two main stages; Liquid (droplet) combustion and solid coke combustion. The liquid combustion stage is complicated as it includes many distinctive sub-stages such as; pre-ignition heating, vaporisation, thermal cracking (decomposition) and polymerisation. The solid coke combustion consists of the heterogeneous oxidation of coke residue. Baert [11] developed a simple vaporisation and pyrolysis model of HFO which predicts the formation of coke and pyrolysis gases. Baert's results demonstrated that asphaltene are the main source of coke formation. Takasaki et al.[12] studied the combustion characteristics of marine fuel oils with good and poor combustion characteristics. Their analysis showed that the poor fuel BFO-A contained lower amounts of (24%) saturated hydrocarbons than the good fuel BFO-S (31%), while aromatic hydrocarbons content was very high in the poor fuel (68%) compared to the good fuel (48%).

Model Development

This paper describes the application of previously developed low-pressure continuous thermodynamics vaporisation and chemical kinetic pyrolysis models [3, 4, 13] using CFD package StarCD v3.24, to carry out the spray combustion simulations of above mentioned good and poor fuels.

Fuel Models

When fuel is injected into the combustion chamber as a spray, heat transfer, phase change, chemical transformation and occur. These processes convert fuel liquid into volatile vapour and gases, which later on burn in the oxidising environment surrounding the spray. In CFD modelling these processes are critical because they control the overall performance of the combustion process. The processes used in simulation for a burning spray of HFO are summarised in Figure 1 and are shown in grey colour while their products and fuel are shown with white background colour.

As the liquid droplet enters the hot combustion chamber, heat transfer between the droplet and the hot surroundings occurs, and vaporisation starts. The more volatile light hydrocarbon molecules continuously vaporise in order of their volatility, leaving the less volatile molecules in the droplet [11]. As droplets are further heated, at sufficiently high temperatures the less volatile molecules (primarily from the heavy residue) decompose into free radicals. These free radicals can further decompose, either through cracking into small molecules, or recombination through polymerisation to form large molecules. Pyrolysis involves this simultaneous process of cracking and polymerisation, converting the heavy molecules into low molecular weight volatile compounds (containing up to C₁₀ atoms together with H₂O, H₂ and CO₂) and coke [11].

The weakest bonds of HFO begin breaking at around 625 K and consequently when the droplet reaches this temperature, the heavy molecules of the residual portion of HFO start decomposing [11]. Furthermore, as the temperature of a droplet approaches 650 K, non-volatile paraffinic and naphthenic

molecules also begin cracking into low molecular weight compounds. However, for a significant rate of thermal cracking, temperatures in excess of 800 K are needed. Chen & El-Wakil [14] showed that thermal cracking occurs during the initial stage (vaporisation) but it becomes more important when a droplet reaches 700 K and heavy molecules in the droplet start decomposing and forming volatiles. Thermal cracking results in a decrease in the molecular weight of the fuel, but only the non-aromatic (aliphatic) part of the molecules produces volatiles [11].

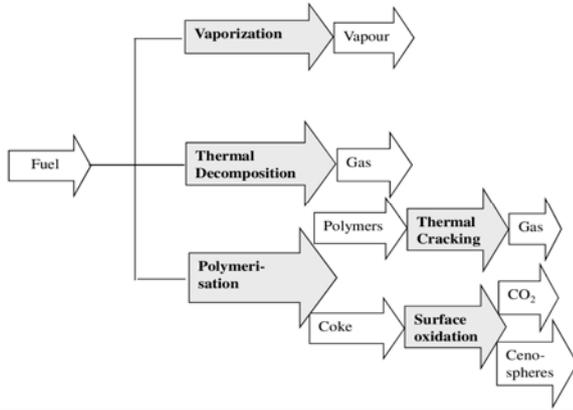


Figure 1: The processes of a burning droplet in a burning HFO spray.

Polymerisation of HFO usually starts around 840 K [10]. Thermal cracking reduces the large molecules in the fuel to their aromatic nuclei, which are very stable and begin to decompose at 1000 K. Most of these aromatic nuclei either evaporate or recombine to form polymers. Polymerisation combines the aromatic part of the molecules to form polymers. Hence it does not affect the mean molecular weight of the fuel [11, 13]. Polymer forms continuously during pyrolysis, but at the same time, the non-aromatic (aliphatic) part of the polymer undergoes further cracking due to high temperature. Eventually the remaining polymer becomes a coke residue.

As shown in Table 1, HFO is assumed to contain four chemical components; n-paraffins, aromatics, naphthenes and heavy residue. Each component (fraction) contains a range of species with different molecular weights which is represented by a gamma distribution function in the continuous thermodynamics approach. While the properties of n-paraffins, aromatics and naphthenes have been determined experimentally, little is known about the properties of the residue. The residue may have a higher molecular weight than is used in this modelling, as it consists mainly of asphaltenes and large aromatics. However it is less important to use an accurate distribution function for the residue since it evaporates negligibly. Overall, the present HFO sample is assumed to comprise of 30% cutter stock and 70% residue.

Table 1: Compositions of the good and poor fuel oils used in simulations.

Components	Mass Fractions		Mean Molecular weights
	Good fuel	Poor fuel	
n-Paraffins	0.15	0.05	340.00
Aromatics	0.05	0.15	300.00
Naphthenes	0.10	0.10	370.00
<i>Total Cutter</i>	0.3	0.3	
Residue	0.7	0.7	850.00

Raoult's law together with the Clausius-Clapeyron equation is used for the vapour-liquid equilibrium of light components. All the processes were implemented in the *drmast* subroutine of StarCD using FORTRAN code.

Soot Models

Mainly two types of emissions are reported in combustion studies, one originates in the liquid phase and another in the gas phase. The incomplete combustion of liquid droplets produces particles known as cenospheres, while gas phase soot results from chemical reactions of fuel vapour and pyrolysis gases in the fuel rich core of the spray [15].

Coke Burnout Model

At high temperatures when most of the volatile products of vaporisation and thermal cracking have left the droplet, the coke molecules begin to oxidise via heterogeneous surface oxidation which is referred to as the coke burnout phase. However, if insufficient oxygen is present or non-volatile compounds are formed within the droplet, then the liquid droplet (which includes original liquid and formed coke) cannot fully oxidise. This unoxidised residue is referred to as cenospheres [16], which are carbonaceous residues of the spray droplets containing voids [17]. The literature [14, 18] cites that coke burnout starts after the completion of vaporisation and pyrolysis. In other words; when the droplet mainly contains coke, which cannot be further decomposed. It is postulated here that heterogeneous surface oxidation (burnout) begins when the aromaticity of the liquid reaches 0.9 or more, and the droplet contains 95% coke (polymer). In the present simulation, StarCD's char burnout model for coal combustion was employed for the burnout of polymer.

Gas Phase Soot Model

The basic model utilised by Goldsworthy [2] for the gas phase soot formation and burnout was used. The production of soot in each computational cell is determined by the difference between the rates of soot formation and consumption.

Physical Properties of Liquid Fuel and Vapour

The overall density of HFO is taken as a function of composition [3]. The density of individual fractions is assumed to remain constant because while it increases with the increase in the mean molecular weight, at the same time it decreases with the increase in droplet temperature. However, the total density of HFO varies as the vaporisation of light fractions (n-paraffins, aromatics and naphthenes) occurs. The droplet temperature is increasing but its density and mean molecular weight are increasing. Thus, droplet viscosity is held constant at 15 mm²/s, which is representative of the viscosity at the point of injection for HFO [2]. Similarly, the surface tension coefficient is also taken constant as 0.04 N/m. The vaporisation enthalpy for the light components of HFO was simulated using the critical temperature relationship given by Garaniya [3], while the vaporisation enthalpy of the heavy component (residue) has not been determined experimentally, and the constant value of 232 kJ/kg used by Goldsworthy [2] was assumed. The residue cracks (decomposes) into volatile compounds and then these volatile compounds have to leave the droplet through vaporisation, hence this vaporisation enthalpy must be added to the decomposition enthalpy of the component [11]. In the present simulations, a similar approach to Baert [11] is employed, whereby 1000 kJ/kg is used for the combined enthalpy of decomposition and vaporisation. The mean specific heat capacities of the droplet components were simulated as a second order polynomial function of temperature for each of the four components. In StarCD when the droplet reaches its critical temperature it is assumed to evaporate completely and is removed it from the computation. The critical temperature of the entire droplet which is needed as an input in StarCD was set artificially high at 2000 K. This allows the droplet to remain in the computation and undergo surface oxidation. All properties of the vapour phase reactants and product molecules were adopted from the standard StarCD database excluding the LHV of fuel, which was set to the LHV of HFO by modifying the formation

enthalpy of the vapour scalar. All numerical relationships for the properties were developed in the *dropro* subroutine in StarCD.

Other Associated Models

Ignition delay is the main criterion for the ignition quality of fuels, and in HFO combustion it is determined by the quality of the cutter stock. Cutter stock containing paraffinic hydrocarbons has a shorter ignition delay than the cutter stock with aromatic hydrocarbons [2]. During the ignition delay, a flammable mixture of evaporated vapour and surrounding gas is formed. After ignition, this mixture burns very quickly giving rise to a sharp increase in ambient pressure. An ignition model similar to Goldsworthy's model was used for HFO. The combustion model provides the reaction rate subsequent to ignition. This appears in the source terms of the enthalpy and the species transport equations. A combined time model is used whereby the rate of combustion can be controlled either by turbulence, kinetics, or the combination of both [2]. The rate of combustion is also determined by the local concentration of fuel and oxidant. The Reitz & Diwakar atomization model for primary droplet breakup, the k-ε High Reynolds Number turbulence model and three dimensional grids as developed by Goldsworthy [2] were used.

Results and Discussions

Experimental data from a constant volume combustion chamber (CVCC) were compared with modelled results. This chamber was developed at Kyushu University in Japan and it is used to visualise the spray/flame and study combustion [12]. The visual chamber has a bore of 150 mm, greater than 275 mm length and is electrically heated. Optical windows provide a view of the full length of the spray. The CVCC provided the flame and spray observations. In the model, it is assumed that a higher percentage of paraffins in the cutter stock characterises a good fuel oil whereas a higher percentage of aromatics in the cutter stock characterises a poor fuel oil. Both good and poor fuel oils were assumed to contain 30% cutter stock and 70% residue and the compositions of their cutter stocks used in simulations are given in Table 1. In total 50% of the cutter stock in the good fuel oil is paraffinic so that the poor fuel contains 15% n-paraffins by mass. On the other hand, the cutter stock of the poor fuel oil contains 50% aromatics hence the poor HFO contains 15% aromatics by mass. Further, the combustion properties of the fuels were altered in the model by altering the ignition model settings and the activation energy for combustion.

Good Quality Fuel Oil

Figure 2 shows the CVCC simulation results for the good fuel oil from the present model compared with Takasaki et al.'s measured spray results for soot/spray and visual flame extent, at a consistent spatial scale. The BDL image is produced by backlighting the burning spray with diffuse light. The dark region represents the extent of unevaporated fuel and soot. Chamber pressure is 2.5 MPa and initial temperature 600K.

The present results show good quantitative agreement with both the modelled and the experimental results at 6 ms after the start of combustion, which is 9 ms after the start of injection. The ignition delay in the modelled fuel oil is determined as the time from the start of injection to the attaining of an ambient temperature of 1500 K or more. The ignition delay in the CVCC experiments was determined as the time from the start of injection to the first appearance of a bright flame.

Modelled soot formation in the present case is divided into two different mechanisms (coke and gas phase soot), and only the gas phase soot mass fraction and its consumption rate are shown in the figure. In the centre and towards the bottom of the spray, it appears that the droplets in that region are still undergoing pyrolysis and therefore absorbing energy from the surroundings, resulting in a lower temperature. The highest values of heat release rate shown in Figure 2 coincide with the high temperature region (2300-2500K). The unburnt/unevaporated droplets

apparent in the BDL image are (1) still pyrolysing forming coke (polymer) and volatile compounds, (2) coke burning through surface oxidation, (3) cenospheres remaining at the end of surface oxidation. The model results are qualitatively similar to the experimental results of Takasaki et al. The modelled flame penetration and flame lift-off length are similar to the measured results of Takasaki et al.

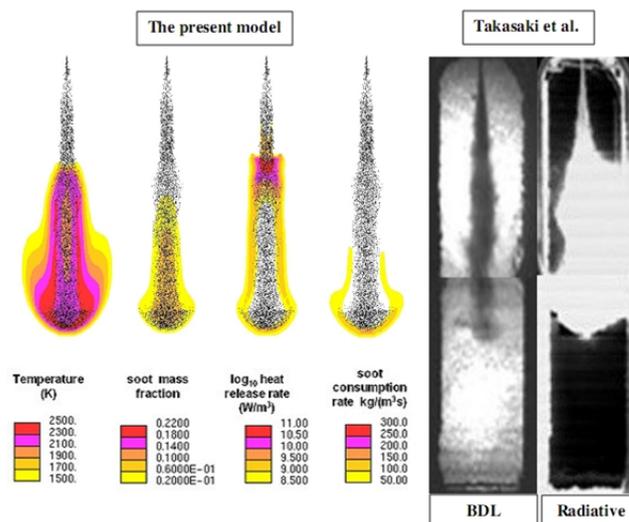


Figure 2: Comparison of the present model with Takasaki et al.'s measurements at 9 ms after start of injection.

Figure 3 shows the mass balance for a selected parcel in the burning fuel spray. A parcel represents a group of droplets having similar properties such as velocity, density, temperature, etc. This parcel was injected 35 μs after the start of injection. This parcel is fully burnt in the spray and no residue remains at the completion of combustion.

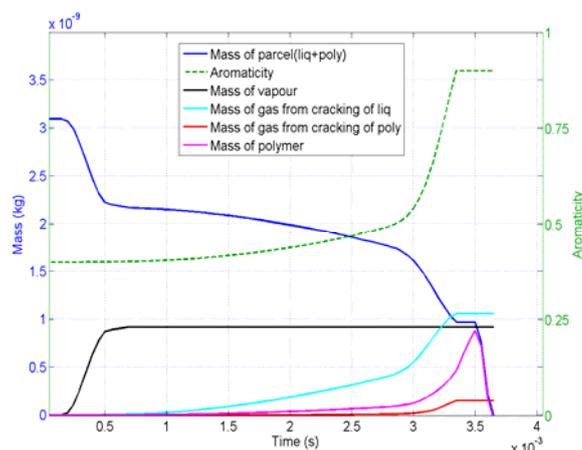


Figure 3: Mass balance of a single parcel (original liquid + products) with respect to the lifetime of the parcel for the good fuel oil in the CVCC.

The light components evaporate rapidly ("mass of vapour"). The resulting vapour mixes with the surrounding air and burns. As the droplet temperature increases thermal cracking begins in the droplet producing volatile compounds from the non-aromatic parts of the original liquid and formed polymer. Thermal cracking leaves the heavy aromatics in the droplet and thus the droplet becomes more carbon rich. The aromaticity of the liquid remains constant after the completion of thermal cracking. Thermal cracking also reduces the non-aromatic portion of the polymer producing gases which is shown by a red line. Surface oxidation of the polymer begins at 3.5 ms.

Poor Quality Fuel Oil

As shown in Figure 4, the present model for the poor fuel show good qualitative agreement with experimental results at 6 ms after the start of combustion, which is 13 ms after the start of injection due to an observed ignition delay of 7 ms.

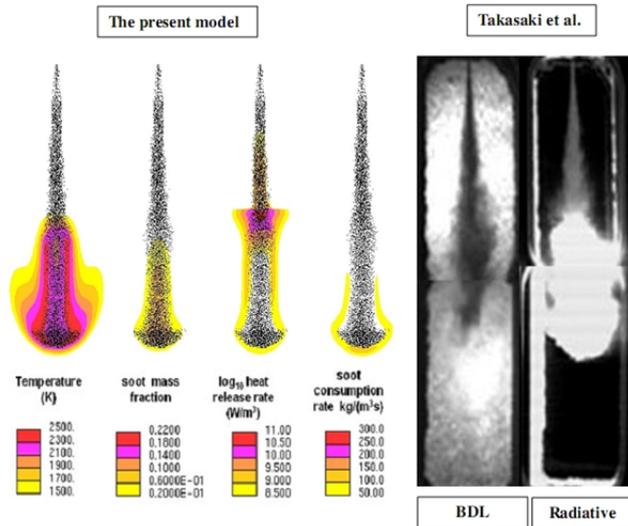


Figure 4: Comparison of the present model with Takasaki et al.'s measurements at 13ms after start of injection.

Comparison of the behaviour of the good and poor fuel oils shows that the mass transfer rate of poor fuel oil is slower due to lower ambient temperature due to later ignition. Poor fuel oil has a lower ignition quality and consequently ignites later, and vaporisation and pyrolysis which are a function of the droplet temperature begin later. The total amount of vapour and pyrolysis gas produced from good and poor parcels are almost the same at the end of the droplet lifetime, but their production rates vary according to the ignition behaviour of the fuel. A typical good fuel parcel required 0.7 ms for vaporisation of its cutter stock while a typical poor fuel required 1 ms. The observed droplet lifetime for the good fuel was 3.7 ms, which is about half that observed for the poor fuel oil (8 ms). On the other hand, the rate of combustion of coke observed for the poor fuel was higher than for good fuel oil. Complete burnout of the coke is predicted for both fuels in the present model but no qualitative data in the literature are available to validate this result. Unburnt coke could damage engines or be emitted as Black Carbon.

Conclusions

The paper describes a model for HFO vaporisation, decomposition and combustion. The developed models were applied to a constant volume spray combustion chamber for two representative fuels; one with good combustion quality and the other with poor. Qualitatively the developed models compare well with the limited available data from a visual combustion chamber. Details of the complex processes a droplet undergoes within a burning spray were given. Limitations were faced in attempting first principles modelling because HFO is comprised of many dissimilar and complex compounds and in addition many processes occur simultaneously during combustion. Further, little information is available in the literature on HFO spray combustion.

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