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A multi-dimensional quasi-discrete model for the analysis of Diesel fuel droplet heating and evaporation

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HIGHLIGHTS

- Multi-dimensional quasi-discrete model taking into account liquid species diffusion in realistic Diesel fuel.
- The dependence of the properties of components of Diesel fuels on temperature.
- The modelling of heating and evaporation of Diesel fuel droplets.

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ABSTRACT

A new multi-dimensional quasi-discrete model is suggested and tested for the analysis of heating and evaporation of Diesel fuel droplets. As in the original quasi-discrete model suggested earlier, the components of Diesel fuel with close thermodynamic and transport properties are grouped together to form quasi-components. In contrast to the original quasi-discrete model, the new model takes into account the contribution of not only alkanes, but also various other groups of hydrocarbons in Diesel fuels; quasi-components are formed within individual groups. Also, in contrast to the original quasi-discrete model, the contributions of individual components are not approximated by the distribution function of carbon numbers. The formation of quasi-components is based on taking into account the contributions of individual components without any approximations. Groups contributing small molar fractions to the composition of Diesel fuel (less than about 1.5%) are replaced with characteristic components. The actual Diesel fuel is simplified to form six groups: alkanes, cycloalkanes, bicycloalkanes, alkylbenzenes, indanes & tetralines, and naphthalenes, and 3 components $C_{19}H_{34}$ (tricycloalkane), $C_{13}H_{12}$ (diaromatic), and $C_{14}H_{10}$ (phenanthrene). It is shown that the approximation of Diesel fuel by 15 quasi-components and components, leads to errors in estimated temperatures and evaporation times in typical Diesel engine conditions not exceeding about 3.7% and 2.5% respectively, which is acceptable for most engineering applications.

1. Introduction

Diesel fuel droplet heating and evaporation is an important part of the processes leading to fuel combustion in Diesel engines [1]. Accurate modelling of these processes is essential for their understanding and ultimately improving engine design. The simplest model of Diesel fuel droplet heating and evaporation is based on a number of assumptions. These include the assumptions that Diesel fuel can be approximated by a single component (n-dodecane in most cases), temperature gradients inside droplets can be ignored, the droplet interface is stationary during the time step, and kinetic/molecular dynamic effects during heating and evaporation can be ignored [2].

Some of these assumptions were relaxed in several advanced models of droplet heating and evaporation, described in a number

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of papers including [3–6]. As demonstrated in our recent publications [7–9], the most important of the above-mentioned assumptions is that Diesel fuel can be approximated by a single component. The early models, taking into account the effect of multiple components in Diesel engines, could be subdivided into two main families: those based on the analysis of individual components (Discrete Component Models (DCM)) (e.g. [10,11]), applicable in the case when a relatively small number of components needs to be taken into account, and those based on the probabilistic analysis of a large number of components (e.g. Continuous Thermodynamics approach [12–14] and the Distillation Curve Model [15]). In the second family of models, a number of additional simplifying assumptions were used, including the assumption that species inside droplets mix instantaneously or do not mix at all. Models containing features of both these families were suggested in [16,17].

A new approach to modelling the heating and evaporation of multi-component Diesel fuel droplets, suitable for the case when a large number of components is present in the droplets, was suggested in [7]. This approach is based on the introduction of hypothetical components with non-integer numbers of carbon atoms. These hypothetical components were called quasi-components. There are some similarities between the quasi-components introduced in [7] and the pseudo-components used in [17], but these quasi-components and pseudo-components were introduced in different ways. In contrast to the previously suggested models, designed for large numbers of components, the model suggested in [7] took into account the diffusion of liquid species and thermal diffusion, as in the classical Discrete Component Models, alongside recirculation inside droplets. This model was called the 'quasi-discrete model'. In [8], this model was generalised to take into account the differences in liquid density, viscosity, specific heat capacity, and thermal conductivity for liquid components in Diesel and gasoline fuels.

Although the usefulness and efficiency of the quasi-discrete model was clearly demonstrated in [7–9], this model still has a number of serious limitations the most important of which is that it is based on the assumption that Diesel and gasoline fuels consist only of n-alkanes. At the same time, as will be shown later in this paper, the total molar fraction of alkanes (n-alkanes and iso-alkanes) is only about 40% of the overall composition of Diesel fuels (a similar conclusion could be drawn for gasoline fuel [18]). Hence, the contribution of other components apart from alkanes cannot be ignored.

In this paper, the model originally suggested in [7] is generalised to take into account the realistic composition of Diesel fuels. This composition is described in the following section. The model used in our analysis is introduced in Section 3. The new elements of the model are described alongside the previously developed elements to make the whole paper self-sufficient for practical application of the results. The solution algorithm is described in Section 4. The results of calculations are presented in Section 5. The main results of the paper are summarised in Section 6.

2. Composition of Diesel fuel

The commercial Diesel fuel selected in the present work conforms to standard European Union fuel (EN590). The detailed chemical species composition was obtained using comprehensive two-dimensional gas chromatography (GCXGC) which is a very convenient tool for the characterisation of petroleum-based fuels [19–21]. Molar fractions of various components in this fuel are presented in Table 1 [22]. The results presented in this table were simplified, taking into account that the properties of n-alkanes and iso-alkanes are rather close. Also, one can observe in Table 1 that the contributions of tricycloalkanes, diaromatics and phenanthrenes to Diesel fuel are rather small (less than about 1.6% for each of these components). This allows us to ignore the dependence of the properties of these components on the number of carbon atoms and replace these three groups with three components, tricycloalkane, diaromatic and phenanthrene, with particular arbitrary chosen values of carbon numbers. A simplified version of Table 1, in which n-alkanes and iso-alkanes are merged into one group of alkanes, and tricycloalkanes, diaromatics and phenanthrenes are excluded, is presented as Table 2. Transport and thermodynamic properties of the components included in Table 2 are summarised in Appendices A,B,C,D,E and F. Transport and thermodynamic properties of three components, tricycloalkane, diaromatic and phenanthrene, are summarised in Appendix G. Based on the results presented in Table 1, we assume that the molar fraction of tricycloalkanes is 1.5647%, while the molar fraction of diaromatics and phenanthrenes are equal to 1.2240% and 0.6577%, respectively.

Table 1
The composition (molar fractions) of a realistic Diesel fuel sample (gas chromatography data) used in the analysis.

Number C atoms	n-Alkanes	iso-Alkanes	Cycloalkanes	Bicycloalkanes	Tricycloalkanes	Alkylbenzenes	Indanes & tetralines	Naphthalenes	Diaromatics	Phenanthrenes
C8	0.3080	0	0	0	0	0.4970	0	0	0	0
C9	1.0513	1.9807	0	0	0	3.2357	0	0	0	0
C10	1.2635	3.7906	0.6408	0.6926	0	5.3584	1.3157	1.9366	0	0
C11	1.1002	2.0628	1.8745	1.0524	0	0.9492	1.3632	2.5290	0	0
C12	0.9866	1.6290	1.6951	0.9753	0	1.9149	1.1951	1.4012	0	0
C13	0.9646	1.5793	1.2646	0.6611	0	0.6873	1.0652	0.7692	0.3834	0
C14	1.0146	1.6351	1.3633	0.5631	0.0914	0.6469	0.8406	0.4879	0.3217	0.0768
C15	1.2051	1.9595	1.2353	0.4314	0.1799	0.4782	0.7051	0.3843	0.2589	0.2033
C16	1.0442	1.6137	1.0449	0.4921	0.1773	0.4564	0.6684	0.2854	0.2602	0.1705
C17	1.0564	1.8041	1.0162	0.6529	0.4001	0.4204	0.5598	0.2072	0	0.1154
C18	1.0596	2.1807	1.2848	0.6554	0.3304	0.5234	0.5357	0.2358	0	0.0917
C19	1.0916	2.4380	1.3566	0.9901	0.2159	0.3226	0.3403	0.2151	0	0
C20	0.7054	1.5284	0.9961	0.1965	0.1696	0.2848	0.3227	0.2256	0	0
C21	0.3756	1.0674	0.5374	0.0935	0	0.2032	0.1638	0	0	0
C22	0.2328	0.5662	0.3040	0.0701	0	0.0969	0.0781	0	0	0
C23	0.1083	0.2889	0.1090	0.0488	0	0.0494	0	0	0	0
C24	0.0461	0.1442	0.0755	0.0234	0	0.0473	0	0	0	0
C25	0.0221	0.0776	0.0445	0.0169	0	0	0	0	0	0
C26	0.0106	0.0319	0.0214	0	0	0	0	0	0	0
C27	0.0052	0.0257	0.0155	0	0	0	0	0	0	0
Mol%	13.6518	26.4039	14.8795	7.6154	1.5647	16.1719	9.1537	8.6773	1.2240	0.6577