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Effect of realistic multicomponent diesel surrogates on predicted in-nozzle flow and cavitation

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Abstract

In-nozzle flow dominates primary break-up characteristics and therefore the combustion efficiency. However, predictive methods of the internal nozzle flow and its link with the spray characteristics have traditionally used constant fuel properties, which may lead to large inaccuracies. Surprisingly enough, neither the effects of using realistic surrogates have been closely examined. In this work, the fuel property variation as function of pressure and temperature of three diesel surrogates are modelled using the PC-SAFT state-of-the-art EoS; these include n-dodecane and two mixtures comprising four and eight components, named V0 and V1 respectively, based on a grade no. 2 diesel emissions-certification fuel. Then, the surrogates used in simulations for a common rail 5-hole tip injector. The needle is assumed to be still at a lift of $105\mu\text{m}$, similar to that used for pilot injections. The injector operating pressure is 180MPa and the collector back pressure is 5MPa. Heat effects are omitted and no turbulence model is used. The bulk fluid is considered to be a single phase whose density varies according to a barotropic-like scheme, following an isentropic line. Results show that the mixture surrogates V0 and V1 have a greater vapour pressure than that of n-dodecane, although they are significantly heavier both in density and viscosity. Predicted cavitation clouds occupied a $\sim 14\%$ larger volume for V1 than that for n-dodecane. Slight differences were observed on mass flux, where V1 gave an increase of $\sim 7\%$ with respect to n-dodecane. Interestingly, the amount of vaporised components which appear simultaneously in the two mixtures were not the same, which may show that there exists an interaction between the components during the vaporisation process. Despite its exploratory nature, this study offers some insight for the first time into the use of complex EoS and surrogate mixtures, which may be worth to capture the particular properties of diesel fuel during high pressure injections.

Introduction

Recent studies on global energy demand and supply has shown that the demand for heavy duty transportation is expected to grow the most by volume [1] in the forthcoming years. As a consequence, the diesel oil demand will rise accordingly. Modern diesel engines operate with upstream pressures around 200MPa, although the current trend is to increase them up to 300MPa, as included in the forthcoming EU emission regulations. However, due to the micrometre scales of injectors, high injection pressures will irremediably cause very high fuel velocities which, added to the sharp geometric changes in the injector passages, lead to significant pressure gradients and local depressurization. Then, if the pressure decreases beyond the saturation point, the fuel may vaporise in a phenomenon known as cavitation, which in turn is related to injector erosion and underperformance [2]. On the other hand, it has been observed that cavitation enhances atomisation performance, increases the spray cone angle, and it is related to mass flux choke due to hampering of the free flow, enhancing then the nozzle outlet velocity [3].

Research on the modelling of in-nozzle cavitation has been thorough in approaches. For example, the fluid inside the nozzle has been already modelled as one-fluid or two-fluid mixtures, the latter combined with a mass transfer term between the phases to obtain asymmetric flow features closer to experiments [4]. Moreover, EulerianLagrangian and Rayleigh-Plesset models can be used for the tracking of dispersed bubbles and estimating the bubble growth and collapse, respectively. Other models, such as the homogeneous equilibrium model (HEM), considers the fluid as a homogeneous mixture on the sub-grid scale. This model can be used to study the formation and transport of vapour bubbles, the turbulent fluctuations in velocity and pressure and the effect of noncondensable gases [5]. It has been made also possible to look into the effect of liquid and vapour compressibility on supercavitation formation [6].

To date, in most of injector simulations the properties of the fluid in liquid the state are assumed to follow a barotropic evolution, i.e. pressure and density are one to one related, if not assumed constant. On the other hand, the vapour properties are often assumed to remain constant. For the liquid, the barotropic equation is

usually derived following Kolev's diesel properties collection [7] or single component approximations using the NIST REFPROP [8] database. However, the use of constant properties may lead to large deviations in discharge coefficient and

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Compound	M_w	T_b	mol %	
	[g/mol]	[K]	C ₁₂ VO	V1
n-hexadecane	226.4	560.0	- 27.8	2.7
n-octadecane	254.5	590.0	-	- 20.2
heptamethylnonane	226.4	520.0	- 36.3	29.2
n-dodecane	170.3	489.4	100.0	-
n-butylcyclohexane	140.3	456.2	-	- 5.1
trans-decalin	138.2	460.5	- 14.8	5.5
1,2,4-trimethylbenzene	120.2	442.6	-	- 7.5
tetralin	132.2	480.9	-	- 15.4
1-methylnaphthalene	142.2	518.0	- 21.1	14.4

Table 1: Molar composition for the two mixture diesel surrogates [11] modelled here. Boiling points at 0.1 MPa taken from the literature.

fuel heating predictions, particularly in cases of high pressure injections [9]. Moreover, composition effects in diesel fuel are related to changes in the cavitation cloud size, the spray atomisation, and spray tip penetration [10]. Surprisingly, the effects of using realistic surrogates have not been closely examined.

The aim of the current work is to simulate the in-nozzle flow and cavitation of diesel injectors using single and multicomponent diesel surrogates, studying the differences from their outcomes. The surrogates are n-dodecane and two mixtures of four and eight components, based on a grade no. 2 diesel emissions-certification fuel [11]. In their original research, the mixture surrogates were tested to mimic the characteristic composition, ignition quality, volatility, density, and other properties from the real diesel fuel. The surrogate compositions are listed in Table 1.

The modelling of the surrogates is made through the PC-SAFT equation of state (EoS) [12]. Several advantages are realised when using the PC-SAFT EoS compared to the widely used cubic EoS for calculating fluid properties. The PC-SAFT EoS more accurately predicts derivative properties, reducing errors by a factor of up to eight [13], as compared to predictions with a cubic EoS, such as the Peng-Robinson EoS [14]. Density predictions with the PC-SAFT EoS exhibit six times lower error for a widely used surrogate such as dodecane [15]. The PC-SAFT EoS provides satisfactory agreement between calculated and experimental properties of reservoir fluids, natural gas and asphaltene phase behaviour [16]. These studies suggest the PC-SAFT EoS should provide reasonable predictions of diesel fuel properties at extreme operating conditions, for which a paucity of data exist.

The overall structure of the study takes the form of four sections. After the already shown introductory first section, the second section gives the outline of the case set-up, the CFD model used for the simulations and the description of the PC-SAFT EoS. Then, the results are shown including the calculated properties of the surrogates and the in-nozzle flow and cavitation characteristics, alongside the discussion of this results. Lastly, the final section gives a summary and critique of the findings.

Numerical Methods

Injector geometry and operating conditions

The examined injector geometry was based on a common rail 5-hole tip injector. As focus is given here on the effect of fuel properties, complications arising from the needle valve motion have been ignored. Although the simulation is transient, the needle was assumed to be still at a lift of $105\mu\text{m}$, similar to that characteristic pilot injections. Incorporation needle motion would obviously change the flow field, however at the expense of great computational cost and without interfering on the preferential vaporisation mechanism, i.e. the main topic of this

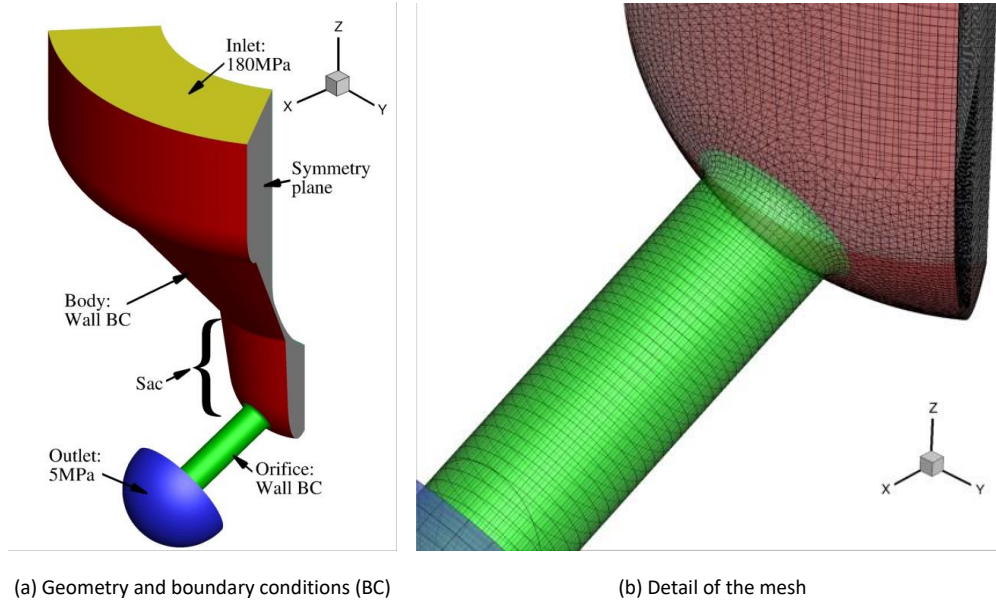


Figure 1: Simulated geometry, one fifth of the total structure.

work. The simulated geometry consisted on 1/5 of the total structure, as shown in Figure 1a, imposing periodic boundary conditions at the walls. Although more accurate results would be calculated at the expense, again, of a great computational cost by taking into account the complete 360° geometry.

Pressure boundary conditions are imposed to 180MPa at the inlet and 5MPa at the outlet. Note also that there is a hemispherical volume attached to the nozzle exit. This volume is added to be able to capture the complete cavitation cloud, which may extend out of the orifice.

Regarding the computational mesh, two topologies have been used, as shown in Figure 1b. Before the orifice entrance, in the sac volume, there is an unstructured tetrahedral mesh. For the rest of the domain, an hexahedral block-structured mesh is used. The total number of cells in the numerical mesh was $\sim 200\text{k}$. A finer mesh may resolve better the small instabilities of the flow; however, the averaged values are not expected to change significantly.

The Reynolds number at the needle/needle seat passage was estimated to be 7000, which corresponds to a transitional regime and is characteristic of low needle lift injections. Regarding the use of turbulence model, studies have shown that RANS models suffer from significant pitfalls when resolving the cavitation cloud [17], while the more accurate LES models need a significantly finer mesh, which is out of the exploratory nature of this work. Therefore, no turbulence model was used in the simulations.

CFD model

The in-house density-based CFD code used in this work solves thus a laminar, compressible and viscous Navier-Stokes system in the open-access OpenFOAM platform. The energy equation was omitted here by assuming constant entropy. Using this assumption, density is a function of pressure only, greatly simplifying the simulation. Although it is an obvious simplification, it is also an asymptotic limit that would happen for a discharge coefficient equal to unity and adiabatic walls, which can give significant insight in the in-nozzle flow.

The flow has been considered compressible. Due to formation of cavitation there is a wide range of Mach numbers operating during the process, ranging from $O(10^{-1})$ to $O(10^2)$. For density-based solvers, low Mach

numbers are related to convergence problems and dispersion, so a modification in the fluxes is used for accounting for all Mach ranges.

The two phase flow is assumed to be an homogeneous mixture of vapour and liquid in mechanical equilibrium, i.e. both phases share the same pressure and velocity fields.

A state-of-the-art EoS

The PC-SAFT EoS [12] is a theoretically derived model, it splits the intermolecular potential energy of the fluid into a reference term accounting for repulsive interactions and a perturbation term accounting for attractive interactions. The reference fluid is composed of spherical segments comprising a hard sphere fluid that then forms Palette Cmpd. Name

Palette Cmpd. Name	m	$\sigma[\text{\AA}]$	$\epsilon/k[K]$
n-hexadecane	6.669	3.944	253.59
n-octadecane	7.438	3.948	254.90
heptamethylnonane	5.603	4.164	266.46
n-dodecane	5.306	3.896	249.21
n-butylcyclohexane	3.682	4.036	282.41
trans-decalin	3.291	4.067	307.98
1,2,4-trimethylbenzene	3.610	3.749	284.25
tetralin	3.088	3.996	337.46
1-methylnaphthalene	3.422	3.901	337.14

Table 2: PC-SAFT pure component parameters for the compounds within the diesel surrogate mixtures listed in Table 1.

molecular chains to create the hard-chain fluid. The attractive interactions, perturbations to the reference system, are accounted for with the dispersion term. Hence, each component is characterized by three pure component parameters, which are a temperature-independent segment diameter, σ , a segment interaction energy, ϵ , and a number of segments per molecule m . Values for the components used in this work can be found in Table 2.

The PC-SAFT EoS is derived as summations of the residual Helmholtz free energy, as shown in Equation (1).

$$\frac{A^{res}}{RT} = a^{res} = a - a^{ig} = a^{hc} + a^{disp} \quad (1)$$

Results and Discussion *Isentropic properties*

The first set of results, as shown in Figure 2, provides the isentropic properties of the surrogates studied here. The given properties as function of increasing pressure are vapour fraction, density, temperature, speed of sound and viscosity at constant entropy.

As shown in Figure 2a, it is apparent that the mixture surrogates V0 and V1 have a greater vapour pressure than that of n-dodecane. As a consequence, for the same depressurization V1 will be the first to vaporise, followed by V0 and, lastly, n-dodecane. What is interesting about the data in this figure is that V0 and V1 are significantly heavier than n-dodecane, so one would assume that they would generally vaporise less at same

conditions, as most of heavier hydrocarbons would. Nevertheless, this result corroborates the findings of diesel gas chromatography [11] and it also supports the use of surrogate mixtures, as the existence of light hydrocarbons within the heavy diesel fuel is key to its vaporisation. Figure 2b explicitly shows that n-dodecane is lighter than V0 and V1 in the liquid state. However, close to the vapour pressure of the mixtures, n-dodecane is still liquid and, therefore, denser.

From Figure 2c, it is clear that the temperature profile is similar for all surrogates within the liquid state. What is striking about the data is that as V1 vaporises, its temperature drops accordingly while the other surrogates are still liquid. This situation causes temperature differences as high as $\sim 17\text{K}$ between V1 and dodecane, when close to full vaporisation. Similar conclusions can be drawn for the speed of sound, presented in Figure 2d. The bump in the speed of sound seen for pressures below saturation is characteristic of the Wallis formula [18].

The greatest discrepancy is seen in viscosity, Figure 2e, where the viscosity of V1 is, at times, even three times that of n-dodecane. The spike at $p \sim p_{sat}$ is consequence of the two-phase model for viscosity [19]. Similarly to what happened with density, n-dodecane viscosity is larger than that of V0 and V1 when the latter are close to their vapour pressure.

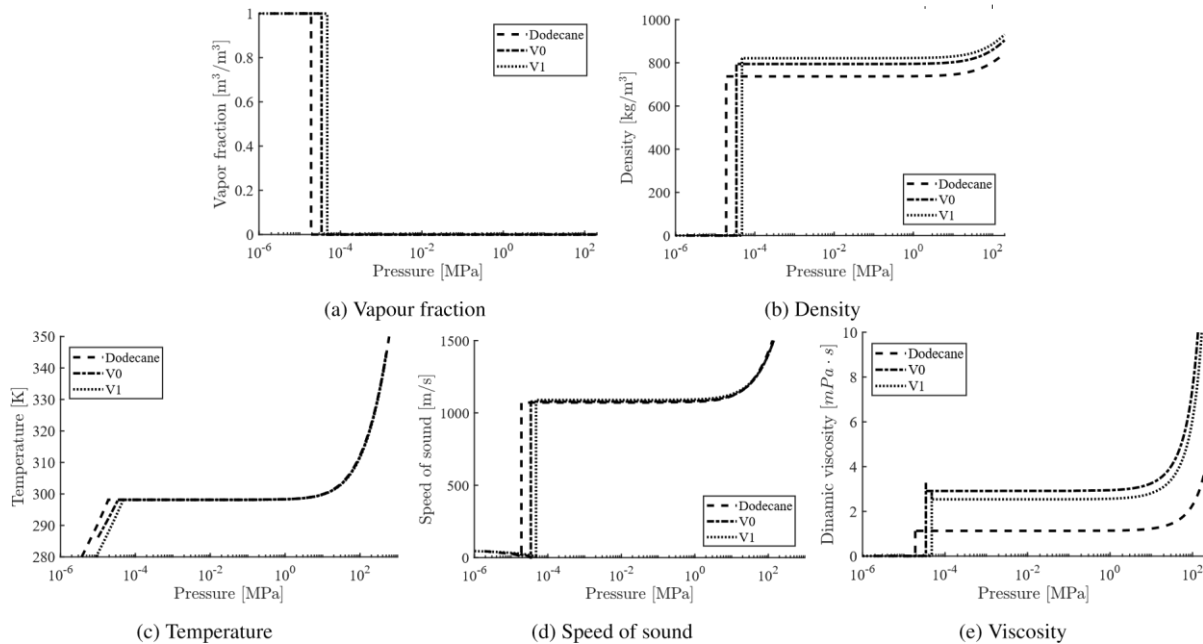


Figure 2: Isentropic lines for every surrogate. The chosen entropy is that of each substance at 293K and 0.1MPa.

In addition, Figure 3 shows the individual vaporisation of selected components in relation to the global mixture molar vapour fraction. The selected components are those that appear in both mixture surrogates, i.e. from heavier to lighter: n-hexadecane, heptamethylnonane, 1-methylnaphthalene and trans-decalin. As some components within the mixtures vaporise at different rates, it will be expected to observe different vaporisation patterns in the injection simulations.

In-nozzle flow and cavitation

Figure 4 illustrates the average vapour fraction recorded in the simulations using the three surrogates. This comparison indicates a clear difference between the surrogates, where the mixture surrogates produced larger vaporisation than the n-dodecane. This difference is highlighted in Figure 5a, where it is shown the averaged volume of the cavitation cloud in the nozzle, normalised by that of n-dodecane. From this bar graph, it can be seen that V1 resulted in the greatest volume, covering about a $\sim 14\%$ larger volume than that of n-dodecane. This also accords with the previous subsection, where due to the lighter components found in V0 and V1, they cavitate slightly earlier and, therefore, the resulting vaporised cloud is larger.

Figure 5b shows the average mass flux at the nozzle exit, normalised by that of n-dodecane. In average, it can be seen from the figure that there are differences up to $\sim 7\%$, as heavier surrogates produce a slightly higher mass flux. Most experimental research on in-nozzle cavitation and its effect on in-nozzle flow suggest that, when cavitation occurs, the mass flow is choked due to the hampering of the free flow by the vapour cloud [3]. This is shown in the mass flow evolution in Figure 5c. The evolution has been smoothed out for better readability. What stands out in the figure is the appearance of peaks in rather random time-steps. These peaks are associated with a decrease or thinning of the cavitation cloud, the absence of cavitation shedding or a combination of those.

Individual vaporisation

Perhaps, the most interesting result on this research is the vaporisation of the individual components within the mixture surrogates. Due to the use of a realistic EoS, the contents of each component in the vapour phase can be accurately predicted.

Figure 6 shows the volume fraction of vaporised component in the mixture surrogates. The volume is obtained for vapour fractions between 10% and 100%. For the two figures, the lighter the component, the larger the volume of vapour produced. Interestingly, the amount of vaporised components which appear simultaneously in the two cases is not the same. As an example, the volume fraction of n-hexadecane vaporised in V0 (~ 3%) is much smaller than that in V1 (~ 8%). In a more extreme case, the lightest component in V0, i.e. trans-decalin, covered a volume ~ 52% while for V1 it did not reach 40%. Thus, this result may show that there exists an interaction

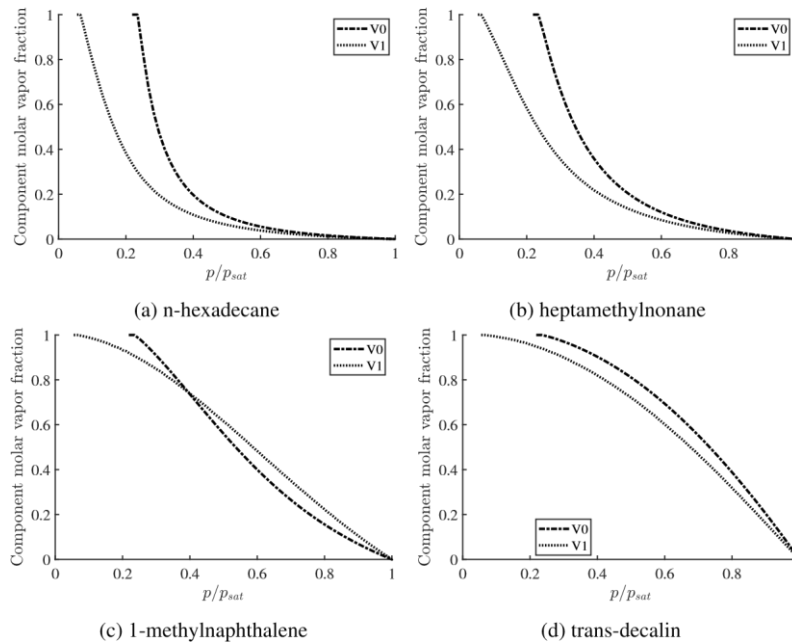


Figure 3: Individual vaporisation

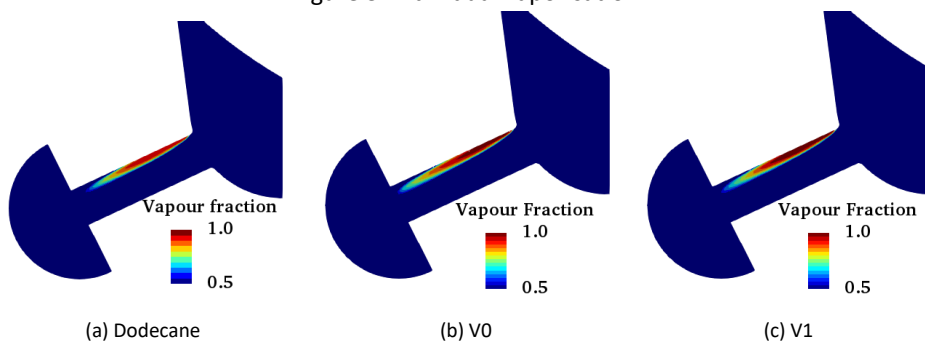


Figure 4: Average vapour volume fraction

between the components during the vaporisation process. It is also striking that the lighter components in V1 are vaporised in approximately the same amount. The 4 lighter components within V1 vaporised covering a volume in a range from 30.5% to 31.2%.

Figure 7 and 8 show the individual vaporised isosurfaces, on average, of each component within V0 and V1 for vapour fractions above 10%. As stated in the previous paragraph, the vaporised volume is different in both cases for the same components, as seen for instance for n-hexadecane and trans-decalin. In the same manner, the 4 lighter components of V1 have almost indistinguishable cavitation clouds.

Lastly, the higher the intensity of the cavitation the larger blocking of the liquid flow, reducing the discharge. If there is vaporisation at the nozzle exit, as seen for the lightest components, the discharge reduction is significant. This phenomenon is also known as choking [20].

Summary and Conclusions

This study has examined the impact of realistic diesel surrogates on the in-nozzle flow and cavitation formation, using PC-SAFT. For this, three surrogates have been used: n-dodecane and two mixtures, one with 4 components and one with 8 which are named V0 and V1, respectively. The injection process has been the same for all the cases. The geometry used was a $105\mu\text{m}$ fixed lift 5-hole injector, for which only a 1-5th was simulated while imposing periodicity conditions at the lateral walls. The upstream/downstream pressures were fixed to 180MPa and 5MPa, respectively. The properties of the surrogates introduced in the simulations were calculated in advance by imposing a constant entropy, of that given at 293K and 0.1MPa, for each case.

The isentropic properties calculated show interesting results. The main differences between the surrogates are

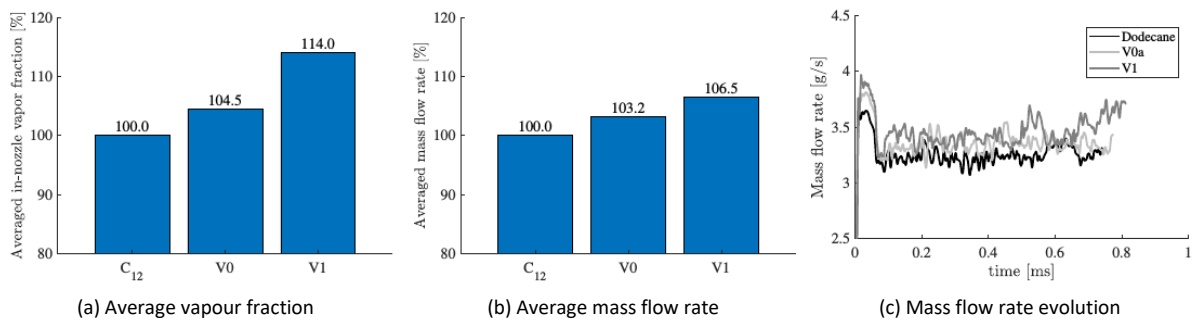


Figure 5: In-nozzle flow characteristics

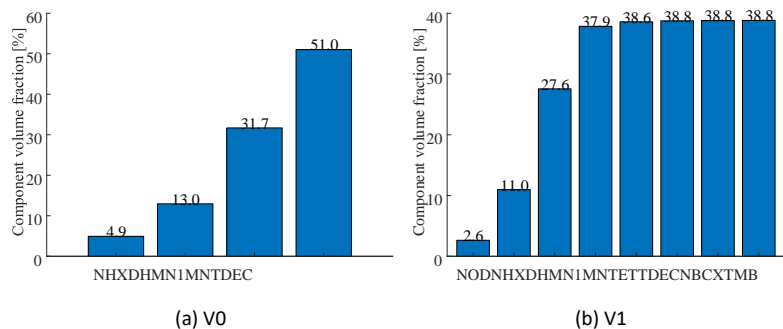


Figure 6: Individual vaporisation within the mixture surrogates. Abbreviations: NOD: n-octadecane, NHXD: nhexadecane, HMN: heptamethylnonane, 1MN: 1-methylnaphthalene, TET: tetralin, TDEC: trans-decalin, NBCX: n-butylcyclohexane, TMB: trimethylbenzene.

focused in the density and viscosity, while other properties are different only the VLE and vapour state, with no apparent differences in the liquid phase. Although V1 and V0 are heavier than dodecane, they start vaporising earlier. This result may be explained by the fact that the mixtures contain lighter hydrocarbons, influencing thus the vaporisation process by anticipating it.

Regarding the results of the simulations, the most compelling differences are in the size of cavitation clouds. With respect to the volume of cavitation cloud of dodecane, V1 was observed to give an increased cavitation cloud of $\sim 14\%$. On the other hand, slight differences were observed on mass flux, where V1 gave an increase of $\sim 7\%$ with respect to n-dodecane. Perhaps one of the most striking results are found within the individual vaporisation of each component in the mixtures. Same components are found to vaporise in different amounts depending on the mixtures they are found within.

Despite its exploratory nature, this study offers some insight for the first time into the use of complex EoS and surrogate mixtures, which may be worth to capture the particular properties of diesel fuel during high

pressure injections. The findings in this report are subject to at least three limitations. First, presuming an isentropic process introduces an idealism which is not able to capture such non-ideal situations as friction induced heating. Second, the barotropic nature of the simulations makes the mixture to be treated as a pseudo-single component, thus in every cell the global composition of the fuel is conserved. Third, the absence of a turbulence model causes the results to be taken only as averages. Further work needs to be done to establish whether more flow characteristics may be impacted by the use of more mixture surrogates and its potential effect on spray atomisation and combustion.

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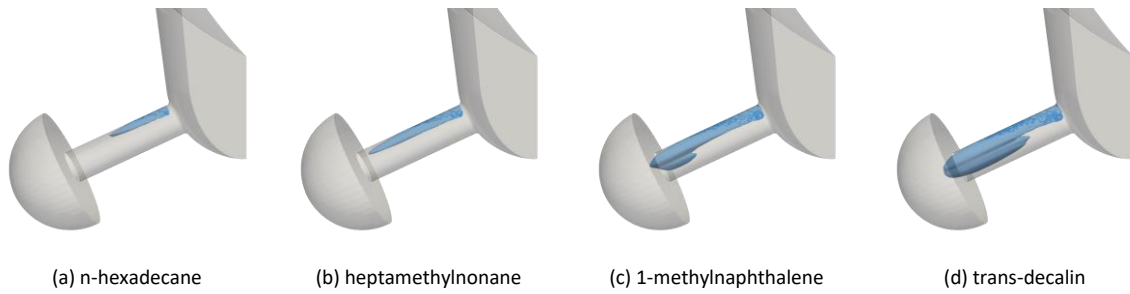


Figure 7: 10% average vapour fraction isosurface per component in V0 surrogate

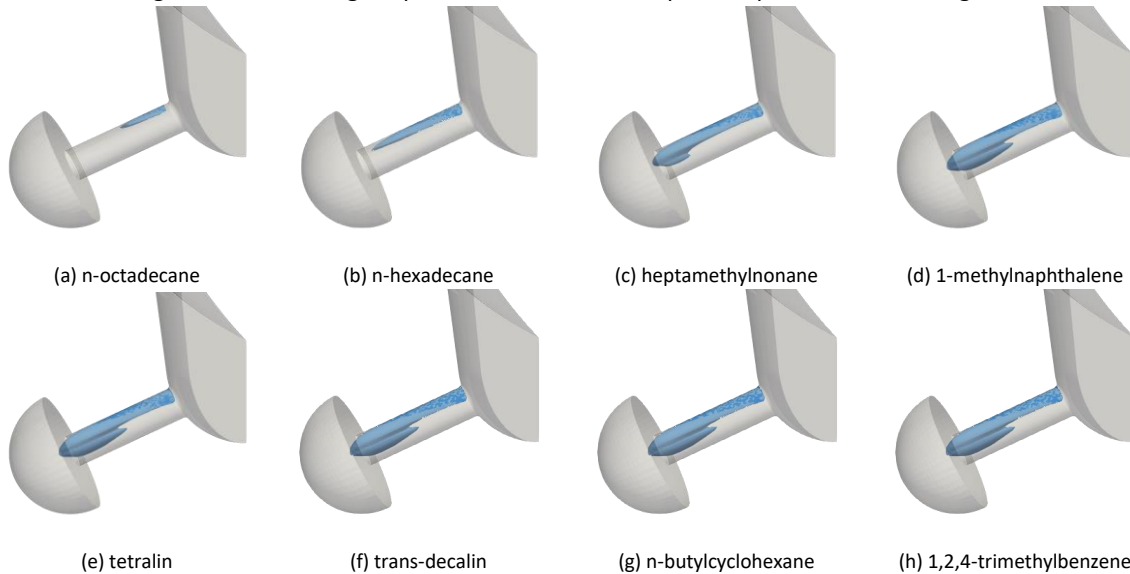


Figure 8: 10% average vapour fraction isosurface per component in V1 surrogate

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