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## CFD simulation of pseudo-diesel injections at high-load conditions employing the PC-SAFT EoS and VLE calculations

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### Abstract

The molecular-based Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) equation of state (EoS) is coupled with Vapor-Liquid Equilibrium (VLE) calculations in a density-based solver of the Navier-Stokes equations to perform multicomponent two-phase simulations of Diesel injections at high-pressure conditions. The PC-SAFT EoS requires three parameters, which can be fitted to experimental data or calculated using group contribution methods, to model the properties of a specific component. Therefore, there is no need for extensive model calibration, as is typically the case when the NIST library is utilised. PC-SAFT can flexibly handle the thermodynamic properties of multi-component mixtures for which the NIST (REFPROP) library supports only limited component combinations. Moreover, complex hydrocarbon mixtures can be modelled as a single pseudo-component knowing its number averaged molecular weight and the hydrogen-to-carbon ratio. One and two-dimensional simulations are included to demonstrate the multidimensional, multispecies and multiphase capability of the numerical framework.

### Keywords

PC-SAFT EoS; Pseudo-component; Diesel Fuel Injection

### Introduction

Road freight is the most energy-intensive freight mode (per tonne-kilometre) and practically only employs fossil fuels [1]. It generates approximately 16% of the CO<sub>2</sub> emissions worldwide [1] and its demand is expected to grow +160% in tonne-kilometre until 2050 [2]. The study performed by [1], which explored the technical limits of electrification in this sector using real data from the Swiss truck fleet, points out how full electrification is particularly difficult to be carried out. Even when considerably improving the gravimetric energy density of the battery cells, three additional conditions must be met to have a high electrification potential: (1) a change in the maximum permissible weight; (2) to have access to a high-capacity grid for charging; and (3) backing an intra-day energy infrastructure (such as swapping stations). Therefore, there is a real need to improve our understanding of Diesel engines to continue reducing emissions until gradual replacement with electrification becomes effective.

This paper is presenting an improved thermodynamic model for simulating air-fuel mixing at Diesel engine relevant conditions. According to experiments performed by several authors (see selectively [3]–[7]), supercritical mixing occurs at pressures near or slightly higher than the critical pressure of the injected liquid fuel. [8], [9] stated that the convection-diffusion phenomena described by the Navier-Stokes equations governs Diesel injections. The authors derived a mathematical model combining real-fluid thermodynamics and Linear Gradient Theory to specify under what conditions exists a classical non-continuum “jump” between the phases or a continuous gas-liquid interfacial diffusion layer. According to the results, high-temperature interfaces presented a significantly reduced surface tension and a wider interface when compared to low-temperature interfaces. There is a reduction in the mean free molecular path and a broadening of the interfaces (which places the interface in the continuum length scale regime). More recently, [10] investigated the atomization and mixing processes of sprays injected into progressively higher pressure and temperature ambient conditions. It was determined that the surface tension remains in effect at the gas-liquid interfaces in ambient conditions slightly above the critical point of the fuel. However, the surface tension at higher pressure and temperature conditions diminishes, as expected for supercritical fuel-air mixtures. In a following study [11], the authors carried out systematic macroscopic droplet evaporation measurements using high-speed long-distance microscopy for three single-component fuels (n-heptane, n-dodecane, n-hexadecane) injected into gas (89.71% N<sub>2</sub>, 6.52% CO<sub>2</sub> and 3.77% H<sub>2</sub>O) at elevated temperatures (700–1200 K) and pressures (2–11 MPa). They observed that the classical evaporation/diffusive mixing boundaries was applicable even at high pressures and temperatures. In [12] the evaporation of n-alkane fuels into nitrogen was investigated at different pressure and temperature conditions carrying out molecular dynamics simulations. The aim of this work was to understand how the transition from classical two-phase evaporation to one-phase diffusion-controlled mixing takes place. Two regimes are identified: (1) subcritical evaporation where a distinctive interface exists separating the liquid core and the ambient gases; and (2) supercritical evaporation where initially the liquid has a surface tension that decreases rapidly and vanishes. During the subcritical stage, the evaporation rate increases and reaches a maximum after which there is a transition to the supercritical stage. The results obtained have a high degree of agreement against the experimental results obtained by [11].

Turning to numerical simulations, numerous studies on Diesel sprays exist that employ Lagrangian methods considering a sharp gas-liquid interface which evolve according to primary and secondary breakup models and evaporation [13]–[15]. However, this approximation presents some limitations to accurately capture dense flow

regimes near the nozzle where the liquid fuels disintegrate into ligaments that then form droplets; some numerical improvements for applications to dense grids relative to the volume fraction of the Lagrangian phase have been reported in [16]. Still, they are sensitive to calibration parameters; unfortunately, there is no quantitative experimental droplet size measurements near the injector nozzle at Diesel engine conditions [17]. In [18], [19] an Eulerian density-based methodology was used to model the primary atomisation of the injected liquid accounting for compressibility effects associated with the high-pressure and injection velocity. A single-phase dense-gas approach was combined with the Peng-Robinson (PR) EoS. However, n-dodecane/nitrogen mixtures are a TYPE IV mixture, which means that the critical temperature of the mixture is higher than the lower critical temperature of the components and lower than then the higher critical temperature of the compounds. On the other hand, the critical pressure is higher than the critical pressure of the components. Considering that the pressures that can be found in the combustion chamber of Diesel engines are lower than the critical pressure of some nitrogen/fuel mixtures, the VLE state must be included in the simulation. In [17], [20] a multi-species two-phase model was developed using Large Eddy Simulations (LES) for accounting the turbulent mixing under high pressures. A thermodynamic solver that can compute the properties of a homogenous mixture in supercritical or subcritical states was implemented. The LES including VLE thermodynamics of the so-called Spray A benchmark case of the Engine Combustion Network (ECN) performed by [17] shows a high degree of agreement against the available experimental data. Although according to [11], [12] the ambient conditions of the so-called ‘Spray A’ (900K, 6MPa) fall in the classic evaporation regime, the authors of [17] justified the use of a diffuse interface due to the high Weber number and low Stokes number. The authors pointed out the issues of employing cubic EoS for modelling hydrocarbon properties at temperatures found inside the injection system [21]–[23]. In [17], due to the 8.6% error when compared to NIST in the density prediction of n-dodecane at 363K, it was necessary to increase the injection velocity to match the mass-flow measurement leading to an error in the predicted velocity of 50 m/s. These problems could be overcome by applying SAFT models.

The novelty in this paper is to present a numerical framework that combines Perturbed-Chain SAFT (PC-SAFT) and VLE calculations in a density-based, fully conservative solver of the Navier-Stokes and energy conservation equations. VLE calculations allow to perform simulations where the fuel enters the combustion chamber at low temperatures (subcritical injections). A purely predictive method that employs the PC-SAFT EoS for developing pseudo-components, which are defined to replicate the properties of complex hydrocarbon mixtures (e.g., diesel fuels), has been completed and validated to be used in CFD simulations. Then, complex hydrocarbon mixtures can be modelled as a single pseudo-component knowing its number averaged molecular weight (MW) and hydrogen-to-carbon (HN/CN) ratio.

### Material and methods

The Navier-Stokes equations have been solved employing the finite volume method on a Cartesian numerical grid. Operator splitting as described in [24] is utilised to separate the hyperbolic and parabolic operators. The global time step is computed using the CFL (Courant-Friedrichs-Lewy) criterion of the hyperbolic part. A thermodynamic solver inspired by the work of [17] is employed to approximate the mixture thermophysical properties by performing PC-SAFT and VLE calculations.

The Navier-Stokes equations for a non-reacting multi-component mixture containing N species in a x-y 2D Cartesian system are given by:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \frac{\partial \mathbf{F}_v}{\partial x} + \frac{\partial \mathbf{G}_v}{\partial y} \quad (1)$$

The vectors of eq. 1 are:

$$\mathbf{U} = \begin{bmatrix} \rho Y_1 \\ \vdots \\ \rho Y_N \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \mathbf{F} = \begin{bmatrix} \rho u Y_1 \\ \vdots \\ \rho u Y_N \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \end{bmatrix}, \mathbf{G} = \begin{bmatrix} \rho v Y_1 \\ \vdots \\ \rho v Y_N \\ \rho vu \\ \rho v^2 + p \\ (\rho E + p)v \end{bmatrix}, \mathbf{F}_v = \begin{bmatrix} J_{x,1} \\ \vdots \\ J_{x,N} \\ \sigma_{xx} \\ \sigma_{xy} \\ u\sigma_{xx} + v\sigma_{xy} - q_x \end{bmatrix}, \quad (2)$$

$$\mathbf{G}_v = \begin{bmatrix} J_{y,1} \\ \vdots \\ J_{y,N} \\ \sigma_{yx} \\ \sigma_{yy} \\ u\sigma_{yx} + v\sigma_{yy} - q_y \end{bmatrix}$$

where  $\rho$  is the fluid density,  $u$  and  $v$  are the velocity components,  $p$  is the pressure,  $E$  is the total energy,  $J_i$  is the mass diffusion flux of species  $i$ ,  $\sigma$  is the deviatoric stress tensor and  $q$  is the diffusion heat flux vector.

The conservative variables, pressure and speed of sound values needed to solve the Riemann problem are interpolated at the cell faces from cell centres using the fifth order reconstruction scheme described in [21]. This technique decreases the computational time and smooths-out the spurious pressure oscillations associated with fully conservative (FC) schemes employed along with real-fluid EoS. The temporal integration is carried out using a second-order Runge–Kutta (RK2) scheme applying the filter presented in [21]. The model developed by [25] is used to calculate the dynamic viscosity and the thermal conductivity.

#### Diesel fuel properties modelling

Two approximations have been considered to model the properties of Diesel: (i) the multicomponent Diesel surrogate and (ii) the single pseudo-component method. These are briefly explained below:

##### (i) Multicomponent Diesel surrogates

In [26] four Diesel surrogates have been proposed. The V0A and V0B are two low-accuracy surrogates while V1 and V2 are the two higher-accuracy surrogates. Their molar composition is summarized in [26]. As pointed out in [27], the PC-SAFT EoS shows much better agreement with the experimental values in comparison with the results obtained using the model developed at NIST [26].

##### (ii) Pseudo-component method

In [28] a technique was developed that defines a single pseudo-component to represent the compounds found in a hydrocarbon mixture. It only requires two mixture properties as inputs, the number averaged MW and the HN/CN ratio. Here we briefly describe how to achieve the pseudo-component PC-SAFT parameters needed in this study. The group contribution (GC) parameters of [29] are used to develop the correlations for n-alkanes and poly-nuclear aromatics (PNAs) that numerically bound the pseudo-component PC-SAFT parameter values. An averaging parameter,  $Z$ , is used to calculate the pseudo-component parameters.  $Z$  is calculated using the mixture number averaged MW and HN/CN ratio, which can be directly calculated if the components comprising the mixture, and their relative concentrations, are known or can be obtained using elemental analysis. Considering that the PC-SAFT is implemented using an iterative approach, whose computational intensiveness depends on the number of components solved, this method allows for modelling of complex hydrocarbon mixtures as one component, thus, it reduces significantly the computational requirements of the simulation but without decreasing its accuracy. The methodology developed by [28] was validated for modelling density, isothermal compressibility and volumetric thermal expansion coefficient of hydrocarbon mixtures and jet and Diesel fuels. However, the pseudo-component must correctly model the internal energy (employed in the conservation of the total energy equation) speed of sound (used to calculate the hyperbolic fluxes and time step), enthalpy (employed in the parabolic operator of the Navier-Stokes equations) and fugacity coefficients (to perform VLE calculations). Using PC-SAFT, the internal energy, enthalpy and heat capacities at constant pressure and volume (needed to compute the speed of sound) are computed as the sum of ideal and residual contributions. PC-SAFT pure component parameters obtained employing the method of [28] are used to calculate the residual contributions. The ideal enthalpy of each component is calculated by integrating the ideal heat capacity at constant pressure with respect to temperature [30]. The molar composition of the mixture is used to calculate the ideal enthalpy of the mixture. The mixture ideal internal energy is computed employing its ideal enthalpy. The ideal heat capacities at constant pressure of each component is computed employing the correlations published in [30]; then, molar fractions are used to compute the ideal heat capacity at constant pressure of the mixture, which is employed to calculate the ideal heat capacity at constant volume.

**Table 1.** Comparison between experimentally measured surrogate densities (kg/m<sup>3</sup>) at 293.15 K and 0.1 MPa with the NIST and PC-SAFT predictions [27].

Surrogate	Experiment[26]	NIST	PC-SAFT
V0A	818.0	809.1	814.9
V0B	837.5	821.6	833.2
V1	828.4	814.1	825.2
V2	853.0	839.9	861.8

**Table 2.** Molar composition for the four Diesel fuel surrogates (V0A, V0B, V1, V2) [26]

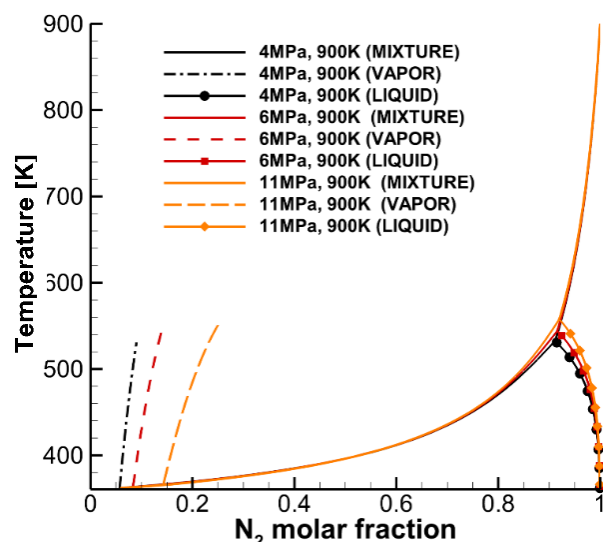
Compound	V0A	V0B	V1	V2
n-hexadecane	27.8	-	2.70	-
n-octadecane	-	23.5	20.2	10.8
n-eicosane	-	-	-	0.80
heptamethylnonane	36.3	27.0	29.2	-
2-methylheptadecane	-	-	-	7.3
n-butylcyclohexane	-	-	5.10	19.1
triisopropylcyclohexane	-	-	-	11.0
trans-decalin	14.8	-	5.50	-
perhydrophenanthrene	-	-	-	6.00
1,2,4-trimethylbenzene	-	12.5	7.5	-
1,3,5-triisopropylbenzene	-	-	-	14.7
tetralin	-	20.9	15.4	16.4
1-methylnaphthalene	21.1	16.1	14.4	13.9

#### Thermodynamic solver (PC-SAFT + VLE)

The thermodynamic solver is employed to compute temperature, pressure, sound speed and enthalpy once the conservative variables have been updated [21]. The inputs are the density, internal energy and mass fraction of the components. The three PC-SAFT parameters per compound (number of segments per chain, energy parameter and segment diameter) are specified for initialisation.

#### Algorithm

- 1) Filter. This step is employed to decrease the computational time by reducing VLE calculations. By checking the molar fractions of the components, it can be determined whether only one phase exists. Isobaric-adiabatic lines can be computed using the initial conditions of the case of interest (temperature in the chamber, temperature of the fuel injected and pressure in the combustion chamber) to determine the molar fractions at which VLE is not expected. As we can see in Figure 1, by performing an injection of n-dodecane at 363K in a combustion chamber at 900K and 11MPa, the nitrogen mole fraction at which the fuel starts vaporizing is close to 0.15.



**Figure 1.** Isobaric-adiabatic mixing lines at different pressures in the combustion chamber

- 2) One phase. When knowing that the mixture is stable the molecular density of the mixture can be computed and used as an input to the PC-SAFT model. The Newton-Raphson method is employed to compute the temperature that is needed to calculate the value of all other thermodynamic variables. The temperature dependent function used in the iterative method is the internal energy. The derivative of the internal energy with respect to the temperature at constant molecular density can be directly obtained as these are the independent variables of the PC-SAFT model.
- 3) Two phases. If the state of the mixture is unknown the density cannot be used as an input. The pressure and the temperature are iterated employing a multidimensional Newton-Raphson method until the density

and the internal energy obtained using the PC-SAFT + VLE calculations are the ones obtained from the conservative variables. For each P-T calculation a stability analysis is performed to determine if the mixture is stable using a successive substitution iteration (SSI) method to perform equilibrium calculations.

- Stable mixture: The PC-SAFT model is solved. The reduced density is iterated until the computed pressure equals the input pressure.
- Unstable mixture: The isothermal-isobaric flash problem (TPn flash) is solved and the properties of the fluid in a VLE state are computed.

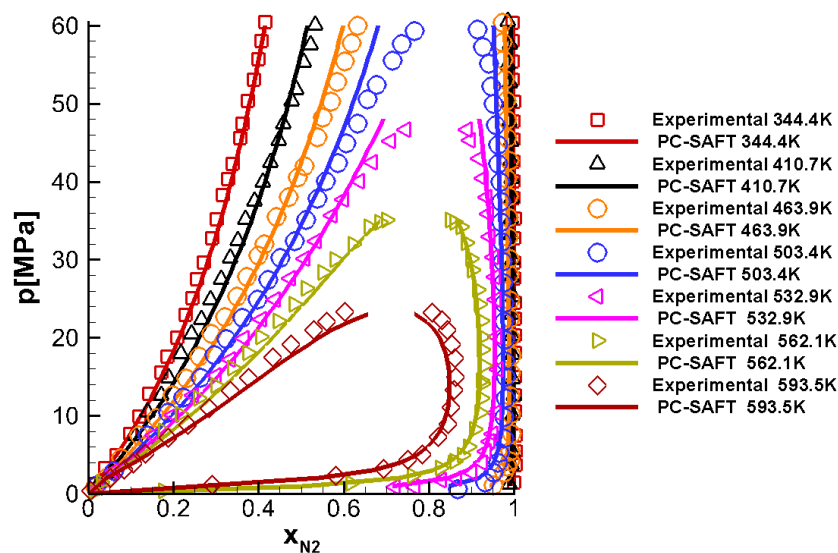
The validation of the thermodynamic solver was performed employing the experimental results of [31], see Figure 2.

## Results and discussion

The working fluids employed are the following: (i) a mixture of n-octane, n-dodecane and n-hexadecane; (ii) a pseudo-component that replicate the properties of the previous mixture; (iii) a pseudo-component that replicate the properties of the VOA Diesel.

### (i) Shock Tube Problem

The working fluids employed are a mixture of n-octane, n-dodecane and n-hexadecane (Table 3) and a pseudo-component that replicate the properties of the mixture (Table 4). The domain is  $x \in [-0.5, 0.5]$  m; 800 equally spaced cells were employed; wave transmissive boundary conditions are used in the left and right sides; the simulated time is  $5 \cdot 10^{-4}$  s; the initial conditions in the left state are  $\rho_L=438\text{kg/m}^3$ ,  $T_L=859.5\text{K}$ ,  $u_L=0\text{m/s}$ ; and in the right state are  $\rho_R=100\text{kg/m}^3$ ,  $T_R=1744\text{K}$ ,  $u_R=0\text{m/s}$ . Figure 3 presents the density, temperature, pressure, velocity, speed of sound and internal energy results. The pseudo-component results are the same as the multicomponent ones indicating that the methodology developed by [28] can be used to model complex hydrocarbon mixtures as a pseudo-component in CFD simulations.



**Figure 2.** Experimental [31] and calculated pressure-composition phase diagram for the  $\text{N}_2$  (1) +  $\text{C}_{12}\text{H}_{26}$  (2) system. Solid lines: PC-SAFT EoS with  $k_{ij} = 0.144$  [31].

### (ii) Diesel jet

A structured mesh is applied with a uniform cell distribution; the domain used is 12mm x 6mm; 1,216,800 cells are employed; the parabolic sub-step is included into these simulations without sub-grid scale modelling for turbulence or heat/species diffusion; the CFL number is set at 0.5; the fifth-order WENO discretization scheme presented in [21] is used; transmissive boundary conditions are applied at the top, bottom and right boundaries while a wall condition is employed at the left boundary; a flat velocity profile is imposed at the inlet; the velocity of the jet is 600 m/s; the diameter of the exit nozzle is 0.1mm; the case is initialized using a pressure in the chamber of 11 MPa; the temperature of the nitrogen is 973 K; and the temperature of the injected fuel is 363K. The loops where the hyperbolic fluxes, parabolic fluxes, update of conservative variables and thermodynamic solver are solved (see Appendix) were paralleled employing OpenMP (24 physical cores were employed). Some instabilities were observed in the initialization as [17] reported. To solve this problem, a ramp is used to accelerate the fuel to 600m/s. The binary interaction parameter applied is  $k_{ij} = 0.1446$ . Figure 4 shows the density, temperature, pressure and overall vapor fraction on a molar basis at  $3.04 \times 10^{-5}$  s. The computational time required to solve  $3.3 \times 10^{-5}$  s was 92.1 hours. A lot of time is invested on solving the multidimensional Newton-Raphson method of the cells that are in a VLE state. At these conditions, the derivatives of the Jacobian matrix are calculated numerically. The developed methodology is fast enough to perform simulations at affordable time scales. It should also be considered that the results are equivalent to a multicomponent injection of a Diesel surrogate of 4 components that vaporize when

mixed with hot nitrogen. This methodology makes the simulation time independent of the number of compounds present in the fuel and thus, allowing the real composition of a specific fuel to be utilised in CFD simulations.

### Conclusions

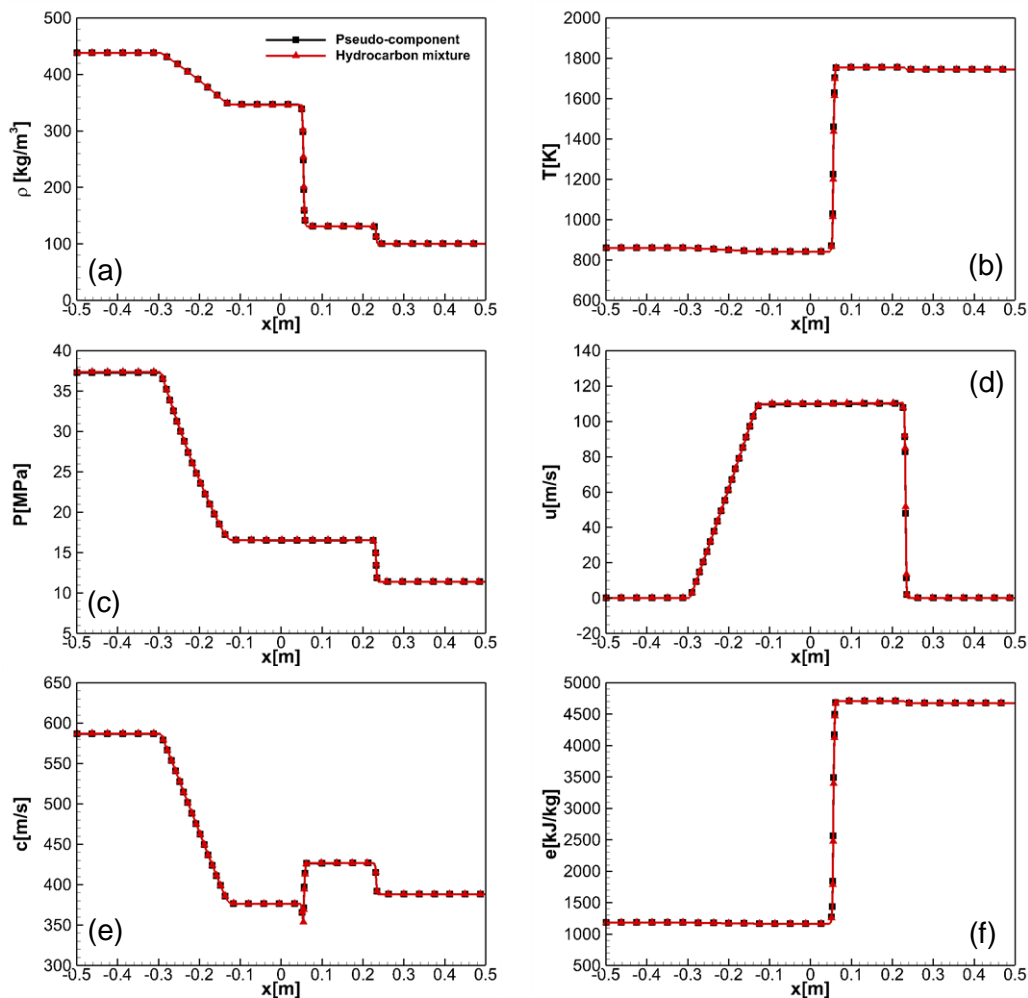
This conference paper presents a novel numerical framework that combines PC-SAFT and VLE calculations in a density-based, fully conservative solver of the Navier-Stokes and energy conservation equations to simulate fuel-air mixing at high-pressure conditions. By coupling VLE calculations with the PC-SAFT model, subcritical simulations can be carried out. A purely predictive method that employs the PC-SAFT EoS for developing pseudo-components, which are defined to replicate the properties of complex hydrocarbon mixtures (e.g., diesel fuels), has been completed and validated to be used in CFD simulations. Then, complex hydrocarbon mixtures can be modelled as a single pseudo-component knowing its number averaged molecular weight and the hydrogen-to-carbon ratio. This methodology makes the simulation time independent of the number of compounds present in the fuel and thus, allowing the real composition of a specific fuel to be utilised in CFD simulations.

**Table 3.** Molar composition of hydrocarbon mixture employed in the shock tube problem [28]

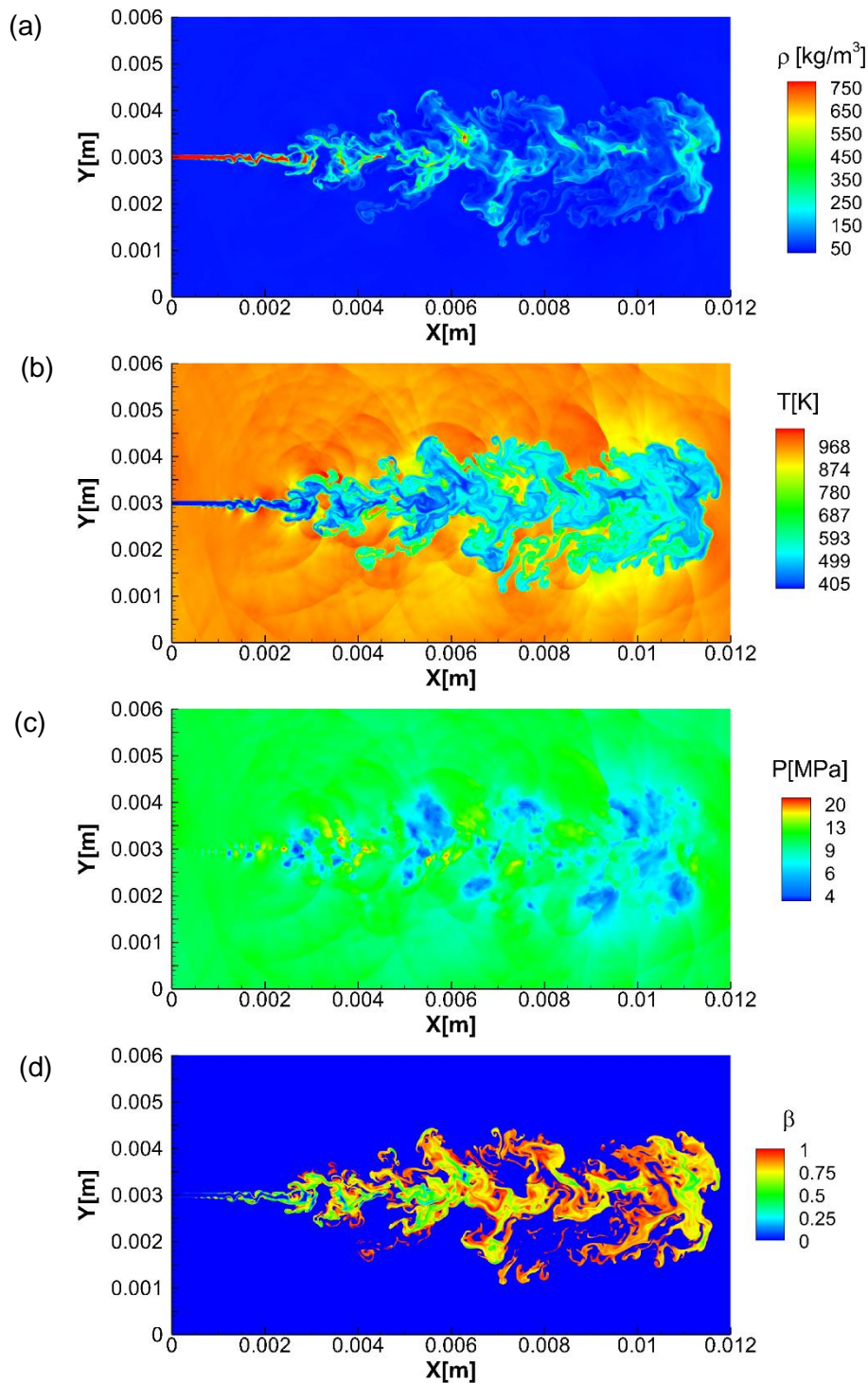
Compound	Hydrocarbon mixture (Molar composition)
n-hexadecane	0.232
n-octane	0.460
n-dodecane	0.232

**Table 4.** PC-SAFT pure component parameters employed to model the pseudo-component employed in the shock tube problem

Compound	$m$	$\sigma$ (Å)	$\epsilon/k$ (K)
Pseudo-component	7.387	3.400	234.47



**Figure 3.** Shock Tube Problem. CFL = 0.5, 800 cells,  $t=5 \cdot 10^{-4}$  s. Comparison of the (a) density, (b) temperature, (c) pressure, (d) x-velocity, (e) sonic fluid velocity, (f) internal energy using as working fluids are a mixture of n-octane, n-dodecane and n-hexadecane (Table 3) and a pseudo-component that replicate the properties of the mixture (Table 4) [28].



**Figure 4.** CFL = 0.5, 1,216,800 cells. Results of the simulation of the V0A Diesel pseudo-component jet at  $t = 3.04 \times 10^{-5}$  s.: (a) density, (b) temperature, (c) pressure, and (d) overall vapor fraction on a molar basis.

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### Nomenclature

#### List of abbreviations

CFL	Courant–Friedrichs–Lewy
EoS	Equation of State
HLLC	Harten-Lax-van Leer-Contact
PR	Peng-Robinson
PC-SAFT	Perturbed Chain Statistical Associating Fluid Theory
VLE	Vapor-Liquid Equilibrium
WENO	Weighted Essentially Non-Oscillatory



### List of Symbols

$c$	Sound speed [ $\text{m s}^{-1}$ ]
$\beta$	Overall vapor fraction on a molar basis
$p$	Pressure [Pa]
$T$	Temperature [K]
$\mathbf{U}$	Conservative variable vector
$\mathbf{F}$	x-convective flux vector
$\mathbf{G}$	y-convective flux vector
$\mathbf{F}_V$	x-diffusive flux vector
$\mathbf{G}_V$	y-diffusive flux vector

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