Complex multicomponent real-fluid thermodynamic model for high-pressure Diesel fuel injection

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Introduction

To correctly model the combustion in Diesel engines one needs to characterise the atomisation and mixing of sprays. 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 [1]–[3]. However, this approximation presents some limitations to accurately model 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 [4]. Still, they are sensitive to calibration parameters. In [5], [6] an Eulerian density-based methodology was employed to simulate the primary atomisation of the injected liquid considering compressibility effects. A single-phase dense-gas approach was applied. However, in n-dodecane/nitrogen mixtures the critical temperature 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/n-dodecane mixtures, the Vapor-Liquid Equilibrium (VLE) state must be included in the simulation. In [7], [8], a thermodynamic solver that can compute the properties of a homogenous mixture in supercritical or subcritical states was implemented in a multi-species two-phase model. The Large Eddy Simulations (LES) of the Spray A benchmark case of the Engine Combustion Network (ECN) performed in [7], [8], show a high degree of agreement against the available experimental data. However, the authors pointed out the issues of employing cubic EoS for modelling hydrocarbon properties at temperatures found inside the injection system. Due to the error in the density prediction of n-dodecane, it was necessary to increase the injection velocity to match the mass-flow measurement leading to an error in the predicted velocity. As a solution to these issues, we have coupled the molecular-based Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) with Vapor-Liquid Equilibrium (VLE) calculations in a density-based solver of the Navier-Stokes equations. The PC-SAFT EoS presents a precision similar to NIST (REFPROP), but without the need of an extensive calibration. Moreover, PC-SAFT can flexibly handle the thermodynamic properties of multi-component mixtures, and complex hydrocarbon mixtures can be modelled as a single pseudo-component [9]. All the details about the developed numerical algorithm have can be found in [10].

Material and methods

The Navier-Stokes equations for a non-reacting multi-component mixture containing N species have been solved employing the finite volume method on a Cartesian numerical grid. Operator splitting 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. The temporal integration is carried out using a second-order Runge–Kutta (RK2) scheme. The model developed by [11] is used to calculate the dynamic viscosity and the thermal conductivity. The HLLC (Harten-Lax-van Leer-Contact) solver is employed to compute the convective fluxes. A thermodynamic solver inspired by the work of [7] is employed to approximate the mixture thermophysical properties by performing PC-SAFT and VLE calculations. It is employed to compute temperature, pressure, sound speed and enthalpy once the conservative variables have been updated. The inputs are the density, internal energy and mass fraction of the components. Three PC-SAFT parameters per compound (number of segments per chain, energy parameter and segment diameter) are specified in the initialisation. By checking the molar fractions of the components, it can be determined whether only one phase exists or the state of the mixture is unknown. If the state of 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. If the state of the mixture is unknown, 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. The isothermal-isobaric flash problem (TPn flash) is solved if the stability analysis reveals an unstable mixture.

Diesel jet

Diesel is modelled using a technique developed by [9], which employs the PC-SAFT to define a single pseudo-component that represent the compounds found in a complex hydrocarbon mixture. This model allows to consider the actual composition of the Diesel fuel in CFD simulations, and makes the simulation time independent of the number of Diesel compounds. A structured mesh is applied with a uniform cell distribution; the domain used is 12mm × 6mm; 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 10.5 MPa; the temperature of the nitrogen is 970 K; and the temperature of the injected fuel is 360K. The evaporation of the Diesel can be observed in Figure 1, which shows the overall vapor fraction of the Diesel jet on a molar basis at different times.

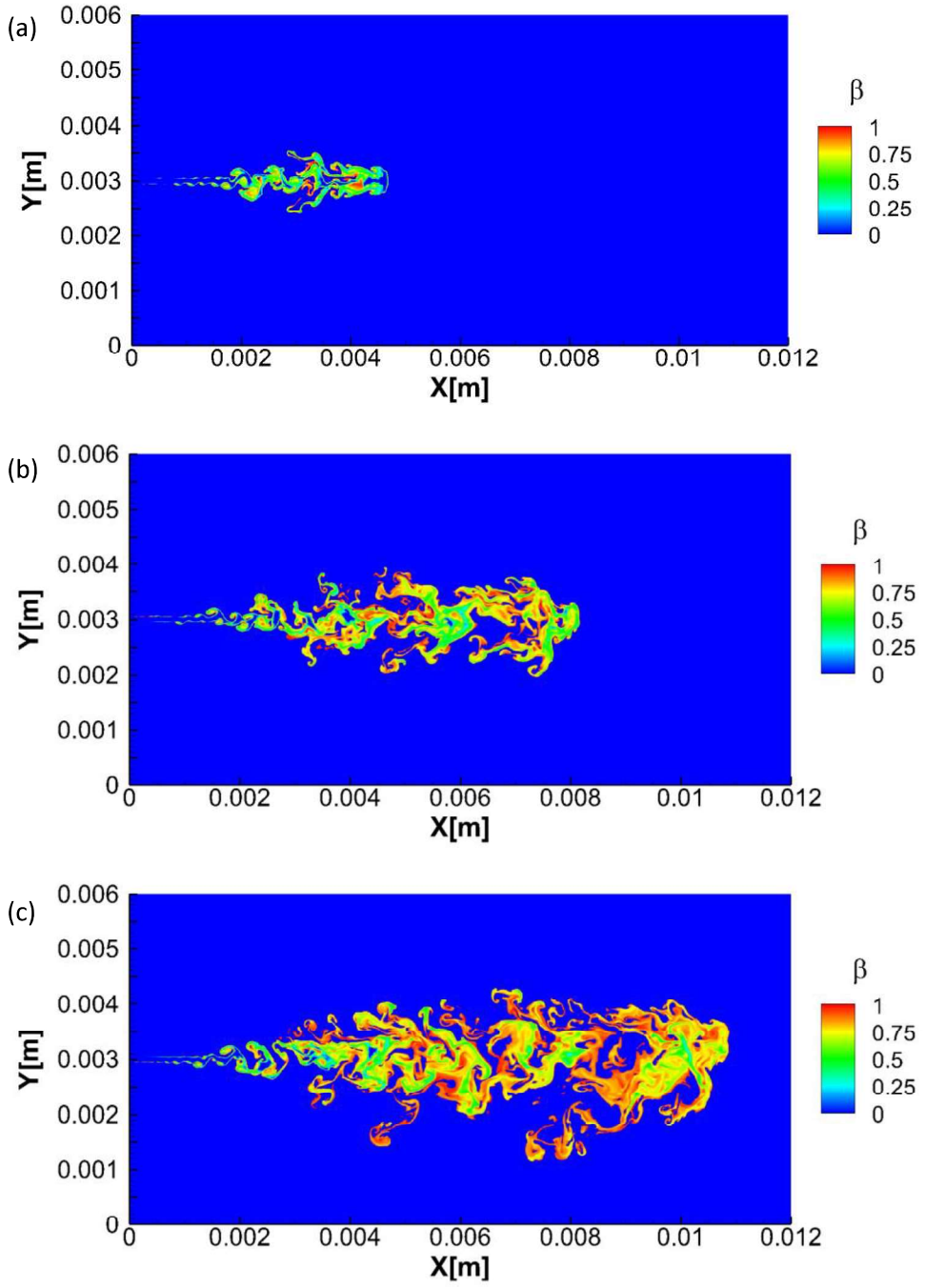

Figure 1. Overall vapor fraction on a molar basis of the Diesel injection at (a) t = 1.06×10^{-5} s, (b) t = 1.87×10^{-5} s and (c) t = 2.7×10^{-5} s.

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 [m s-1]
β	Overall vapor fraction on a molar basis
p	Pressure [Pa]
T	Temperature [K]

References

[1] Y. Pei, E. R. Hawkes, S. Kook, G. M. Goldin, and T. Lu, "Modelling n -dodecane spray and combustion with the transported probability density function method," *Combust. Flame*, 2015.

[2] Y. Pei *et al.*, "Large eddy simulation of a reacting spray flame with multiple realizations under compression ignition engine conditions," *Combust. Flame*, vol. 000, pp. 1–14, 2015.

[3] M. Jangi, R. Solsjo, B. Johansson, and X. Bai, "International Journal of Heat and Fluid Flow On large eddy simulation of diesel spray for internal combustion engines," *Int. J. HEAT FLUID FLOW*, vol. 53, pp. 68–80, 2015.

[4] S. Tonini, M. Gavaises, and A. Theodorakakos, "Modelling of high-pressure dense diesel sprays with adaptive local grid refinement," *Int. J. Heat Fluid Flow*, 2008.

[5] L. Hakim, G. Lacaze, and J. Oefelein, "Large Eddy Simulation of Autoignition Transients in a Model Diesel Injector Configuration," 2016.

[6] G. Lacaze, A. Misdariis, A. Ruiz, and J. C. Oefelein, "Analysis of high-pressure Diesel fuel injection processes using LES with real-fluid thermodynamics and transport," *Proc. Combust. Inst.*, 2015.

[7] J. Matheis and S. Hickel, "Multi-component vapor-liquid equilibrium model for LES of high-pressure fuel injection and application to ECN Spray A," *Int. J. Multiph. Flow*, vol. 99, pp. 294–311, 2017.

[8] J. Matheis and S. Hickel, "Multi-component vapor-liquid equilibrium model for LES and application to ECN Spray A," *arXiv Prepr. arXiv1609.08533*, 2016.

[9] H. B. Rokni, A. Gupta, J. D. Moore, M. A. McHugh, B. A. Bamgbade, and M. Gavaises, "Purely predictive method for density, compressibility, and expansivity for hydrocarbon mixtures and diesel and jet fuels up to high temperatures and pressures," *Fuel*, vol. 236, no. August 2018, pp. 1377–1390, 2019.

[10] C. Rodriguez, H. B. Rokni, P. Koukouvinis, A. Gupta, and M. Gavaises, "Complex multicomponent real-fluid thermodynamic model for high-pressure Diesel fuel injection," *Fuel*, p. Accepted Manuscript, 2019.

[11] T. H. Chung, M. Ajlan, L. L. Lee, and K. E. Starling, "Generalized multiparameter correlation for nonpolar and polar fluid transport properties," *Ind. Eng. Chem. Res.*, vol. 27, no. 4, pp. 671–679, Apr. 1988.