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Exploring the interaction between phase separation and turbulent fluid dynamics in multi-species supercritical jets using a tabulated real-fluid model

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1. Abstract

Today, injection of liquid fuels at supercritical pressures is a frequently used technique to improve the efficiency of energy systems and address environmental constraints. This paper focuses on the analysis of the coupling between the hydrodynamics and thermodynamics of multi-species supercritical jets. Various phase transition phenomena, such as droplet formation process by condensation, which have been shown experimentally to significantly affect the flow and mixing dynamics of the jet, are studied. For this purpose, a tabulated multicomponent real fluid model assuming vapor-liquid equilibrium is proposed for the simulation of turbulent n-hexane jets injected with different inflow temperatures (480 K, 560 K, 600 K) into supercritical nitrogen at 5 MPa and 293 K. Numerical results are compared with available experimental data but also with published numerical studies, showing a good agreement. In addition, comparisons between different turbulence models, including the LES Sigma, Smagorinsky and RANS $K - \epsilon$ models have been performed, showing the relevance of the LES Sigma model for these very complex two-phase flows.

Keywords: Real fluid model; Vapor-liquid equilibrium; Tabulation; Multicomponent; Large-eddy simulation; Condensation; Droplet formation process.

2. Introduction

In modern high-performance engines, the operating pressures now approach or exceed the critical pressures of the working fluids to increase the engine's efficiency and reduce CO_2 emissions. However, the injection is such that the propellant may enter the chamber at subcritical (cryogenic temperature) or supercritical temperature, corresponding to liquid-like (LL) or gas-like (GL) states, respectively [1–3]. The properties in these states significantly deviate from the ideal gas as they introduce some thermodynamics' non-idealities and transports anomalies. Two-phase flows covering (LL) and (GL) conditions are known in the literature as the transcritical regime [1–9]. At subcritical conditions, the phase transition phenomena are either classified as evaporation or condensation. Generally, it has been accepted that the subcritical liquid-to-gas transition is characterized by a structural change from an ordered (liquid) to a disordered (gas) state. In this case, density can be chosen as the appropriate order parameter, which exhibits a sharp discontinuity when phase transition occurs [10–12]. Besides, pseudo phase transition (i.e. pseudo-boiling or pseudo-condensation) may occur in the supercritical state at the crossover between LL and GL fluids, where the density changes sharply but continuously. The locus where this sharp transition from LL and GL fluids is currently not well understood. The Widom line [3, 8, 10, 11], defined as the heat capacity maximum, is usually used to separate the LL and

GL supercritical fluids. However, the Widom line cannot be clearly defined at high pressure and high temperature (see Figure 1(b)), where the minima of the thermal diffusivity coefficients are found to be more appropriate by Gorelli et al. [12] for tracking the transition between the supercritical LL and GL fluids. In the pseudo-boiling transition, no structural change has been observed in macroscopic light scattering experiments [6, 7]. As such, these phenomena share a nonlinear behavior similar to that of the subcritical condition when the coexistence line is crossed, as illustrated in Figure 1. For pure n-Hexane (C_6H_{14}), this figure shows the phase transition in subcritical states (i.e., evaporation and condensation processes) when the coexistence line is crossed. Also, the gradual phase-change processes in the transcritical regime (i.e., pseudo-boiling and pseudo-condensation) as soon as it meets the Widom line. This illustrates that phase transition, including bubble or droplet formation process, evaporation, and condensation, are mainly driven by changes in pressure or temperature for a single-component fluid.

As a matter of fact, researcher's interest in the behavior of supercritical fluids dates back to at least 1869 [13]. However, despite recent theoretical, experimental, and computational efforts, these phenomena are still not fully understood especially for multicomponent systems. In the past decades, extensive studies have been performed for understanding the behavior of a single-component phase transition [3, 8, 9, 12, 14–18]. One of the pioneering and remarkable studies was conducted by Chehroudi et al. [15]. They experimentally studied the jet behavior of pure liquid nitrogen injected into gaseous nitrogen at subcritical and supercritical pressures. They observed that in subcritical pressures, due to the significant surface tension, the interface between the liquid and the gas plays an important role, and it leads to the appearance of the primary and secondary breakup, known as classical atomization. However, as the pressure increases, the magnitude of the surface tension decreases and vanishes at the critical point, which suppresses the formation of ligaments and droplets for supercritical pressures. However, liquid-like ligaments (also called finger-like) could be seen in their shadowgraphy experimental results despite the absence of surface tension, especially for the transcritical injection regime. Therefore, injection above the critical pressure of a single-component propellant can be considered as a diffuse

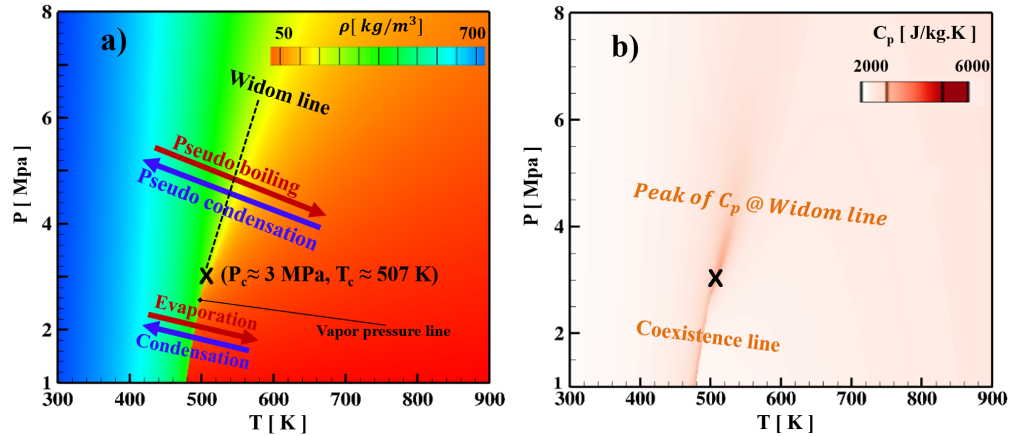


Fig. 1. Illustration of the phase transition in subcritical states (i.e., evaporation and condensation processes) when the coexistence line is crossed, and gradual phase change processes in the transcritical regime (i.e., pseudo-boiling and pseudo-condensation) when crossing the Widom line. Pressure-Temperature diagram: (a) Density contour mapped by coexistence and Widom lines, and (b) Heat capacity contour for C_6H_{14} . Nonlinear behavior is present along the Widom line but also along the liquid-vapor coexistence line.

interface mixing process rather than a classical atomization of the interface. However, the same is not valid for multicomponent systems for which the local critical pressure of the mixture could dramatically exceed the value of the pure components. Indeed, various studies have been carried out for multicomponent systems, and their interfacial phase transition has been revealed to be more complex than for a single-component system, mainly due to the variation of the mixture critical point with the local composition of the fluid [8, 17, 19–25]. Furthermore, this difference in phase transition mechanisms between single and multicomponent systems leads to various interface structures that influence the jet behavior [1, 8, 21, 22]. Crua et al. [1] studied the injection of liquid (n-heptane, n-dodecane, n-hexadecane) into supercritical nitrogen at different temperatures and pressures. They investigated the transition from a two-phase to a single-phase mixing regime and established a criterion for switching between the two regimes as a function of the critical temperature and pressure of the pure fuels. However, due to the limited accuracy of the experimental setup, reliable data are still lacking for the precise identification of the transition between the two-phase and single-phase mixing regime that could be used for validating numerical models. In addition, there are still multiple doubts and questions about the conditions and mechanisms behind the interface disappearance for multicomponent systems.

Other interesting experimental studies have recently been done by Gerber et al. [6, 7]. These studies focused in particular, on under-relaxed jets for which a shock waves train was observed in the near nozzle region. They concluded that high-pressure jets have the same scattering footprint and morphological properties as low-pressure jets. However, enhanced scattering is only observed upon multiple crossings of the Widom region, e.g., due to the series of rapid recompressions caused by the shock train. This enhanced scattering is caused by the enhancement in compressibility and density fluctuation when the fluid switches between LL and GL. Therefore, the experimental findings of Gerber et al. [6, 7] show that density fluctuations are not negligible across the Widom line. They can be detected both at the macroscopic (continuum) and molecular scale. Indeed, these findings were confirmed at molecular scales by the small-angle X-ray scattering experiments in [26]. This completely changes the physical meaning of pseudo-boiling/pseudo-condensation transition from the subcritical counterpart (evaporation/condensation).

Another interesting study was recently carried out by Traxinger et al. [21]. They experimentally and numerically studied a multicomponent system consisting of a high-pressure n-hexane jet at three different temperatures (480K, 560K, 600K), injected into a chamber filled with supercritical nitrogen at ($P = 5\text{ MPa}$ and $T = 293\text{ K}$). Specifically, the focus was on the phase separation of an initially supercritical fluid due to the interaction with its surrounding. Simultaneous shadowgraphy and elastic light scattering (ELS) experiments were conducted by Traxinger et al. [21] to capture both the flow structure as well as the phase separation. Remarkable results have been shown experimentally for the case of supercritical n-hexane with $T=560\text{ K}$, exceeding its critical temperature and pressure, injected into supercritical nitrogen at $T = 293\text{ K}$ and $P = 5\text{ MPa}$. Indeed, the condensation of n-hexane has been observed in these conditions, as expected from their prior thermodynamic study. The phase transition is initiated in the mixing layer some distance downstream of the nozzle and eventually mixes with the jet core at large distances. In addition, at a higher injection temperature of n-hexane ($T = 600\text{ K}$), this phenomenon of phase transition does not occur, and the gaseous fuel injected into the chamber gradually mixes with the ambient gas. Finally, a classical subcritical atomizing n-hexane jet was imaged at the lowest n-hexane injection temperature ($T = 480\text{ K}$). The various experimental and numerical results of Traxinger et al. [21] will be used in the present work to validate our Computational Fluid Dynamics (CFD) tabulated Real-Fluid Model (RFM) presented in Section 3.

Developing a CFD model capable of handling subcritical, transcritical, and supercritical conditions, including possible phase transition, is crucial to enable a more accurate analysis of multicomponent systems. To study these complex behaviors, it is therefore essential to use a real fluid model capable of automatically switching from a single-phase flow to a two-phase

flow, and vice versa [8, 17, 21, 24, 25]. However, real fluid simulations have been proven to be computationally time-consuming. Indeed, it has been found that the complexity of cubic EoS and solving the Vapor-Liquid-Equilibrium (VLE) iteratively using the isoenergetic-isochoric (UVn)-flash set of equations are computationally expensive [8, 17, 24, 25, 27–30]. Therefore, an accurate, robust, and most importantly an efficient real-fluid model is required, which is one of the main objectives of the presented work. A remedy for this problem is to set up a table before the start of the simulation and store the values of the required thermodynamic properties in it. Then, rapid searching, as well as an interpolation, are carried out in the table during the simulation. This process of searching and interpolation is usually called “a look-up table” in the literature. More details about tabulation, interpolation, and look-up of data can be found in [8, 31–36].

In summary, in this study, a fully compressible, multicomponent real fluid model accounting for VLE is proposed using a generalized three-dimensional (3D) tabulation method [8, 30, 31]. The tabulated thermodynamic properties of the binary mixture are calculated as a function of temperature (T), pressure (P), and mass fraction of the first species in the mixture (Y). In this model, an in-house thermodynamic library IFPEN-Carnot is used to generate a 3D table (with T-P-Y as the axis for a binary mixture) based on various real fluid EoS. This IFPEN-Carnot thermodynamic library includes different EoSs, such as Peng-Robinson (PR-EoS) [37], Soave-Redlich-Kwong (SRK-EoS) [38], and Cubic Plus Association (CPA-EoS) [39], which also represents one of its main advantages [8, 40]. For computational speed and robustness, a uniform look-up table is generated based on an isothermal-isobaric TPn-flash [8, 17, 25, 29]. The RFM model was implemented together with the generalized 3D tabulation method in CONVERGE solver [41].

This paper is organized as follows. Section 3 is dedicated to the explanation of the numerical and theoretical methods, including the governing equations, thermodynamic tabulation, and look-up methods. Section 4 is devoted to understanding the condensation phenomenon during the supercritical injection of hexane into nitrogen using the proposed RFM model. In addition, comparisons between various turbulence models, including large-eddy simulations (LES Sigma [42] and Smagorinsky [43]) models as well as a Reynolds Averaged Navier-Stokes (RANS $K-\epsilon$) [44] model will be carried out and discussed. Subsequently, the numerical results in sections 4 and 5 are compared with available experimental data, but also with published numerical studies. Finally, this paper is summarized and the conclusions are presented in section 6.

3. The real-fluid RFM model

The real-fluid RFM model [8, 40, 45] used in the current work is presented in this section. It is a fully compressible model developed under the homogeneous equilibrium modeling (HEM) assumption, considering multicomponent in both phases. Indeed, the RFM model has been developed assuming the two-phase system to be under the assumptions of thermodynamic equilibrium (i.e., equilibrium of the velocity, pressure, temperature, and chemical potential at liquid-vapor interfaces). This assumption guarantees the required hyperbolic mathematical formulation for the RFM model. The set of governing equations as employed in the CONVERGE CFD solver [41] has been used as a base framework for the development of the tabulated RFM model presented below. More details about this modelling approach could be found in Jafari et al. [8].

3.1. Governing equations of the flow solver

The set of governing equations are presented through equations (1 - 4) including the density transport equation, species transport equation, mixture momentum equation and mixture specific internal energy equation, respectively. (ρ , u_i , P , T , e) are the mixture’s density, velocity, pressure, temperature, and specific internal energy, respectively. (Y_m , h_m) are mass fraction and enthalpy

of species (m) in the mixture, respectively. N_s is the total number of species.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial \rho Y_m}{\partial t} + \frac{\partial \rho Y_m u_j}{\partial x_j} = \frac{\partial}{\partial x_j} (\rho D \frac{\partial Y_m}{\partial x_j}), m = \{1 \dots N_s - 1\} \quad (2)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (3)$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u_j}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} (\lambda \frac{\partial T}{\partial x_j}) + \frac{\partial}{\partial x_j} (\rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j}) \quad (4)$$

where the viscous stress tensor (τ_{ij}) is given by

$$\tau_{ij} = \mu (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) - 2/3 \mu (\frac{\partial u_k}{\partial x_k}) \delta_{ij} \quad (5)$$

It is worth mention that the calculations of the real fluid thermodynamic properties are performed based on the residual approach [17,46]. In this approach, any thermodynamic function is computed from the sum of an ideal gas part and a residual part. The ideal gas part is determined from a specific polynomial equation [47]. While the residual part, which represents the deviation from the ideal gas behavior is deduced from the employed equation of state (EoS). More details can be found in our previous studies [17,25]. Besides, the thermal conductivity (λ) and the dynamic viscosity (μ) cover laminar and turbulent contributions, as cumulative transport properties of the fluid. The laminar contribution of (λ, μ) is computed by Chung et al. [48] correlations. The turbulent conductivity is calculated using a given turbulent Prandtl number Pr_t , as ($\lambda_t = \frac{C_p \mu_t}{Pr_t}$), where (C_p) is the isobaric heat capacity and the turbulent viscosity (μ_t) is computed by the adopted turbulence model. Also, the laminar, and turbulent diffusion coefficients are estimated using given laminar and turbulent Schmidt numbers, (Sc) for $D = \mu/(\rho Sc)$, and (Sc_t) for $D_t = \mu_t/(\rho Sc_t)$, respectively. In this regard, various turbulence models including large-eddy simulations (LES Sigma [42] and Smagorinsky [43]) models as well as a Reynolds Averaged Navier-Stokes (RANS $K-\epsilon$) [44] model have been considered in this study (See Section 4) to investigate the effect of the turbulence modeling on the numerical results.

3.2. Numerical schemes

The above set of governing equations (1 - 4) of the two-phase RFM model is solved numerically using a diffuse interface modeling approach (DIM). In the CONVERGE CFD solver, all the dependent parameters are collocated at the center of the computational cell. To prevent checkerboarding, the Rhie-Chow algorithm is employed [49]. Besides, a second-order-accurate spatial discretization scheme, plus a first-order Euler temporal scheme, are used for the governing conservation equations discretization. The transport equations are solved using a density-based solver, where an extended Pressure Implicit with Splitting of Operators (PISO) algorithm, method of Issa [50], has been adapted for real fluid equations of state. More details on the modified PISO algorithm can be found Jafari et al. [8].

3.3. Equilibrium thermodynamic closure of the flow solver, and the tabulation look-up

For the supercritical jet with (C_6H_{14}, N_2) binary mixture, the real-fluid Peng-Robinson (PR) [37] equation of state (EOS) has been selected for the thermodynamic closure of the RFM model transport equations (1 - 4). A general form of this cubic EoS can be written as equations (6,7), along with the various parameters that are listed in Table 1 [37], where index (c) stands for

Table 1. Parameters for PR equation of state (index c stands for critical value)

δ_1	δ_2	$(a_c)_i$	m_i	b_i
$1 + \sqrt{2}$	$1 - \sqrt{2}$	$0.45727 \frac{R^2 T_c^2}{P_c}$	$0.37464 + 1.54226\omega - 0.26992\omega^2$	$0.0778 \frac{RT_c}{P_c}$

critical point value for a pure component when it appears as in T_c or P_c . Also, it is worth noting that local mixture critical point values are denoted by a (c, mix) index.

$$P = \frac{RT}{v - b} - \frac{a(T)}{(v + \delta_1 b)(v + \delta_2 b)} \quad (6)$$

$$a_i(T) = (a_c)_i \left[1 + m_i \left(1 - \sqrt{\frac{T}{T_c}} \right) \right]^2 \quad (7)$$

Besides, when the PR-EoS is used for mixtures, van der Waals mixing rules are applied as equation (8), where (k_{ij}) is the binary interaction parameter (BIP) that can be fitted to experimental data to well represent the phase diagram of a binary system, x_i is the molar fraction, and $a_i(T)$ is the parameter calculated using Equation (7) for component i. In this study, k_{ij} is set to zero.

$$a(T) = \sum_i \sum_j x_i x_j \sqrt{a_i(T) \cdot a_j(T) (1 - k_{ij})}$$

$$b = \sum_i x_i \cdot b_i \quad (8)$$

Generally, it is well known that cubic EoSs with van der Waals (vdW) mixing rule are not really well suited for computing densities [8, 25]. However, our achievement in this study demonstrate that the PR EoS [37] can acceptably predict the density and specific heat capacity for n-hexane (a relatively light component) at $P = 5 \text{ MPa}$, which are in an excellent agreement with the reference data taken from NIST [51], as shown in Figure 2.

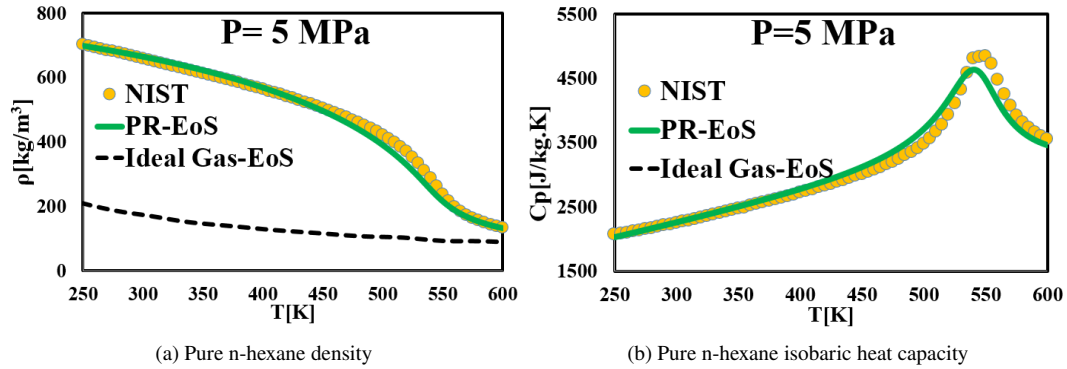


Fig. 2. Comparison of PR-EoS and ideal gas EoS with reference data obtained from NIST [51] for n-hexane at $P = 5 \text{ MPa}$ showing a) Density, and b) Isobaric heat capacity profiles. The results, using PR-EoS, Peng Robinson equation of state, are in a good agreement with NIST data [51], however the fluid properties specially for isobaric heat capacity (outside the range) significantly differ from an ideal gas at this high pressure $P = 5 \text{ MPa}$.

The current work adopts a tabulation approach, where the thermal and transport properties, as well as the phase states and compositions, are tabulated before the CFD simulation. During the simulation, the various tabulated properties, such as density, specific internal energy, isobaric heat capacity, isochoric heat capacity, viscosity, conductivity, gas volume fraction, and species liquid mass fraction in each phase, are linearly interpolated using three inputs, which are temperature (T), pressure (P), and species mass fraction in the mixture (Y_m , $m = 1 : N_s - 1$), where N_s is the total number of species. As we saw above for the binary systems ($N_s = 2$), Y_1 is subsequently denoted Y , as the third axis of the 3D-Table. In this study, this table is generated based on the IFPEN-Carnot thermodynamic library, which uses a robust isothermal-isobaric (TPn)-flash algorithm coupled with the PR-EoS. This tabulation approach offers the advantage of avoiding the direct evaluation of the non-linear cubic EoS along with the VLE calculation during the simulation, which has been proven to be computationally demanding and costly [8, 17, 25, 30, 31]. Moreover, the tabulation approach based on the IFPEN-Carnot thermodynamic library allows simulating different fuels and surrogates without the need of hard coding a (TPn) flash for each EoS of interest.

With respect to interpolating the data in the table during runtime, the simplistic inverse distance weighting (IDW) is implemented [52]. This critical step is mainly carried out during the simulation for two main tasks:

1. **A Table look-up function:**
Compute the thermal, transport properties as well as the phase state using the input parameters (T, P, Y_m) with $m = 1 : N_s - 1$.
2. **A Reverse look-up function:**
Compute/Update the temperature using the inputs (e, Y_m, P) once the mixture mass fraction (Y_m) and the energy (e) transport equations are solved for each pressure (P) in the PISO loop.

A general form of finding an interpolated value of u_i at a given point X based on samples $u_i = u(X_i)$, $i = 1, \dots, N$ using IDW can be expressed as equation (9), where $\omega_i(X) = \frac{1}{d(X, X_i)}$, X denotes an interpolated (arbitrary) point, X_i is an interpolating (known) point, d is the given distance from the known point X_i to the unknown point X , N is the total number of known points used in each local interpolation. $N = 8$ for uniform 3D table.

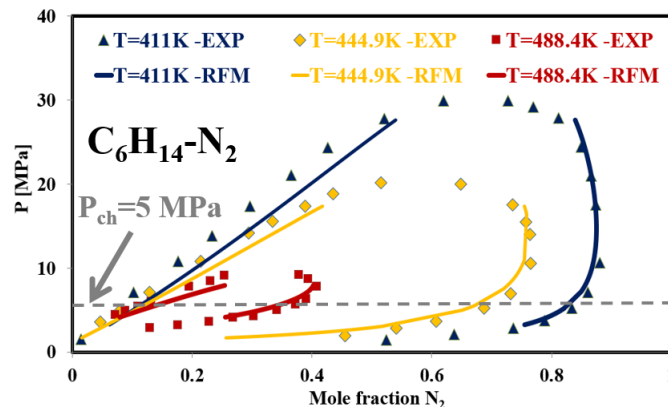


Fig. 3. Vapor-Liquid equilibrium of $C_6H_{14} - N_2$ calculated in this study using PR-EoS compared to the experimental data [53]

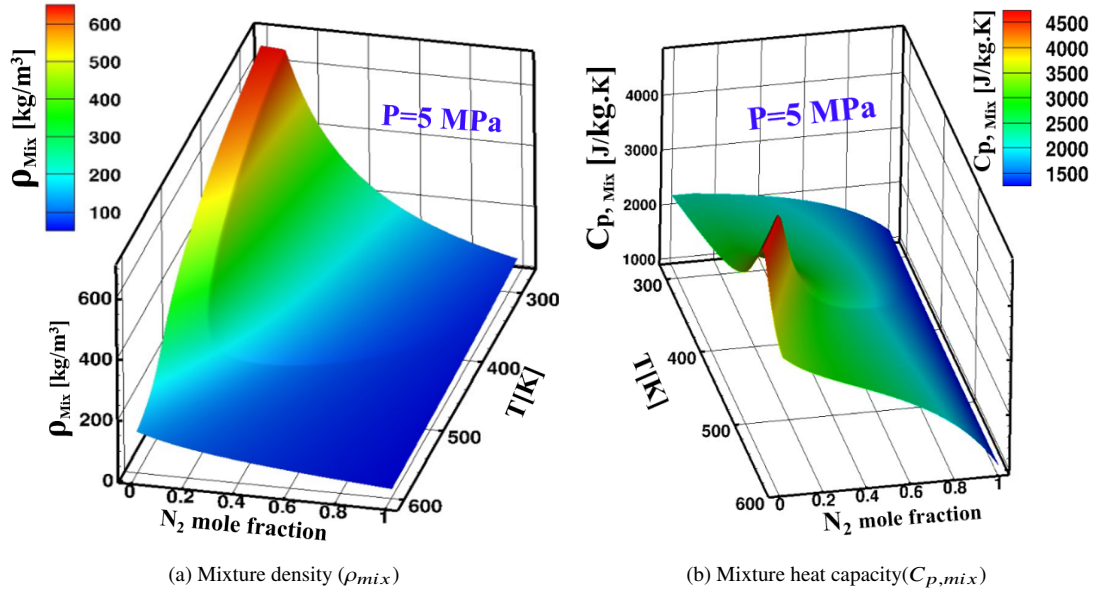


Fig. 4. Contour plots of (a) mixture density, and (b) mixture heat capacity for $C_6H_{14} - N_2$ at $P_{ch} = 5 MPa$. As the plots show, due to the different non-linearity for various properties, the grid independency for having a refined thermodynamic table is mandatory.

248

$$u(X) = \begin{cases} \frac{\sum_{i=1}^N \omega_i(X) u_i}{\sum_{i=1}^N \omega_i(X)} & \text{if } d(X, X_i) \neq 0 \text{ for all } i \\ u_i & \text{if } d(X, X_i) = 0 \text{ for some } i \end{cases} \quad (9)$$

249 3.4. Validation of the VLE solver

250 As explained in the introduction, the state properties deviate considerably from those of the ideal
 251 gas, as they introduce some thermodynamic non-linearity and a transport anomaly at supercritical
 252 pressures, as shown in Figure 2. Indeed, as it can be seen in Figure 2, compared to the density
 253 and isobaric heat capacity from NIST [51] for n-hexane at $P = 5 MPa$, ideal gas EoS cannot
 254 predict the transcritical behavior of such properties, ideal gas EoS is outside the range. However,
 255 more accurate and complex EoS, as PR EoS, can predict the transcritical behavior with a good
 256 agreement, especially for the isobaric heat capacity.
 257 To validate the VLE thermodynamic solver, the VLE for a binary mixture of $C_6H_{14} - N_2$ using
 258 PR-EoS has been compared with the available experimental data [53], as shown in Figure 3.
 259 It can be seen that the calculation results of the VLE solver are in good agreement with the
 260 experimental data over the entire ranges of pressure for the different temperatures. Furthermore,
 261 Figure 4(a,b) shows the variation of the mixture density and heat capacity, respectively, for a
 262 binary mixture of $C_6H_{14} - N_2$ as a function of temperature and N_2 mole fraction at $P=5 MPa$.
 263 These results have been obtained using a uniform table with $\Delta T = 1 K$, $\Delta Y_{N_2} = 0.005$ in grid
 264 sizes on the axis. Due to the different non-linearity of the properties shown in Figure 4(a,b), a
 265 grid independence for the thermodynamic table is mandatory, which should correctly capture
 266 various interesting phenomena such as the heat capacity peak ($C_{p,mix}$) around the Widom line
 267 for certain compositions of this multi-species system, see Figure 4(b). It is worth mentioning that
 268 the values of properties in two-phase region, in the vapor liquid equilibrium dome, are computed

from the mixing of the liquid and vapor phase properties using the vapor fraction, more can be found here [8, 17].

3.5. Analytical study of condensing supercritical jet

This section focuses on the analysis of the thermodynamic states of a condensing supercritical jet. As reported in the introduction, condensation of n-hexane has been recently shown experimentally by Traxinger et al. [21] when it is injected in supercritical state at $T_{inj} = 560K$ into a supercritical nitrogen at $T_{ch} = 293K$ and $P_{ch} = 5MPa$. They observed that condensation is initiated in the mixing layer and eventually mixes in the core of the jet forming a spray of droplets at great distance from the nozzle. In such conditions, the mixture temperature distribution in the chamber is usually varying in the range between $T_{inj} = 560K$ and $T_{ch} = 293K$. Indeed, assuming an adiabatic process neglecting heat exchange, the enthalpy of the mixture at equilibrium H_{mix} is equal to the weighted molar average of the enthalpy of the pure components, H_{N_2} and $H_{C_6H_{14}}$:

$$H_{mix}(T_{AM}, P_{ch}, z_{N_2}) = z_{N_2}H_{N_2}(T_{ch}, P_{ch}) + z_{C_6H_{14}}H_{C_6H_{14}}(T_{inj}, P_{ch}).$$

The adiabatic mixture temperature, denoted (T_{AM}) is the solution of this equation, as the enthalpy values are calculated using PR-EoS using our in-house thermodynamic library. z_{N_2} is the mole fraction of N_2 (with $z_{N_2} + z_{C_6H_{14}} = 1$). T_{inj} , T_{ch} , P_{ch} denote the temperature of the injected n-hexane at the exit of nozzle, the initial temperature of N_2 in the chamber, and the initial chamber pressure (here constant and equal to $5MPa$), respectively. More details on AMT can be found in [55]. Figure 5(a,b) displays the AMT temperatures (dashed lines) for two different chamber pressures at $P = 1MPa$ and $P = 5MPa$ in a T - x_{N_2} phase diagram (triangle) obtained using PR-EoS. As shown in Figure 5(a), the AMT, dash lines, are plotted with the same inflow temperature, $T_{inj} = 554.8K$ and chamber temperature, $T_{ch} = 293K$. For the low pressure case, $P = 1MPa$, the AMT does not cross the corresponding two-phase boundary, and hence the jet is supposed to stay in the single-phase mixing regime. However, for the higher pressure case, $P = 5MPa$, the AMT crosses the corresponding two-phase boundary very close to the N_2 mole fraction of one and it is therefore expected that the jet enters the two-phase region near the periphery of the jet as shown experimentally in Traxinger et al. [21]. In addition, it can be seen in Figure 5(a) that the slope (dT/dx) of the phase diagram (near $x_{N_2} = 1$) can control the phase separation process (condensation) and the formation process of spray droplets for certain temperature and pressure ranges of the supercritical injection regime. Besides, Figure 5(b) shows and confirms the same behavior for a constant pressure, $P = 5MPa$ but at two different n-hexane inflow temperatures, $T_{inj} = 554.8K$, and $T_{inj} = 595K$. Indeed, this figure shows that by increasing the inflow temperature to $595K$, the AMT no longer crosses the phase boundary. Therefore, this theoretical analysis has demonstrated that due to the slope (dT/dx) near $x_{N_2} = 1$ in the phase diagram, the periphery of a supercritical jet may or may not nucleate and condense. This proves that jet structure in a multicomponent system does not follow the same behavior as in a single-component jet. In summary, for supercritical jet of C_6H_{14} injected into N_2 colder ambient, droplet formation process by condensation are expected to be triggered at the jet's periphery when the AMT crosses the two-phase region. Otherwise, the periphery of the supercritical jet is going to mix with the ambient gas remaining in the supercritical regime without any droplet formation process. This supercritical droplet formation process/condensation phenomenon, which has been the subject of some recent studies [21, 22], will be investigated in more detail in the next section based on the tabulated RFM model applied in the LES numerical framework.

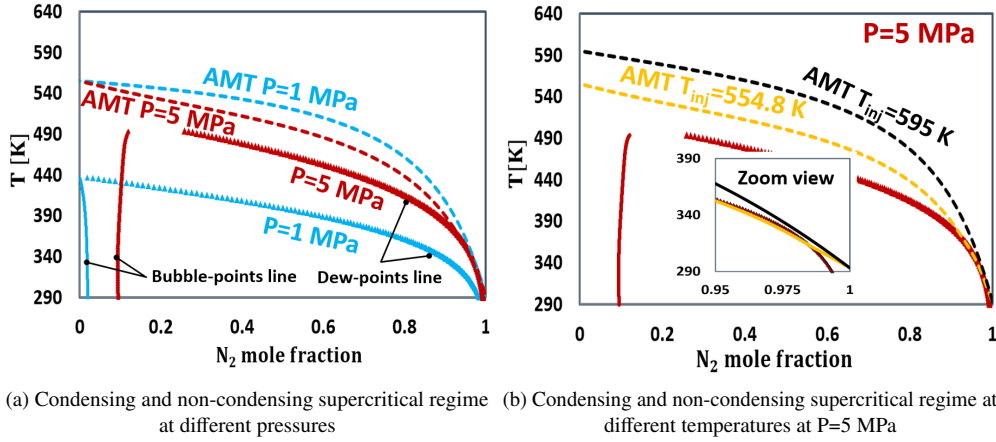


Fig. 5. Condensing and non-condensing supercritical regime (a) at different pressures, (b) at different temperatures. AMT denotes adiabatic mixing temperature, plotted by dash lines, and by crossing the phase boundary(dew points line), the droplet formation process, and the condensation begins and develops at the periphery of the jet. If the AMT doesn't cross the two-phase dome, it will remain at supercritical regime without any droplet formation process, non-condensing supercritical regime (single phase mixing regime).

4. Results and discussion

4.1. Test cases definition

This section is devoted to the numerical study of the turbulent jet mixing process of n-hexane (C_6H_{14}) injected into supercritical nitrogen (N_2). More precisely, following the investigations of Traxinger et al. [21], n-hexane is injected at three temperatures (480K, 560K, 600K) into a chamber initially filled with GN_2 at an ambient pressure of $P_{ch} = 5MPa$. The critical pressure and temperature of pure C_6H_{14} and N_2 are ($P_c \approx 3MPa$, $T_c \approx 507K$) and ($P_c \approx 3.4MPa$, $T_c \approx 126.2K$), respectively. Hence, the ambient pressure, 5MPa correspond to a reduced pressure $P_{r,C_6H_{14}} \approx 1.67$ for pure n-hexane, and $P_{r,N_2} \approx 1.47$ for pure N_2 . However, due to the mixing of two components, the mixture critical point will vary locally as function of the mixture composition. Therefore, with respect to the mixture critical temperature of $C_6H_{14} - N_2$ at $P_{ch} = 5MPa$, n-hexane is injected in subcritical state when it is at 480K and it is injected in a supercritical state when it is heated to 560K or 600K. The three simulation cases are summarized in Table 2, where $T_{t,C_6H_{14}}$ is the temperature in the injector reservoir. The temperature $T_{C_6H_{14}}$ as well as the mean velocity at the nozzle exit $u_{C_6H_{14}}$ were calculated based on the assumption of an isentropic nozzle flow as explained by Traxinger et al. [21].

4.2. Configuration setup

Figure 6(a,b) present the boundary conditions, the computational domain, as well a the mesh structure, respectively, employed in this study. The nozzle orifice diameter (D_i) is $236\mu m$, as can be seen in this figure on the left side of the hexahedral computational domain. The length and width of the grid are $90D_i$ and $40D_i$, respectively. These dimensions proved to be large enough to avoid edge effects on the numerical results. The base grid size was set to $30\mu m$. Besides, fixed embedding has been used to refine the grid at specific locations especially near the nozzle exit, where the grid size was specified to be $7.5\mu m$. This minimum value is the same refined value used in [21]. At the jet inlet, uniform velocity and temperature profiles for $u_{C_6H_{14}}$ and $T_{C_6H_{14}}$ are used, as defined in Table 2. In addition, no-turbulent fluctuations are specified at the inlet

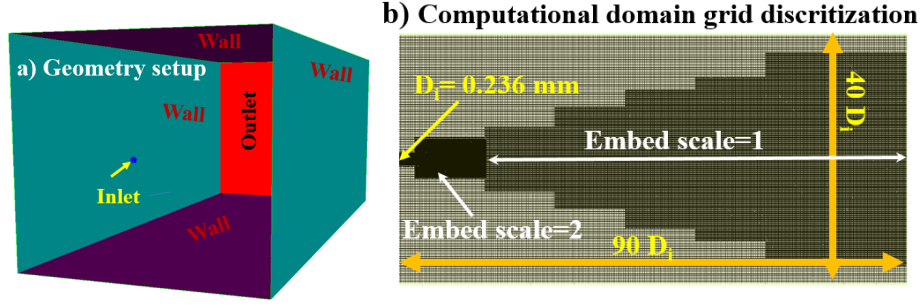


Fig. 6. Schematic of the injector setup as (a) Geometry setup, and (b) Computational domain grid discretization. Fixed embedding has been used to refine the grid at specific locations in the domain. (Local grid size = (Base grid size) / 2^{embed_scale}). The base grid size was set to $30\mu\text{m}$ so that the minimum grid size near the nozzle exit has been specified to be $7.5\mu\text{m}$ using an $embed_scale = 2$.

injection boundary. A pressure outflow boundary condition is used for the outlet boundary. The chamber pressure for all the cases were set to $P_{ch} = 5\text{MPa}$. No-slip and adiabatic conditions are specified for the walls indicated in Figure 6(a). The time step is automatically adjusted in the solver based on a maximum Courant-Friedrichs-Lewy (CFL) number of 50 reaching a value in the range of $[10^{-8} - 10^{-9}]$ seconds.

4.3. RFM model results

Figure 7(a,b), respectively, shows the numerical results of the RFM model, obtained when the LES-Sigma turbulence model [42] is employed, in terms of mixing temperatures versus AMT for the three different test cases (T480, T560, and T600) defined in Table 2. Specifically, Figure 7(a) demonstrates a good agreement between the predicted phase boundary calculated in this study compared with [21]. The low scattering of the LES mixing temperatures in Figure 7(a) indicates almost adiabatic mixing injection (between n-hexane and N_2). The graphical insert shows that the LES mixing temperature scatter plots for the T560 case do intersect the dew line, enter the two-phase region and may induce condensation. Figure 7(b) includes the theoretical AMT (defined in Section 3.5) for the three cases and show the same behavior as the RFM model for case T560.

In Figure 8(a-c), the experimental single-shot images of [21] (left frame 1) are qualitatively

Table 2. Operating conditions used for the current numerical study similar to the experimental study of [21].

Case	$P_{ch}[\text{MPa}]$	$T_{ch}[\text{K}]$	$T_{t,C_6H_{14}}[\text{K}]$	$T_{C_6H_{14}}[\text{K}]$	$u_{C_6H_{14}}[\text{m/s}]$	Injection state
T480	5	293	480	479.3	51	subcritical
T560	5	293	560	554.8	72.1	supercritical (condensing)
T600	5	293	600	595	90.3	supercritical

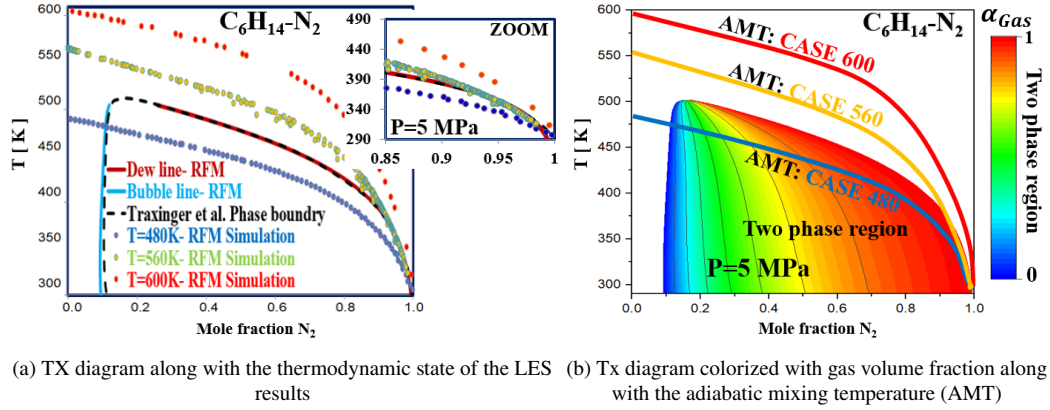
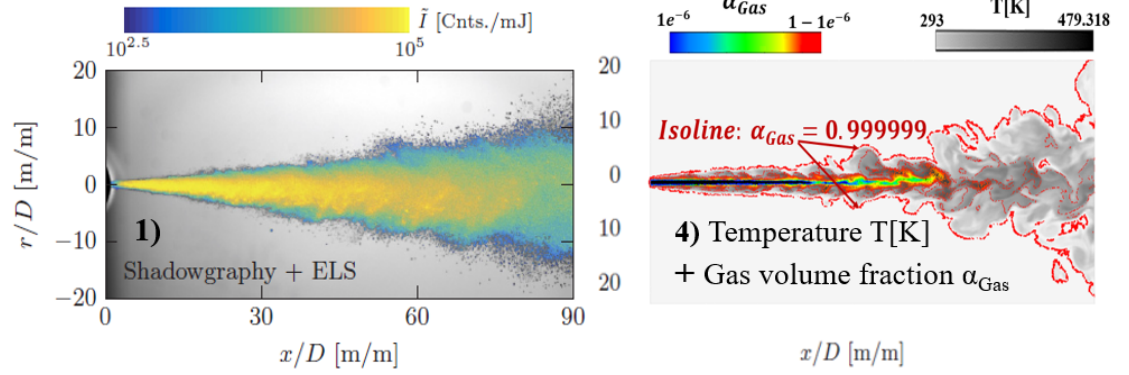


Fig. 7. Temperature N_2 -composition phase diagram for binary mixture of $C_6H_{14} - N_2$ at $P=5$ MPa, calculated by PR-EoS along with the adiabatic mixing temperature (AMT). (a) includes the comparison with [21] along with the three scatter plots of the numerical LES mixing temperature results. The low scattering of the LES mixing temperatures indicate almost adiabatic injection flows. The graphical insert shows that the LES mixing temperature scatterplots for the T560 case do intersect the dew line and enter the two-phase region. (b) includes the theoretical AMT for the three cases and show the same behavior as the RFM model for case T560. The two-phase region background is colored by the gas volume fraction values.

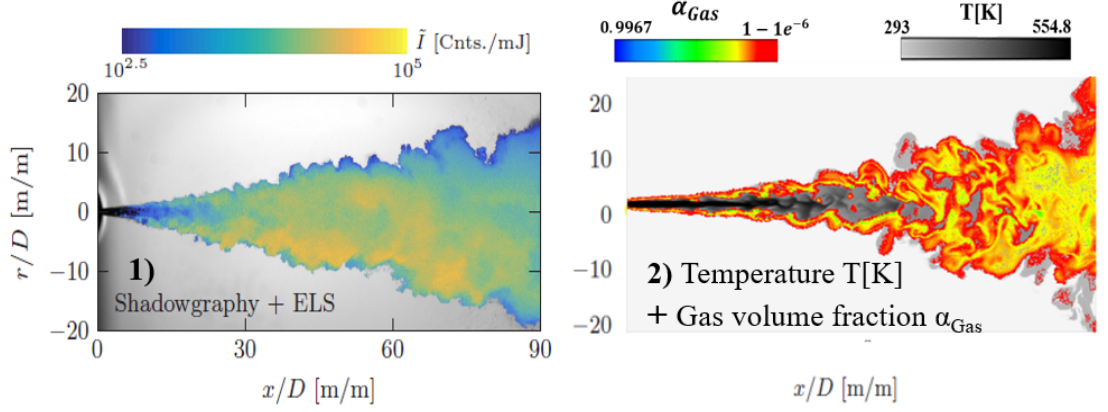
compared with instantaneous numerical snapshots (right frame 2) for the three cases (T480, T560, and T600) obtained using the RFM model, when the LES-Sigma turbulence model [42] is employed. For the experiments, the elastic light scattering (ELS) images superimposed onto shadowgraph images, to visualize both the flow structure and the thermodynamic state. Similarly for the numerical side, the gas volume fraction α_{Gas} distribution is superimposed onto the temperature contours in a plane passing through the axis of the nozzle to indicate regions of two-phase flow and especially the lowest values of α_{Gas} near the periphery of the jet. These numerical results were taken at a point in time so that the jet could be considered as quasi-steady. In doing so, a direct comparison of the two-phase droplet regions in the experiment and LES is rendered in Figure 8(a-b).

More precisely, in the subcritical Case T480, n-hexane is injected in a liquid state as depicted in blue color in Figure 7(b) indicating tiny α_{Gas} in the liquid core. In this case, a classical atomizing jet is shown experimentally in Figure 8(a). A spray can be seen clearly in this (shadowgraph + ELS) experimental image with distinct droplets at the periphery of the jet (especially for $X/D > 50$). Also, the ELS experiments have revealed a strong phase separation within the jet by showing high scattering intensity, (see I the palettes shown in Figure 8). Turbulent diffusion of N_2 into the injected n-hexane liquid core causes this mixture to enter the two-phase dome at a mole fraction of N_2 of about 0.1, as shown in Figure 7. This strong phase change can be seen in the numerical result shown in Figure 8(a) where the liquid core is represented (in blue) as the low gas fraction region. The rest of jet is in two-phase state representing the droplets spray and highlighting the flow structure at its periphery. This flow structures can be also seen in Figure 9 which demonstrates the temporal evolution of superposed temperature and gas volume fraction (α_{Gas}) contours. It is worth noting on Figure 9 that the two-phase jet can be considered as quasi-steady for $t > 4$ ms. Also, the authors would like to remind here that surface tension is not taken into account in the proposed RFM model and that future work should verify its effect on the numerical results of the subcritical T480 case.

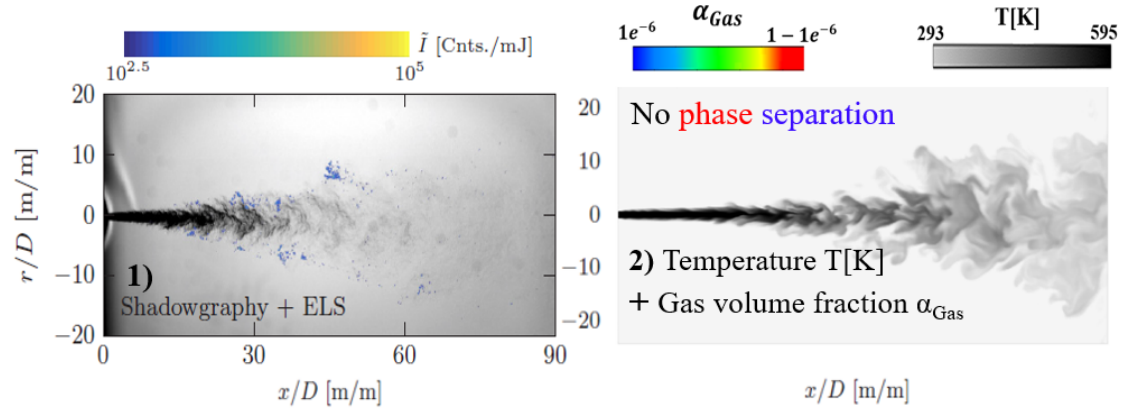
For the second case T560, n-hexane is injected at a supercritical liquid-like state into N_2 which is



(a) Case T480



(b) Case T560



(c) Case T600

Fig. 8. Comparison of experimental (left(1)) and numerical snapshots (right(2)) for the three test cases (T480, T560, and T600). The ELS image superimposed onto the corresponding shadowgraph are used to visualize both the flow structure as well as the thermodynamic state (adapted from [21]) in quasi-steady state condition. α_{Gas} is the gas volume fraction

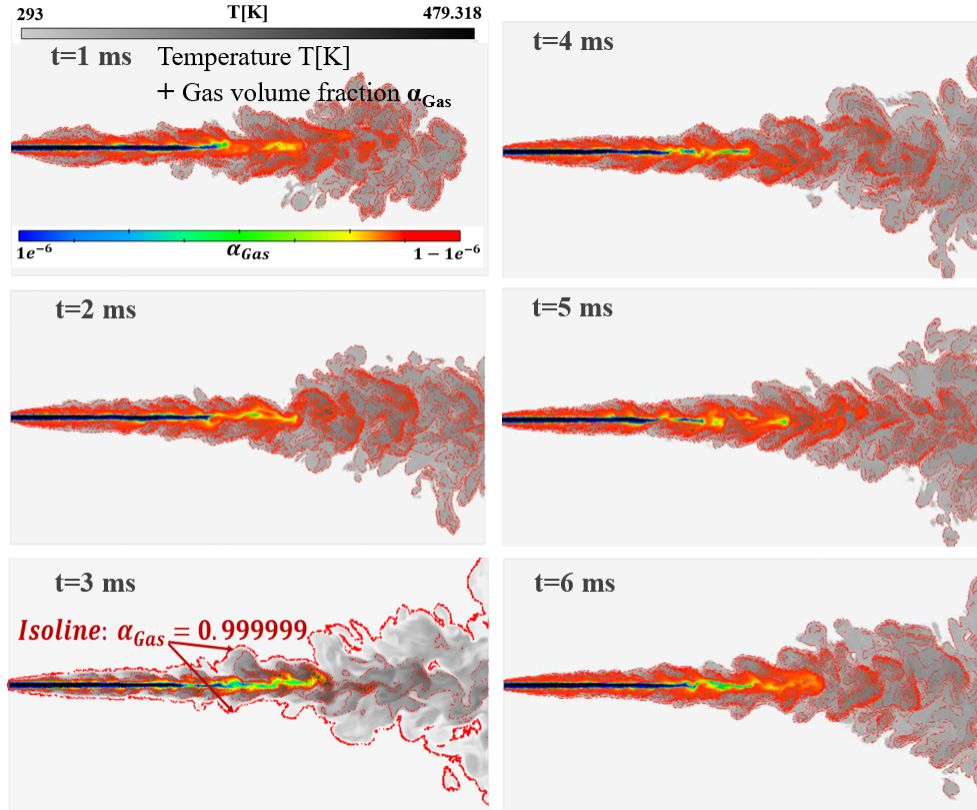


Fig. 9. Temporal evolution of (temperature +gas volume fraction(α_{Gas})) contours using Sigma turbulence model for case T=480.

at supercritical state as well. Although this supercritical condition, the shadowgraph + ELS image (Figure 8(b)) has revealed very rough borders indicating the presence of droplet clusters. This interesting phase change phenomena can be further discussed here using Figure 7(a). Indeed, the zoom inserted in this figure shows that the LES mixing temperature scatter plots for the T560 case has crossed the two-phase dome at high N_2 mole fraction. This means that most of the droplets nucleus have appeared close to the jet periphery. This phase change can be seen in the numerical results of Figure 8(b) and in more detailed time evolution of the jet in Figure 10, in which very low liquid volume fraction is highlighted (see the palette where the value of gas volume fraction changes from around 0.9967 to unity). In this case, the good qualitative validation of the appearance of liquid by condensation at the periphery of the jet could be considered as an a posteriori justification of the VLE assumption on which the proposed RFM model is based. Finally, for case T600, Figure 7(a,b) demonstrates, the jet does not experience any phase change and two-phase regime. Hence, with respect to the mixture critical point, the jet undergoes a single phase mixing regime. The shadowgraph + ELS experiments have revealed this single-phase regime within the jet by showing no significant scattering signal, as shown in Figure 8(c). As shown in this figure, this single-phase (dense-gas) behavior within the jet has been also well predicted by the RFM model.

It is worth noting that the comparison between the simulation and the experiment has shown some differences regarding the jet penetration length and dispersion. This can be attributed to the experimental uncertainty of the velocity and unknown turbulence at the nozzle exit. In addition, there is some probability of uncertainty in the numerical simulation as well. However,

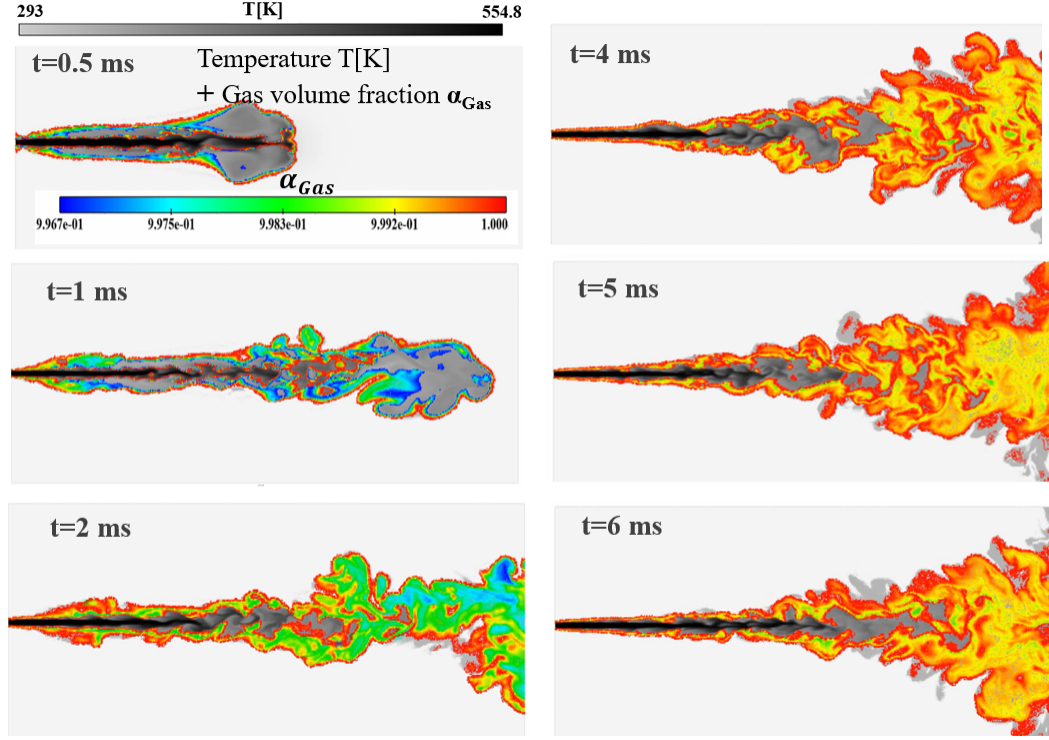


Fig. 10. Temporal evolution of (temperature + gas volume fraction (α_{Gas})) contours using Sigma turbulence model for case 560 (see table 2).

the current validation has demonstrated that the RFM model can efficiently capture the main physics in various conditions.

4.4. Analysis of droplet formation process for binary systems at supercritical regime

With the phase equilibrium model employed in this study, a detailed analysis of the droplet formation process becomes possible in the condition the metastability relaxation time is smaller than the CFD time step. Obviously, VLE assumption is not valid in case the metastability duration is much longer than the CFD time step. In this case, detailed models for nucleation and droplet growth under non-equilibrium condition are required [54].

Here, the case T560 is discussed based on Figure 11(a-d) in order to further illustrate the phase transition and droplet formation near to the jet border of an initially supercritical n-hexane fluid ($T_{inj} > T_c$) due to the interaction with its surrounding supercritical nitrogen. More specifically, Figure 11 shows the contour plots of a) the temperature, b) the C_6H_{14} mass fraction in the mixture, c) the phase indicator $\text{PHI} = 1, 2$ which designates the gas state and the two-phase state, respectively, and finally d) the C_6H_{14} mass fraction in the liquid phase defined as follows: The mass fraction of each component (for a system with (k) components), in any phase (p), ($Y_{k,p}$) is defined as the ratio of component (k) density in the phase (p) considered with respect to the phase density (ρ_p), as $Y_{k,p} = \frac{\alpha_p \rho_{k,p}}{\sum_k \alpha_p \rho_{k,p}}$.

As the phase indicator shows in Figure 11(c), the periphery of the jet goes to two phase regions. This can also be seen in the mass fraction contour of C_6H_{14} , in Figure 11(b). In this figure, a small mass fraction of C_6H_{14} (black color) is present near the boundary of the jet at near room temperature (light gray color in the temperature contour in Figure 11(a)). More importantly,

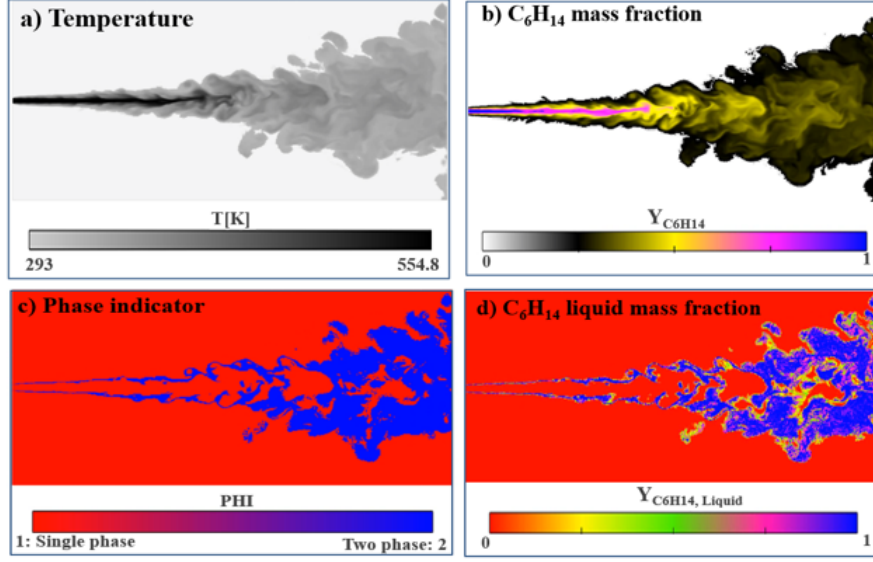


Fig. 11. T560 case results: contour plot of (a) Temperature, (b) C_6H_{14} mass fraction, (c) Phase indicator in which $\text{PHI}=1, 2$ denotes single phase and two-phase states, respectively, and (d) C_6H_{14} liquid mass fraction. This mass fraction ($Y_{C_6H_{14},l}$) is defined as the ratio of C_6H_{14} density in the liquid phase (index l) with respect to the liquid density (ρ_l), as $Y_{C_6H_{14},l} = \alpha_l \rho_{C_6H_{14},l} / \rho_l$.

Figure 11(d) reveals the mass fraction of C_6H_{14} in the liquid phase formed by condensation, mostly near the jet periphery. It worth to mention that as $\sum_k Y_{k,l} = 1$, the mass fraction of N_2 in the liquid phase formed by condensation is revealed to be very small in Figure 11(d).

4.5. Turbulence modelling impacts on two phase jets

Turbulence is known to significantly enhance the mixing rate of species, momentum and energy. This convective process occurs at different length scales as it results from the occurrence of turbulent eddies with different characteristic sizes, in high Reynolds number flows. Currently, only the direct numerical simulation (DNS) method can handle turbulent flows, but only for single-phase gas flows. In general, if a simulation does not use a sufficiently refined grid (DNS), it cannot properly account for turbulent mixing effects. This is still not practical in most of industrial test cases. Thus, turbulence models are often employed to estimate the additional mixing due to turbulence. As Richard Feynman (the American theoretical physicist, Nobel Prize in Physics in 1965) mentioned: "Turbulence is the most important unsolved problem of classical physics", hence developing a general turbulence model is still complicated due to highly unsteady and intricate interactions between various physical phenomena (turbulence, mixing, multi-phase flows, etc.) along with complex geometries and diverse boundary conditions. Traditionally, RANS (Reynolds-averaged Navier–Stokes equations) models [44] employ an effective turbulent viscosity to model the Reynolds stress term. Besides, in the past few years, Large-Eddy Simulation (LES) [42, 43] as a promising approach for turbulence modeling has been extensively used due to its unique potential to reproduce these unsteady and irregular phenomena. The main difference between LES and RANS models is how the fields are decomposed for modeling. For RANS approaches, the field is decomposed into an ensemble mean and a fluctuating component. However, LES resolves more of the turbulent spectrum by using a more refined grid in such a way that only the isotropic smallest eddies remain for an easier modelling of sub-grid scale.

Hence, for LES approach, the field is decomposed into a resolved field and a sub-grid field, and numerous LES models have been developed to relate the turbulent stresses to a differential operator acting on the resolved velocity field, as Equations (10 - 12). However, recent studies still demonstrate that each approach has some cons and pros, and choosing the best global LES approach for turbulence modeling, especially for internal combustion engines, is a crucial issue due to appearance of various complex phenomena [56, 57]. The oldest and most commonly used approach is the one proposed by Smagorinsky [43]. This model, known as a zero-equation LES model, does not solve any additional transport equations for sub-grid scale. It relates the turbulent viscosity to the magnitude of the strain rate tensor and the filter (usually taken as the cell size). Besides, an other promising zero-equation sub-grid model, called the Sigma model, has been developed by Baya-Toda et al. [43]. This more recent model shows that it can be a better alternative to the Smagorinsky model. It constructs the turbulent viscosity from the singular values of the resolved velocity gradient tensor. Most of the performance study of Sigma model have been performed for combustion [56, 57], and not for two-phase flows. In addition, two-phase turbulence effects have largely been neglected in the current literature. Indeed, most of the current state of the art two-phase flow simulations still consider one-fluid turbulence modelling approach, i.e. assuming that the turbulent structures behave similarly to single-phase turbulence. In this study, the objective is to give some insight to two-phase turbulence modelling by analyzing the interaction between the turbulence and two-phase flows, especially when phase transition (evaporation, condensation) occurs. Generally, the turbulent viscosity in LES zero-equation models are defined as the following Equation 10.

$$\nu_{SGS} = (C_m \bar{\Delta})^2 \bar{D}_m \quad (10)$$

where C_m and D_m are the model (m) specific constant, and differential operator of the model respectively. $\bar{\Delta}$ is the filter width (i.e. the cell size in the context of LES with implicit filtering). D_m as the differential operator of the Smagorinsky and Sigma models are computed as the following Equations (11-12).

$$\bar{D}_{Smag} = \bar{S} = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}, \bar{S}_{ij} = 0.5\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \quad (11)$$

$$\bar{D}_{Sigma} = \frac{\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^2} \quad (12)$$

The differential operator of the Smagorinsky model is based on the resolved characteristic rate of strain (\bar{S}_{ij}). However, the Sigma model employs the singular values of the resolved velocity gradient tensor so that the singular values σ_i ($\sigma_1 \geq \sigma_2 \geq \sigma_3$) are the square roots of the eigenvalues of the matrix $\bar{S}_{ij} * \bar{S}_{ji}$ [43].

As a final comment on the turbulence modelling, it is worth to note that turbulent viscosity (μ_{SGS}) is known to be much greater than laminar one (μ) in single-phase turbulent flows. However, this is not always the case in turbulent two-phase flows, especially at the liquid-gas interface where the laminar viscosity experiences a high gradient. Another important point is that the rate of strain \bar{S}_{ij} in \bar{D}_m equations may vary significantly in the interface region due to a large phase transition. This is also may be the case due to non-linear property (C_p , D_T , ...) behaviors at supercritical state in the Widom line region. The latter two effects are somewhat included in the proposed RFM model through the tabulation of the VLE properties and the impulse effect of the phase change on the momentum. However, a more thorough fundamental study of the interaction between turbulence and EoS should be conducted in future work [58].

Figure 12 shows instantaneous contour plot of temperature, and density for case T480 at $t=2.5$ ms using various turbulent models denoted as RANS, LES-Smagorinsky, and LES-Sigma models, respectively. Noteworthy, it does not make sens to compare ensemble averaged RANS results and

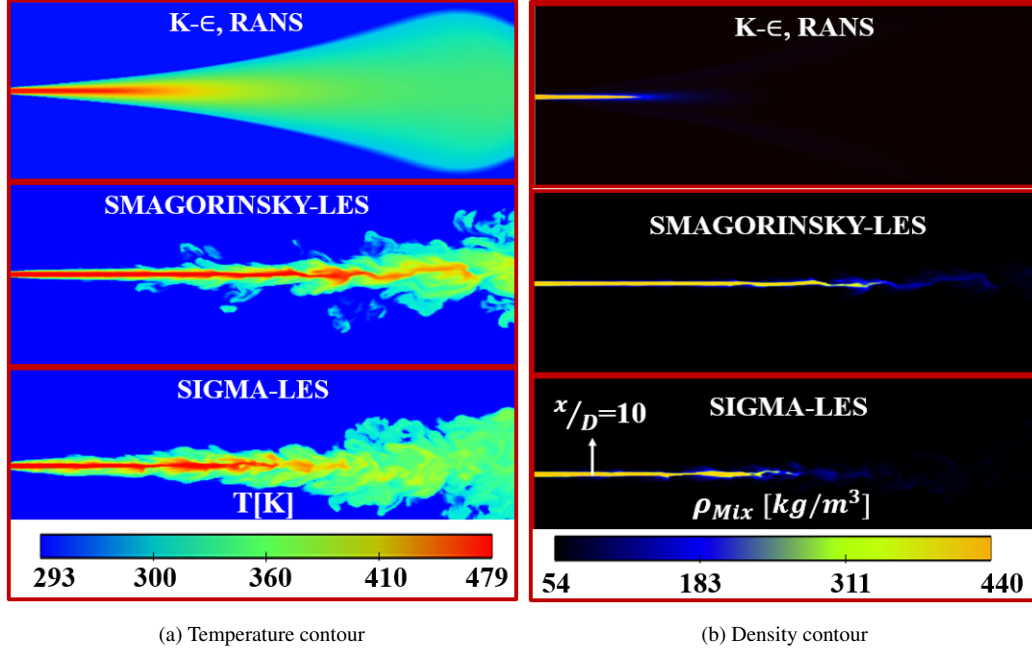


Fig. 12. Impacts of turbulence modellings of the jet structure for various properties for two phase flows using $(k - \epsilon)$ RANS, LES-Smagorinsky, and LES-Sigma models, respectively, from top to down, at $t=2.5$ ms.

instantaneous LES results. However, this Figure demonstrates the different behaviour between RANS and LES models. The liquid core (represented by the mixture density) is very short relatively to the LES results. This is due to the higher turbulent viscosity and kinetic energy (TKE) generated in the RANS simulation (see also Figure 13(a,c)).

The Sigma-LES model gives an initial spray cone angle that better matches the experimental image shown in Figure 8(a) than the LES-Smagorinsky model. Also, the liquid core obtained with Sigma-LES model is shorter than the one obtained by LES-Smagorinsky model. This demonstrates a higher evaporation rate obtained using the LES-Sigma model, and thus the significant effect of turbulence modeling on such two-phase numerical results. However, more simulations should be performed in future work to assert the superiority of LES-Sigma in two-phase flows. To have a better insight, Figure 13(a-c) display a qualitative comparison of some turbulent properties profiles at $X/D = 10$ (see the arrow in Figure 12(b)), as a) Turbulent viscosity (μ_T), b) Turbulent conductivity (λ_T), and c) Turbulent kinetic energy (TKE) using the different turbulence models, respectively at $t=2.5$ ms. Figure 13(a,b) demonstrates the huge values obtained with the RANS model relatively to the LES models. In addition, lower turbulent viscosity and conductivity levels are obtained using the Sigma model compared to the Smagorinsky model in the liquid-gas interface region. This lower turbulent viscosity is expected since Sigma model has been developed to avoid overestimating the SGS turbulence in shear layers, as also reported by [56]. Hence, this lower turbulent viscosity level has led to less dissipation of the turbulent energy, TKE, as shown in Figure 13(c). Besides, some interesting points can be observed in Figure 14 in which is plotted dimensionless radial profiles of the density, density gradient, gas volume fraction and the turbulent conductivity, at $X/D = 10$.

First, it is important to note in this figure that the extrema of the turbulent conductivity and density gradient almost coincide with the locus of the liquid-gas interface at $\alpha_{Gas} = 0.5$. This

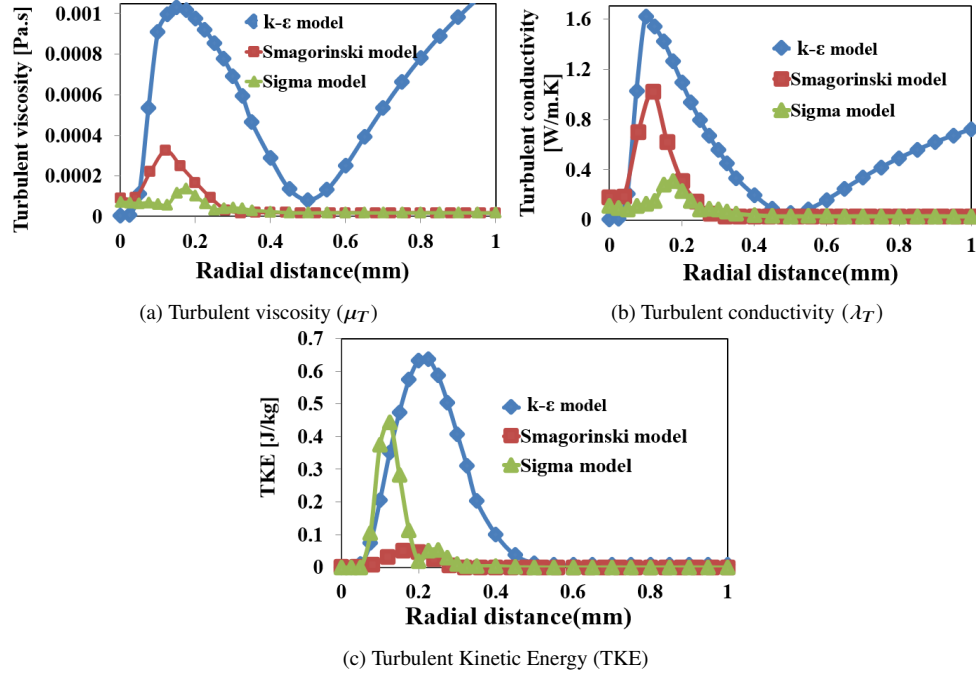


Fig. 13. Impacts of turbulence modellings on different turbulent properties using different ($k - \epsilon$) RANS, LES-Smagorinsky, and LES-Sigma models, respectively, from top to down, at $t=2.5$ ms at $X/D = 10$. Due to the much higher values from the ($k - \epsilon$) model for the different turbulent properties, they have been divided by 100, 100, and 20 for turbulent viscosity, TKE, and turbulent conductivity, respectively, to be in the same range as LES data.

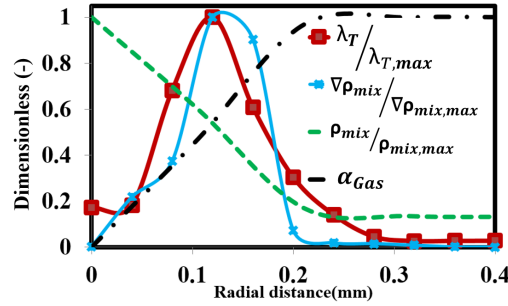


Fig. 14. Impacts of density gradient on the turbulent properties, at $t=2.5$ ms at $X/D = 10$, using LES-Sigma model.

517 demonstrates the high coupling of turbulence with flow characteristics such as density gradient.
 518 Indeed, it is well known that the density gradient in a two-phase flow plays a key role in turbulent
 519 two-phase flows and particularly on liquid atomization.
 520 Generally, vorticity analysis can be used as an appropriate tool for the flow mixing analysis [59,60].
 521 the following Equation 13 gives the total derivative of vorticity ω for compressible flows [59].

$$\frac{D\omega}{Dt} = -\omega(\nabla \cdot u) + (\omega \cdot \nabla)u + \frac{\nabla \rho \times \nabla P}{\rho^2} - \nu \nabla^2 \omega \quad (13)$$

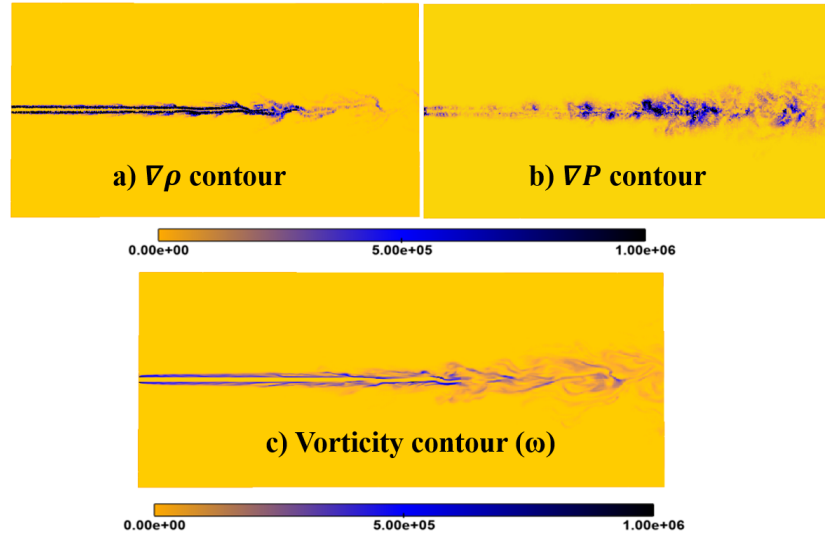


Fig. 15. (a) Density gradient, (b) Pressure gradient and (c) Vorticity contours at the interface at $t=2.5$ ms. The misalignment of spatial pressure and density gradients is at the origin of the baroclinic torque source term.

The first term on the right hand side of Equation 13 represents the expansion of the vorticity due to the compressibility. The second term, called vortex stretching term, is due to the enhancement of vorticity by stretching. The third term, called baroclinic torque, is due to the misalignment of spatial pressure and density gradients. Finally, the viscous diffusion last term expresses the vorticity change due to viscous dissipation. Figure 15(a,b) shows the appearance of a peak at density and pressure gradients contours at the interface, which leads to the formation of high vorticity in at the interface, as shown in Figure 15(c). This demonstrates that real fluid models are required to accurately compute density and pressure gradients and to simulate such turbulent injection flows, as recently reported by [61].

5. Quantitative validation

To quantitatively validate the tabulated RFM-LES results, the numerical results will be compared in this section with the recent experimental data from Baab et al. [62]. They performed quantitative sound speed measurements in jet mixing zones for different configurations with various mixtures at different conditions. The n-hexane case, which corresponds to "Case 1" in Baab et al. [62] is chosen for the comparison to our numerical results. The applied numerical setup is identical to the one used in the previous section. The experimental conditions, listed in Table 3, are very similar to the T600 case in Section 4, as shown in Table 2. One point is worth mentioning is that the nozzle exit temperature $T_e = 627K$ and velocity $u_e = 90m/s$ were estimated in that experimental study based on the assumption of an isentropic flow inside the injector [62].

In this study, another strategy has been adopted, where inflow turbulence fluctuations have been generated and superimposed on the inflow velocity profile using Fourier method, based on the proposals by [63]. This method has been used in order to generate correlated turbulent fluctuations over the mean inlet profile at the nozzle exit. Using synthetic turbulence at the computational domain inlet has shown significant effect on the spray development as demonstrated in [64,65], when the in nozzle flow is not included in the simulation. As pointed out in [64,65], this turbulent intensity ranges between 3% and 5% depending on the turbulence model. Hence, the

Table 3. Operating conditions used for the current numerical study taken from Baab et al [62] experimental study. The nozzle exit temperature T_e was estimated based on the assumption of an isentropic flow inside the injector calculated by [62].

Injection fuel	Chamber gas	P_{ch} [MPa]	T_{ch} [K]	$T_{t,C_6H_{14}}$ [K]	$T_{e,C_6H_{14}}$ [K]
C_6H_{14}	N_2	5	296	630	627

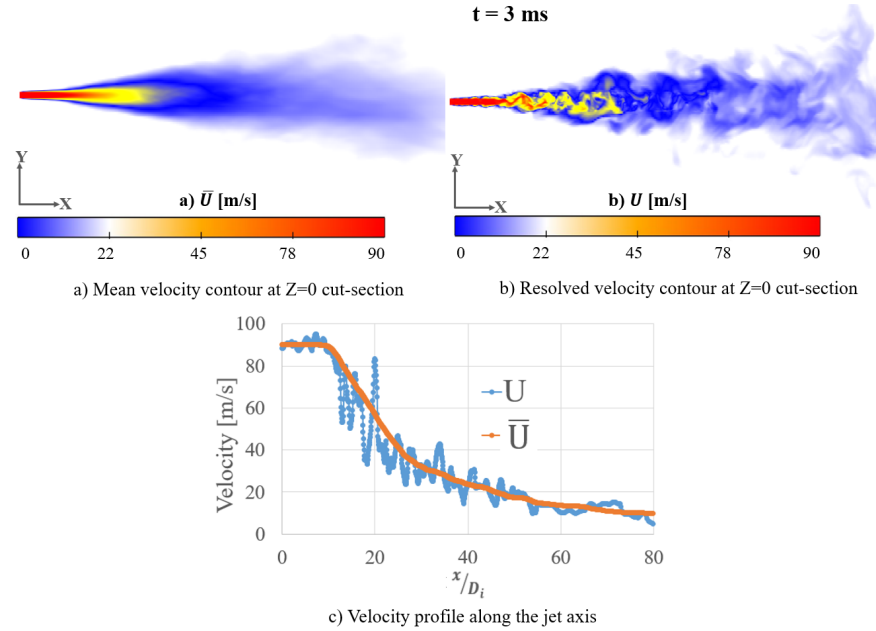


Fig. 16. (a) Mean velocity field (\bar{U}), (b) The resolved velocity (U) at 3 ms, and (c) The velocity profile plotted along the jet axis where the resolved velocity is at 3 ms and the mean velocity is computed using the LES results in the time interval between 2 and 3 ms after the start of injection. For this case, a fluctuating boundary condition has been superimposed on the inflow velocity profile using Fourier method with 5% intensity.

injection boundary conditions in this study are based on the mean inlet velocity of 90 m/s and 5% turbulent intensity superimposed on the inflow velocity profile. In addition, n-hexane is injected with the estimated nozzle temperature of 627K to the chamber filled by N_2 at $T_{ch} = 296K$ and $P_{ch} = 5MPa$. With regard to the numerical setup, the same configuration as shown in Figure 6 is used with the base grid size set to ($40\mu m$) at the far-field of nozzle, and along with different levels of embedding to achieve a fine mesh resolution near the nozzle exit of ($10\mu m$), corresponding to 26 cells in the nozzle diameter. Moreover, the time step is automatically controlled based on a maximum CFL number of 50 reaching a value in the range (10 ns-50ns). Besides, the LES-Sigma model has been used for the turbulence modeling of this test case due to its performance, as shown in the previous section. Figure 16 demonstrates (a) The mean velocity contours computed using the LES results in the time interval between 2 and 3 ms after the start of injection, (b) The resolved velocity, in addition to (c) The velocity profile along the jet axis obtained with an inlet fluctuating boundary condition with 5% intensity. Unfortunately, no experimental velocity and turbulence data are available in this case. Therefore, these numerical results can be used as a reference for future work.

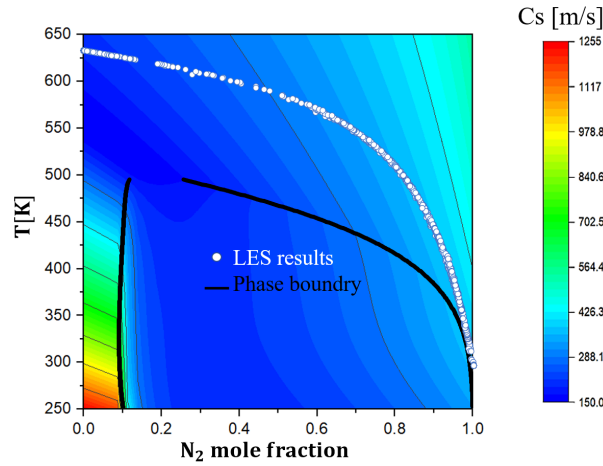


Fig. 17. Temperature- N_2 mole fraction diagram for binary mixture of $N_2 - C_6H_{14}$, colorized with the mixture sound speed, using Wood formula for two phase region [66] at $P = 5 \text{ MPa}$, using PR-EoS, along with the phase boundary (in black). The scatter plots (white points) show the locus of the mixing temperature obtained by the RFM-LES model for the case with $T_e = 627 \text{ K}$ simulation.

Figure 17 shows the Temperature- N_2 mole fraction diagram for the binary mixture of $N_2 - C_6H_{14}$, colorized and mapped with the mixture sound speed, computed using the Wood formula [66] for the two-phase region at $P = 5 \text{ MPa}$, calculated by PR-EoS, along with the scatterplots (white points) locus of the mixing temperature obtained by the RFM-LES model. In this figure, we can observe the sound speed variations along the mixing temperature (white dots). This demonstrates that the flow in the current supercritical condition experiences relatively small sound speed variations. This could be seen more precisely in Figure 18(c) which depicts the instantaneous fully developed $N_2 - C_6H_{14}$ LES results in terms of sound speed contour after $t = 3 \text{ ms}$. Indeed, Figure 18 presents the instantaneous mixture sound speed at axial center-line and at radial direction at $x/D_i = 35$, extracted from the RFM-LES results. An intensely turbulent mixing process of n-hexane with the supercritical nitrogen ambient can be observed in Figure 18(a,b) in terms of the mixture temperature and the hexane mass fraction. The supercritical fuel jet with higher density ($\rho \approx 115 \text{ kg/m}^3$) and temperature ($T = 627 \text{ K}$) enters to the chamber filled with N_2 with lower density ($\rho \approx 58 \text{ kg/m}^3$) and temperature ($T = 296 \text{ K}$), and then n-hexane jet gradually mixes with N_2 inside the chamber. Moreover, as Figure 18(c) shows, the sound speed varies from $C_{s,C_6H_{14}}(P_{ch}, T_e) = 197 \text{ m/s}$ at the exit of nozzle and $C_{s,N_2}(P_{ch}, T_{ch}) = 360 \text{ m/s}$.

Finally, quantitative comparisons of the mixture sound speed with the experimental data from Baab et al. [62] are shown in Figure 19 along the axial and radial axis shown in 18(c). Ten numerical profiles shown as thin gray lines denotes the RFM-LES results in the time range of $t = 2\text{--}3 \text{ ms}$. Furthermore, Figure 20(a) shows the instantaneous contours of the n-hexane mole fraction at $Z=0$ cut section at $t = 3 \text{ ms}$. Besides, Figure 20 demonstrates the instantaneous contours of the n-hexane mole fraction and the validations of LES n-hexane mole fraction with the analytical self-similar solutions calculated by Gerber et al. [6] using REFPROP. Specifically, some instantaneous LES results on the jet axis, as shown in Figure 20(a), are shown (colorized with gray thin lines) in the range of $t = 2\text{--}3 \text{ ms}$. Also, LES simulation results at $t = 3 \text{ ms}$ are highlighted. Overall, a good agreement are found in the sound speed as well as hexane mole fraction predicted results, compared to the reference data, which demonstrate that the RFM-LES solver is able to predict the mixing process of C_6H_{14} and N_2 accurately.

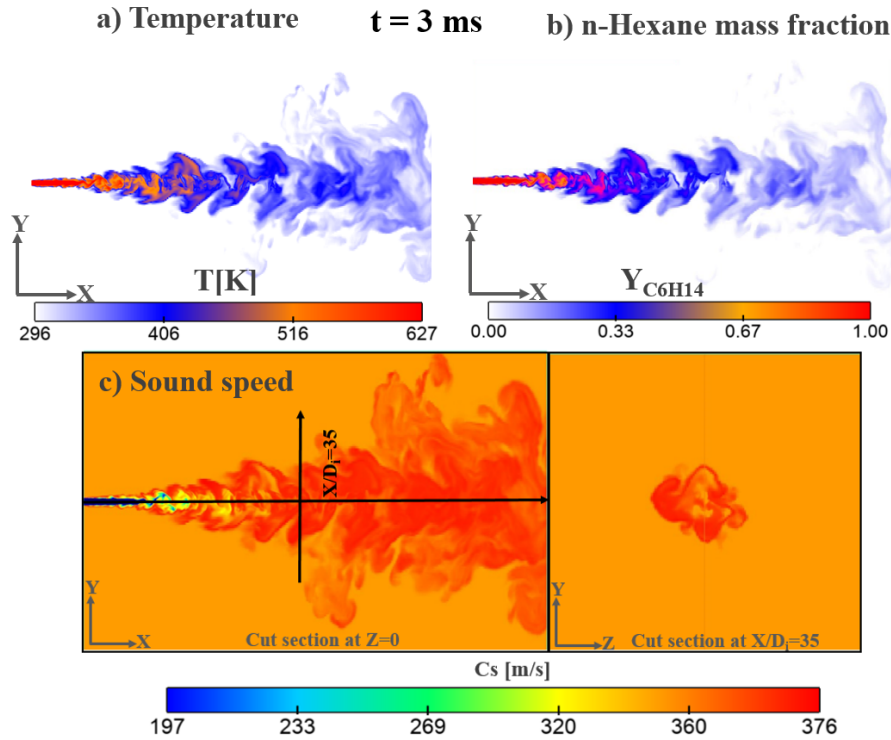


Fig. 18. The top LES results at $t = 3 \text{ ms}$ are: (a) Instantaneous contours of the mixture temperature, (b) n-hexane mass fraction at $Z=0$ cut section. The bottom LES results (c) at $t = 3 \text{ ms}$ are the mixture sound speed at $z = 0$ (left), and at $x/D_i = 35$ cut sections (right). The sound speed in the chamber, filled initially with the N_2 at $T_{ch} = 296 \text{ K}$, is $C_{s,ch} \approx 360 \text{ m/s}$ (orange color). At the nozzle exit where $T_e = 627 \text{ K}$, the sound speed is $C_{s,exit} \approx 197 \text{ m/s}$ (blue color).

6. Conclusion

In this paper, a fully compressible tabulated multicomponent real-fluid (RFM) model has been developed in order to explore the interaction between phase separation and turbulent fluid dynamics in multi-species supercritical flow jets. More specifically, the converge CFD solver has been coupled to the IFPEN-Carnot thermodynamic library using a generalized tabulation method to gain computational efficiency and robustness. This modeling approach has been implemented in the CONVERGE solver for the simulation of the turbulent mixing of n-hexane injected in a chamber filled with nitrogen, considering phase separation processes (condensation) at high pressures conditions with the fluids initially at supercritical state.

First, n-hexane has been injected at three inflow temperatures in the same conditions as the experimental and numerical study of Traxinger et al. [21]. Besides, a more quantitative study has been performed using the experimental study of Baab et al. [62], which has the same setup configuration as [17]. The obtained numerical results have been shown and proved to be in good agreement with the experiments [21, 62]. In addition, the RFM model was shown to be capable of simulating subcritical, transcritical and supercritical jets exhibiting phase separation and condensation processes. As a consequence, if the jet is at a subcritical state, with regard to the mixture critical point, it experiences the classical droplets formation process governed by the liquid atomization. In contrast, if n-hexane is injected at supercritical state in a colder nitrogen

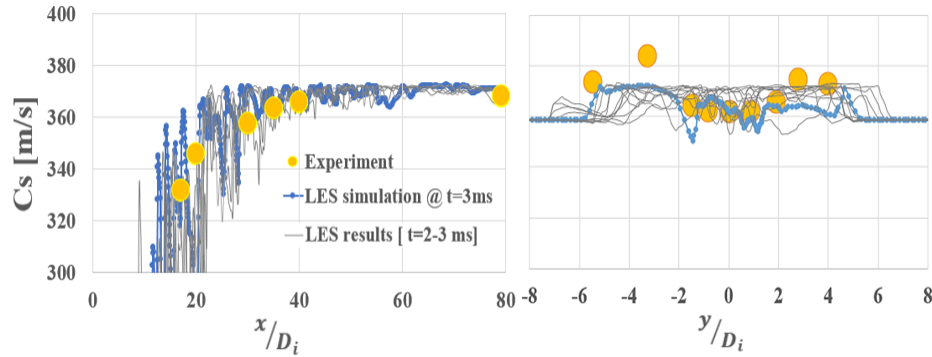


Fig. 19. Validations of mixture sound speed with experimental data of Baab et al. [62], (a) Along the jet axis, and (b) At radial direction at $x/D_i = 35$ determined and plotted at Figure 18. LES results colorized with gray thin line denotes the LES-sigma results for some instantaneous times in the range of $t=2-3$ ms. LES simulation @ $t=3$ ms shows the variations of the mixture sound speed at $t=3$ ms, as shown in Figure 18.

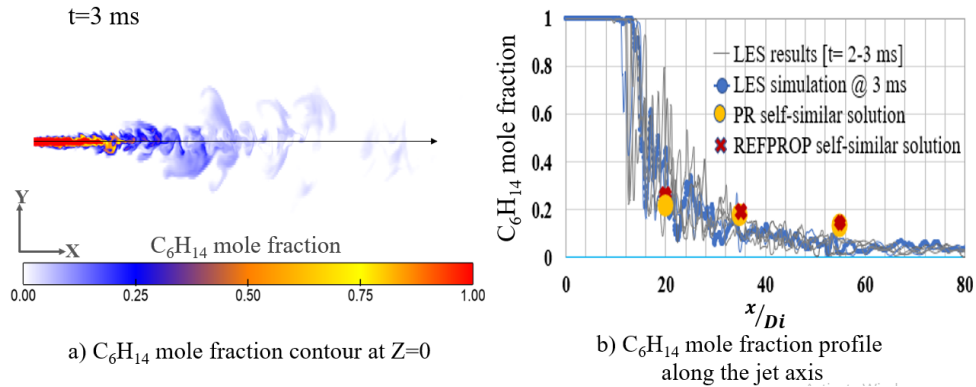


Fig. 20. Instantaneous contours of (a) n-hexane mole fraction, at $Z=0$ cut-section at $t = 3ms$, and (b) Validations of LES n-hexane mole fraction, along the jet axis, with the analytical self-similar solutions calculated by Gerber et al. [6]. They hired PR EoS, and REFPROP data to analytically calculate fuel mole fraction at different distances from the nozzle exit. LES results colorized with gray thin line denotes the LES-sigma results for some instantaneous times in the range of $t=2-3$ ms. LES simulation @ $t=3$ ms, with blue color shows the variations of the n-hexane mole fraction, shown in contour plot in (a).

610 ambient, it may cross the two-phase dome, thus leading to local condensation and droplets
 611 formation mainly at the periphery of the jet. It has been also shown that such condensation does
 612 not occur if the n-hexane is injected at a sufficiently high supercritical temperature.
 613 Next, comparisons between different turbulence models, including large eddy simulation models
 614 (LES Sigma and Smagorinsky) and a Reynolds-averaged Navier-Stokes model (RANS $K - \epsilon$),
 615 have demonstrated the importance of a proper turbulence modeling, and the suitability of the
 616 LES-Sigma model, in addition to accurate thermodynamic and transport properties, for these
 617 highly complex jet flows. Finally, compared to our previous studies [17, 25], the computational
 618 efficiency, accuracy, and robustness of this proposed tabulated RFM model as a remedy to the
 619 direct evaluation of costly phase equilibrium solver have been confirmed.

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