Large-eddy simulation of cryogenic jet injection at supercritical pressures

By J. Matheis, H. Müller†, S. Hickel¶ and M. Pfitzner‡

Institute for Aerodynamics and Fluid Mechanics, Technische Universität München
Boltzmannstr. 15, 85748 Garching b. München
† Institute for Thermodynamics, Universität der Bundeswehr München
Werner-Heisenberg-Weg 39, 85577 Neubiberg
¶ also: Faculty of Aerospace Engineering, Technische Universität Delft, P.O. Box 5058, 2600 GB Delft, The Netherlands

The injection of cryogenic nitrogen with a coflow of warm hydrogen into a supercritical nitrogen atmosphere is studied numerically by means of well resolved large-eddy simulation (LES). The conditions resemble those in liquid-propellant rocket engines. By substituting oxygen with the inert gas nitrogen the setup allows for an isolated view on binary mixing processes near the injector without the influence of combustion. The thermodynamic model is based on the cubic Peng-Robinson equation of state. The LES results are compared with available experimental data demonstrating that the numerical method is suitable to study turbulent binary mixing at transcritical conditions. The following detailed analysis of the thermodynamic conditions that arise in the shear layer reveals that local phase separation may occur for the present injection conditions. The resulting effect on the flow is quantified by an a-posteriori calculation of the two-phase equilibrium conditions in the shear layer. The result indicates a maximum density variation of up to 25% compared to the single-phase calculation.

1. Introduction

In modern high performance Liquid Rocket Engines (LRE) the operating pressure lies well above the critical pressure $p_c$ of the propellants oxygen ($p_{c, O_2} = 5.043$ MPa) and hydrogen ($p_{c, H_2} = 1.296$ MPa). Furthermore, operating conditions are often such that one or both propellants enter the thrust chamber at cryogenic temperatures. For instance, in regeneratively cooled LREs the cryogenic liquid hydrogen is sent through cooling channels where it heats up before being injected through a coaxial injector element at supercritical temperatures ($T > T_{c,H_2} = 33.18$). Oxygen on the other hand is typically injected at temperatures of 100 K, thus subcritical with respect to its critical temperature ($T_{c,O_2} = 154.58$). Hence, the injected oxygen is in a transcritical state, characterized by high liquid-like densities and viscosities. At these conditions the fluid properties significantly deviate from those of an ideal gas. Transcritical jet breakup and atomization behavior differs significantly from injection at lower pressures. Rather than breaking up into droplets, the jet disintegrates by dissolving into finger-like structures [1].

Research in recent years has lead to an improved understanding of the processes in cryogenic rocket engine combustion chambers. Especially cold flow studies, of both pure component and multicomponent systems, contributed to a clearer picture without
introducing the complexities of combustion [1]. With a single and well-defined critical point at which jet disintegration transitions from subcritical to supercritical behavior, the experimental investigation of cryogenic nitrogen injected into a warm nitrogen atmosphere [2–6] became probably the most popular and fundamental of all cases [1, 7]. Along with experimental studies, many groups have investigated this configuration numerically. Due to the availability of high quality quantitative density measurements, the experimental series by [4] has become a mandatory test case for computational fluid dynamics (CFD) validation (see [8–12], e.g.). Additionally to such fundamental studies of single round jets, coaxial injectors have also been subject of intense experimental effort, see, e.g., Refs. [3, 6, 13–16]. In case of multicomponent systems, such as liquid nitrogen (LN2) and gaseous hydrogen (GH2) or gaseous helium (GHe) in [13], LN2 and GH2 in [14], LN2 and GHe in [15], the definition of a point above which jet breakup and atomization transitions from subcritical to supercritical behavior is more difficult. Here, the consideration of multicomponent phase equilibria information is necessary to interpret experimental findings. Even when the operating pressure is well above the critical pressure of the injectants, two phases can coexist and classical spray jet break-up patterns are observed. Comprehensive reviews on that topic can be found, for instance, in [17], [1] and [18], and references therein. In this report, we will study a selected operating point of a series of experiments of [14] in which quantitative density measurements in coaxial LN2 and GH2 jets at supercritical pressures (with respect to the critical pressure of the pure nitrogen and pure hydrogen) were obtained. Emphasis is placed on a quantitative comparison between experimental and numerical data and the assessment of uncertainties related to both of them. In particular, transcritical two-phase phenomena that occur at the present operating conditions will be addressed by means of a novel post-processing of LES data.

This report is organized as follows: Section 2 begins with a brief introduction to the thermodynamics model used for the present simulations. In Sec. 3 and 4 we introduce the experimental setup of [14] followed by a presentation of the numerical approach for the LES. The numerical results are presented in Sec. 5 and the discussion of transcritical two-phase phenomena is found in Sec. 6. Concluding remarks and an outlook to future work are given in the last section.

2. Thermodynamics model

The governing equations, i.e., mass, momentum, and energy equation, are closed by a cubic equation of state (EOS). For brevity we will restrict ourselves here to the Peng-Robinson (PR) EOS [19]:

\[
p = \frac{\mathcal{R}T}{v_{PR} - b} - \frac{a\alpha(T)}{v_{PR}^2 + 2v_{PR}b - b^2}.
\]

In Eq. (2.1) the pressure \( p \) is a function of the (untranslated) molar volume \( v_{PR} \) and temperature \( T \). \( \mathcal{R} \) is the universal gas constant. The \( \alpha \)-function

\[
\alpha(T) = \left[ 1 + c_0(1 - \sqrt{T/T_c}) \right]^2
\]

with

\[
c_0 = 0.37464 + 1.54226\omega - 0.2699\omega^2
\]
accounts for the polarity of a fluid and is a correlation of temperature \( T \), critical temperature \( T_c \) and acentric factor \( \omega \). The parameter

\[
a = 0.45724 \left( \frac{R^2 T^2}{p_c} \right)
\]

represents attractive forces between molecules and the effective molecular volume is represented by the parameter

\[
b = 0.0778 \left( \frac{RT_c}{p_c} \right).
\]

Conventional mixing rules are used in order to extend the PR EOS to a mixture composed of \( N_c \) components. The parameters required in the EOS are calculated from:

\[
a_\alpha = \sum_i \sum_j z_i z_j a_{ij} \alpha_{ij}(T),
\]

\[
b = \sum_i z_i b_i,
\]

with \( z_i \) being the mole fraction of component \( i \). The coefficients \( a_{ij} \) and \( \alpha_{ij}(T) \) are calculated from combination rules where we follow the recommendations given by [20]. Here, off-diagonal elements are calculated using the same expression as for the diagonals together with pseudo-critical parameters. For the present simulations the binary interaction parameter \( \delta'_{ij} \) is set to zero.

Additionally to the thermal EOS, an expression for caloric properties such as internal energy \( e \), enthalpy \( h \) or specific heat at constant pressure \( c_p \) is needed. The departure function formalism provides such expressions as the sum of a low-pressure reference state and the departure from that reference state. The departure function, e.g., for the internal energy, can be written as

\[
e(T, v, z) = e^0(T, z) + \int_v^\infty \left[ T \frac{\partial p}{\partial T} \right] dv.
\]

The solution of the integral on the right hand side only requires relationships provided by the EOS. Analytical solutions for many cubic EOS’s (such as the PR EOS) are available in literature, see, e.g., [22]. In the present work, the ideal reference state (denoted as \( ^0 \)) is evaluated using the 9 coefficient NASA polynomials [23].

In all simulations, viscosity and thermal conductivity are described with the correlation of [24]. We note that the acentric factor of hydrogen was set to zero for the viscosity and thermal conductivity calculations since we observed a singularity in the correlation of Chung for binary \( H_2/N_2 \) mixtures.

Figure 1 depicts the density and the specific heat capacity at constant pressure prediction of the present thermodynamic model in comparison to the NIST [21] reference data. Shown are three isotherms at a temperature of 100 K, 120 K, and 140 K at a constant pressure of 5.5 MPa (left column) and 4 MPa (right column) as function of overall hydrogen mole fraction \( z_{H_2} \).

We observe a very good agreement between the NIST [21] reference data and the PR EOS for 120 K and 140 K. For the isotherm at 100 K, the PR EOS overestimates the NIST [21] density data for nitrogen rich mixtures. This can be corrected using volume translation methods, see e.g. [25] or [26]. However, for the present test case the PR
FIGURE 1. Validation of the real-gas thermodynamics model for a binary nitrogen-hydrogen mixture at 5.5 MPa (left column) and 4 MPa (right column), see panel (a) for the legend. Two-phase region as predicted by the NIST reference data [21] at 100 K and 120 K is indicated by the gray lines.

<table>
<thead>
<tr>
<th>$p$ [MPa]</th>
<th>$T_{N_2}$</th>
<th>$\pi_{N_2}$ [m/s]</th>
<th>$\rho_{N_2}$ [kg/m$^3$]</th>
<th>$\dot{m}_{N_2}$ [g/s]</th>
<th>$T_{H_2}$</th>
<th>$\pi_{H_2}$ [m/s]</th>
<th>$\rho_{H_2}$ [kg/m$^3$]</th>
<th>$\dot{m}_{H_2}$ [g/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>E4</td>
<td>$4^a$</td>
<td>118$^a$</td>
<td>5$^a$</td>
<td>584.43$^b$ / 608.78$^c$</td>
<td>8.29$^b$ / 8.63$^c$</td>
<td>270$^a$</td>
<td>120$^b$</td>
<td>3.55$^b$ / 3.55$^c$</td>
</tr>
<tr>
<td>E4$^{PR}$</td>
<td>4</td>
<td>128.274</td>
<td>7.49</td>
<td>390.18</td>
<td>8.29</td>
<td>270</td>
<td>120</td>
<td>3.55</td>
</tr>
</tbody>
</table>

TABLE 1. Test case definition. $^a$ Nominal experimental operating conditions according to [14]. $^b$ Calculated using NIST. $^c$ Calculated using the PR EOS.

EOS yields a reasonably good approximation of the nitrogen inflow density with an error of about $\sim 4\%$. With respect to the simulation of Oschwald et al.'s configurations we note that a comparison with the reference data at 4 MPa is not possible throughout the whole composition space due to the existence of a two-phase region. The two-phase region as predicted by the NIST [21] reference data at 100 K and 120 K is indicated by the gray lines. Data points that are located within the two-phase region are blanked out. Consequences and modeling requirements associated with the two-phase region at pressures relevant to the present application are addressed separately in Sec. 6.
3. Test case description

We study the coaxial injection of hydrogen and nitrogen into a supercritical nitrogen atmosphere, which resembles the conditions encountered in real rocket engines. By substituting oxygen with the inert gas nitrogen (with its fluid mechanical properties being not too different from oxygen), this setup allows for an isolated view on binary mixing processes near the injector without the influence of combustion [14]. The setup has been investigated experimentally by [14] who performed a series of 2D-Raman density measurements with particular emphasis on atomization and mixing mechanisms. The chamber pressure is 4 MPa, thus, supercritical with respect to the critical pressures of pure nitrogen ($p_{c,N_2} = 3.34$ MPa) and pure hydrogen ($p_{c,H_2} = 1.29$ MPa). The measurement campaign covered experiments with and without the coaxial injection of hydrogen at several injection temperatures and velocities. To the authors’ knowledge, this is currently the only experimental study on inert coaxial injection at LRE relevant conditions that uses laser diagnostic methods in order to obtain quantitative data.

In the following we will discuss LES results achieved for the operating conditions E4, which are summarized in Tab 1. Hydrogen (outer stream) and nitrogen (inner stream) are injected through a coaxial injector element into a cylindrical tank ($D = 10$ cm) filled with nitrogen at 4 MPa and 298.15 K. The inner and outer diameter of the hydrogen annulus are $D_{H_2,i} = 2.4$ mm and $D_{H_2,o} = 3.4$ mm, respectively, the inner nitrogen injector is $D_i = 1.9$ mm in diameter. The nominal bulk velocity of nitrogen is 5 m/s and hydrogen is injected with a bulk velocity of 120 m/s. The ($\rho, T$) diagram shown in Fig. 2 illustrates the nominal operating conditions for the main nitrogen injection. With a temperature of $T_{N_2} = 118$ K, nitrogen is initially in a transcritical state for operating point E4 (liquid-like with $\rho_{N_2} = 584.43$ kg/m$^3$).

Based on the observation that [14] measured the density in the liquid core close to the injector as $\rho_{E4}^{Exp} \sim 390.18$ kg/m$^3$, which according to NIST [21] indicates a nitrogen temperature of about 128.8 K rather than 118 K, we define a second test case E4$^{Fit}$ for which we assume a correct density and mass flow rate (8.29 g/s) measurement and a faulty temperature measurement. We thus obtain $\bar{u}_{N_2} = 7.49$ m/s for the nitrogen
bulk velocity and $T_{N_2} = 128.274$ K for the inflow temperature. This test case will help us to assess uncertainties related to both the experimental and numerical setup. The operating conditions for test case E4 and E4$^{rel}$ are summarized in Tab 1.

4. Numerical approach

The numerical simulations are performed with the flow solver INCA †, which solves the three-dimensional fully compressible multicomponent Navier-Stokes equations in a conservative form. The mass, momentum, and energy equations are closed by a cubic EOS, where an iterative procedure is applied to transform transported variables (density and energy) to primitive variables (temperature and pressure), c.f. [25] and references therein in which details for such an algorithm can be found. The diffusional fluxes are calculated via the Fickian diffusion approximation with an effective binary diffusion coefficient, c.f. [27] and references therein. The physical binary mass diffusion coefficients $D_{ij}$ are modeled according to Chapman and Enskog theory, see, e.g., [28]. The governing equations are discretized by a conservative finite-volume scheme on collocated Cartesian grids with a block structured topology that allows for hanging nodes. In order to avoid spurious oscillations at sharp density gradients, we use a second-order upwind biased numerical flux function together with the van Albada limiter [29] for the advective transport of mass and internal energy. Effects of unresolved subgrid scales

† www.inca-cfd.org
Large-eddy simulation of cryogenic jet injection at supercritical pressures

(SGS) are modeled by the adaptive local deconvolution method (ALDM) of [30]. The formulation ensures that only the compressible modes are affected by the second-order upwind scheme, while vorticity modes and turbulence kinetic energy remain unaffected. The viscous flux is discretized using a 2nd order central difference scheme, and the 3rd order explicit Runge-Kutta scheme of [31] is used for time integration.

The computational domain is shown in Fig. 3. All simulations have been performed in a rectangular domain with the overall dimensions \( L_x = 100 \) mm in the streamwise and \( L_y = L_z = 40 \) mm in the lateral directions. Based on preliminary simulation results, a reasonably good estimate of jet break-up position and spreading angle was available to dimension the grid such that jet dynamics are not spuriously affected by the boundary conditions. An adaptive Cartesian blocking strategy with a static local coarsening/refinement is used with a homogeneous grid resolution in the region of interest. The injector plane, \( 5 \text{ mm} \times 5 \text{ mm} \), is resolved with \( 16348 \) computational cells. Within a cone with an half opening angle of \( \sim 11^\circ \) and a length of \( 20 \text{ mm} \) the grid has a homogeneous resolution in lateral and streamwise direction with \( \Delta y_{\text{min}} = \Delta z_{\text{min}} = 0.0391 \text{ mm} \) and \( \Delta x_{\text{min}} = 2\Delta y_{\text{min}} \). With increasing distance from the surface of the cone, grid coarsening in lateral and streamwise direction is applied. The total number of computational cells is about \( 16.9 \) million. Realistic turbulent inflow data for the \( \text{N}_2 \) pipe and \( \text{H}_2 \) annulus are generated through separate incompressible LES using cyclic boundary conditions in axial direction. At the outlet we prescribe the static pressure of \( 4 \) MPa together with a linear extrapolation procedure of all conservative flow variables. All walls are modeled as adiabatic.

5. LES results

5.1. Instantaneous aspects

Figure 4(a) depicts an instantaneous snapshot of the temperature distribution for case E4 \( (T_{\text{N}_2} = 118 \text{ K}) \). Contour levels are shown for \( 118 \text{ K} < T < 300 \text{ K} \), from dark to light shades, superimposed by a second group of contour levels with \( 110 \text{ K} < T < 118 \text{ K} \), from blue to red shades. Cryogenic nitrogen at \( 118 \text{ K} \) can be identified as ‘dark core’, surrounded by a co-flow of warm hydrogen at \( 270 \text{ K} \). It is interesting to see that the temperature within in the mixing layer drops below its inflow value of \( 118 \text{ K} \) to approximately \( 110 \text{ K} \). A related effect can be observed also for the hydrogen partial density \( \rho_{\text{H}_2} \), which is depicted in Fig. 4(b). Hydrogen is injected with a density of \( \rho_{\text{H}_2} = 3.55 \text{ kg/m}^3 \) and reaches a much higher partial density of almost \( \rho_{\text{H}_2} = 5.35 \text{ kg/m}^3 \) within the mixing layer.

In order to analyze changes in the thermodynamic state throughout the mixing process in greater depth, we show a scatter plot of temperature as function of hydrogen mole fraction in Fig. 5(a) for the same dataset as used for Fig. 4(a). On the left hand side \( (z_{\text{H}_2} = 0) \), pure nitrogen at either \( 118 \text{ K} \) (injection temperature) or \( 298.15 \text{ K} \) (reservoir temperature) can be identified. On the right hand side \( (z_{\text{H}_2} = 1) \), we observe pure hydrogen at \( 270 \text{ K} \). In between, either cryogenic nitrogen from the main injection (follow the line labeled ‘adiabatic mixing temperature’) or warm nitrogen from the reservoir (follow the straight line, top of the figure) is mixed with warm hydrogen. Assuming an isobaric and adiabatic mixing process, the line labeled ‘adiabatic mixing temperature’ can be calculated analytically by solving an enthalpy balance equation

\[
h (T, p, z_1, ..., z_n) - \sum z_i h_i (T_i, p) = 0
\]  

(5.1)
for the temperature $T$. For the molar enthalpy $h(T, p, z_1, ..., z_n)$ the mixing rules of the PR EOS apply. The second term on the left hand side represents the sum of the enthalpies (on a molar basis) of the pure components at $T_{N_2} = 118$ K and $T_{H_2} = 270$ K before mixing. The interested reader is also referred to [32, 33] and [34] who did a similar analysis in the context of high-pressure fuel injection relevant to diesel engines. Following the notation of [34] we call this temperature the 'frozen adiabatic mixing temperature' (FAMT). This analytical model (which neglects heat and mass diffusion and the kinetic energy of the flow) shows that the temperature decrease in the mixing layer can be attributed to real gas mixing effects, i.e., non-linear interaction between molecules introduced via mixing rules (see Sec. 2), and not, as one could also assume, to heat transfer and diffusion mechanisms or to compressibility effects. The isobaric mixing of cryogenic nitrogen and warm hydrogen is endothermic and only scatter away from the adiabatic mixing line can be attributed to transport phenomena (e.g., heat and mass diffusion) not covered by the FAMT model assumptions. Note that the scatter away from the mixing line increases with increasing hydrogen mole fraction. Here, we expect the model assumptions more likely to fail due to the much higher velocity of the hydrogen stream ($u_{H_2} = 120$ m/s) and the resulting turbulent fluctuations (e.g., pressure fluctuations).

A corresponding scatter plot for the hydrogen partial density is shown in Fig. 5(b). Again, there is pure nitrogen (meaning $\rho_{H_2} = 0$) on the left hand side and pure hydrogen at its corresponding density at injection $\rho_{H_2} = 3.55$ kg/m$^3$ on the right hand side. The scattered data is colored by temperature in the same way as done for Figure 4(a). The solid line labeled $\rho_{H_2} (FAMT)$ now corresponds to the hydrogen partial density ($\rho_{H_2} = Y_{H_2} \cdot \rho$) calculated along the adiabatic mixing line of Fig. 5(a). The scattered data follow
closely the analytical solution, and again, this result shows that the hydrogen exceeds its pure component density due to real fluid mixing effects.

Snapshots of temperature and hydrogen partial density for test case $E4^\text{Fit}$ are depicted in Fig. 4(c) and Fig. 4(d), respectively. While we observe a similar effect for the temperature, i.e., a local decrease within the turbulent mixing layer, the hydrogen density does not exceed its pure component inflow value. It is interesting to see that endothermic mixing does not necessarily imply hydrogen partial densities exceeding the inflow value. Figures 5(c) and 5(d) show the corresponding scatter plots. Again, the lines of adiabatic mixing temperature and partial density enclose the scattered data. Compared to the nominal operating conditions, thermodynamic peculiarities are less pronounced for test case $E4^\text{Fit}$ due to the higher nitrogen temperature of $T_{N_2} = 128.274 \text{ K}$.

The scatter plots in Fig. 5(a)-5(d) show that the LES data includes thermodynamic mixture states that lie within the mixture two-phase region, although the operating pressure is well above the critical pressure of the pure components. This aspect is discussed separately in Sec. 6.
In the following we compare our numerical results to the experimental data of [14]. A total time interval of 20 ms has been simulated, which corresponds to 5 flow through times (FTT) with respect to the nitrogen bulk velocity \( \bar{u}_{N_2} = 5 \) m/s and \( L_x = 20 \) mm. A fully developed flow field from coarser grids served as initial solution. Statistical properties have been obtained by averaging in circumferential direction and in time after an initial transient of 6 ms (1.5 FTT). Figure 6(a) and 6(b) depict the axial (centerline) and radial nitrogen density profiles for test case E4. Radial data are extracted at \( x/D_i = 2.1 \). We observe significant differences in the potential core region \( (x/D_i < 3) \) with experimental and numerical nitrogen densities of \( \sim 390.18 \) kg/m\(^3\) and \( \sim 608.78 \) kg/m\(^3\), respectively. Recall Fig. 2: a specification of the inflow boundary condition in terms of temperature and pressure must yield a density within the potential core much higher than what is observed experimentally. With an error of about \( \sim 4\% \) when comparing the PR EOS to the NIST reference data, it becomes apparent that the observed differences in nitrogen density of approximately 200 kg/m\(^3\) can not be attributed to an inaccurate equation of state but rather to measurement uncertainties. A more thorough discussion on this issue is given at the end of this paragraph.

Figures 5.2 and 6(d) show the corresponding hydrogen partial density profiles. Fig-

**Figure 6.** Axial (centerline) and radial nitrogen \( (\rho_{N_2}, \text{(a)/(b) and (e)/(f)}) \) and hydrogen \( (\rho_{H_2}, \text{(c)/(d) and (g)/(h)}) \) partial density profiles for test case \( E4 \) (top) and \( E4^{Fit} \) (bottom). (——) LES results; (⊙) experimental data of [14]. Radial profiles are extracted at 1 mm. Note that Fig. 6 (c)/(g) display the maximum values of the radial hydrogen density distribution that have been recorded experimentally. (■) LES data at the corresponding streamwise locations.

### 5.2. Mean flow

In the following we compare our numerical results to the experimental data of [14]. A total time interval of 20 ms has been simulated, which corresponds to 5 flow through times (FTT) with respect to the nitrogen bulk velocity \( \bar{u}_{N_2} = 5 \) m/s and \( L_x = 20 \) mm. A fully developed flow field from coarser grids served as initial solution. Statistical properties have been obtained by averaging in circumferential direction and in time after an initial transient of 6 ms (1.5 FTT). Figure 6(a) and 6(b) depict the axial (centerline) and radial nitrogen density profiles for test case E4. Radial data are extracted at \( x/D_i = 2.1 \). We observe significant differences in the potential core region \( (x/D_i < 3) \) with experimental and numerical nitrogen densities of \( \sim 390.18 \) kg/m\(^3\) and \( \sim 608.78 \) kg/m\(^3\), respectively. Recall Fig. 2: a specification of the inflow boundary condition in terms of temperature and pressure must yield a density within the potential core much higher than what is observed experimentally. With an error of about \( \sim 4\% \) when comparing the PR EOS to the NIST reference data, it becomes apparent that the observed differences in nitrogen density of approximately 200 kg/m\(^3\) can not be attributed to an inaccurate equation of state but rather to measurement uncertainties. A more thorough discussion on this issue is given at the end of this paragraph.

Figures 5.2 and 6(d) show the corresponding hydrogen partial density profiles. Fig-

**Figure 6.** Axial (centerline) and radial nitrogen \( (\rho_{N_2}, \text{(a)/(b) and (e)/(f)}) \) and hydrogen \( (\rho_{H_2}, \text{(c)/(d) and (g)/(h)}) \) partial density profiles for test case \( E4 \) (top) and \( E4^{Fit} \) (bottom). (——) LES results; (⊙) experimental data of [14]. Radial profiles are extracted at 1 mm. Note that Fig. 6 (c)/(g) display the maximum values of the radial hydrogen density distribution that have been recorded experimentally. (■) LES data at the corresponding streamwise locations.

### 5.2. Mean flow

In the following we compare our numerical results to the experimental data of [14]. A total time interval of 20 ms has been simulated, which corresponds to 5 flow through times (FTT) with respect to the nitrogen bulk velocity \( \bar{u}_{N_2} = 5 \) m/s and \( L_x = 20 \) mm. A fully developed flow field from coarser grids served as initial solution. Statistical properties have been obtained by averaging in circumferential direction and in time after an initial transient of 6 ms (1.5 FTT). Figure 6(a) and 6(b) depict the axial (centerline) and radial nitrogen density profiles for test case E4. Radial data are extracted at \( x/D_i = 2.1 \). We observe significant differences in the potential core region \( (x/D_i < 3) \) with experimental and numerical nitrogen densities of \( \sim 390.18 \) kg/m\(^3\) and \( \sim 608.78 \) kg/m\(^3\), respectively. Recall Fig. 2: a specification of the inflow boundary condition in terms of temperature and pressure must yield a density within the potential core much higher than what is observed experimentally. With an error of about \( \sim 4\% \) when comparing the PR EOS to the NIST reference data, it becomes apparent that the observed differences in nitrogen density of approximately 200 kg/m\(^3\) can not be attributed to an inaccurate equation of state but rather to measurement uncertainties. A more thorough discussion on this issue is given at the end of this paragraph.

Figures 5.2 and 6(d) show the corresponding hydrogen partial density profiles. Fig-

**Figure 6.** Axial (centerline) and radial nitrogen \( (\rho_{N_2}, \text{(a)/(b) and (e)/(f)}) \) and hydrogen \( (\rho_{H_2}, \text{(c)/(d) and (g)/(h)}) \) partial density profiles for test case \( E4 \) (top) and \( E4^{Fit} \) (bottom). (——) LES results; (⊙) experimental data of [14]. Radial profiles are extracted at 1 mm. Note that Fig. 6 (c)/(g) display the maximum values of the radial hydrogen density distribution that have been recorded experimentally. (■) LES data at the corresponding streamwise locations.
Large-eddy simulation of cryogenic jet injection at supercritical pressures

Figure 5.2 displays the observed maximal values of the radial hydrogen density distribution at several stations. Interestingly, [14] report an increase in hydrogen density downstream of the jet break-up that exceeds its pure-component value at injection, which is qualitatively reproduced by the numerical simulation. Quantitatively, we observe a very good agreement for \( x/D_i > 6 \). In the immediate vicinity of the injector, however, large deviations between measured and simulated hydrogen density are present. Recall the snapshot of the hydrogen partial density distribution in Fig. 4(b): as soon as hydrogen and nitrogen start to mix in the recirculation zone downstream of the LN2 post, the hydrogen density rises to about \( \sim 5.3 \) kg/m\(^3\). Therefore, plotting the maximum (mean) value at a streamwise location must yield increased hydrogen densities in the immediate vicinity of the injector. We note that close to the injector, the spatial extent of regions showing increased hydrogen densities is very narrow. The detection of these regions in the near field of the injector may therefore be difficult in an experiment.

In Figs. 6(e)-6(h) we show numerical results for case E4\( ^{E4}_{\text{Fit}} \) where we assumed a correct density and mass flow rate (8.29 g/s) measurement and discarded the temperature measurement. Centerline and radial nitrogen density profiles are shown in Figs. 6(e) and 6(f). We now observe a very good agreement for the nitrogen density, the potential core length and the axial position for which a fully mixed state is obtained (\( x/D_i \sim 10 \)). We note that the two latter observations may depend on the flow solver and grid resolution, whereas the value of the nitrogen density in the potential core does not. These results suggest that the nitrogen temperature at the injector exit could have been higher than the nominal value at the time of data collection. However, using the fitted boundary condition we do not observe the characteristic increase in partial hydrogen density that was recorded experimentally, see Fig. 6(g). With real-gas mixing effects being less pronounced at higher temperatures, this result was to be expected (cf. Figs. 4(d) and 5(d)).

With respect to the hydrogen partial density, the agreement between experimental and numerical data is poor for the fitted boundary condition \( E4\text{Fit} \), both quantitatively and qualitatively.

There are a number of uncertainties related to both the numerical and the experimental setup that may help to explain the observed differences: Laser diagnostics in turbulent flows in a high pressure low temperature environment are very challenging. [14] report difficulties in the quantification of the Raman signal due to refraction index gradients and reflections at the injector face plate. These difficulties may increase the error bar especially at locations very close the injector exit. The temperature measurement by thermocouples took place several diameters upstream of the nozzle exit. Although not explicitly mentioned in Refs. [14] and [5], we expect measurement uncertainties to be in the same order of magnitude as experienced in similar cryogenic nitrogen injection experiments, e.g., [4], [35] and [16]. For the present near critical operating conditions, the nitrogen density is very sensitive to temperature changes. Thus, uncertainties in the temperature measurement can have a significant impact on computational results when used as inflow boundary condition. The Raman signal was detected with a single camera system. Depending on the bandpass filter that was used for the spectral separation of the Raman signals from different species, either nitrogen or hydrogen density measurements could be performed. According to Oschwald, the measurements of the two species are therefore not temporally correlated and the same holds for measurements at different axial positions (private communication). We cannot exclude the possibility that the nitrogen temperature at the injector exit was approximately 128 K during nitrogen density measurements, which could explain the good agreement with respect to the
nitrogen density for case E4, while it had its nominal value of 118 K during hydrogen density measurements, which could explain the good agreement with respect to the exceeding hydrogen density for case E4. However, it is impossible to draw any definite conclusions because of the complexity of the problem and the variety of sources that may contribute to the uncertainties in measurement and simulation.

With respect to the numerical simulation, we note that the location of jet break-up, spreading angle, and downstream evolution (∂ρ/∂x) is very sensitive to both the numerical scheme and grid resolution. For example, in [36] we use a more dissipative numerical scheme compared to the present method and obtain a shorter dense core. Evidence from yet unpublished results indicate that the location of jet break-up moves further downstream for finer grids (∼101 million cells). We therefore consider the present results and the results published in [36] and [37] not grid converged. Non-ideal thermodynamics phenomena like endothermic mixing and exceeding partial densities, however, can be reproduced with any numerical scheme (and turbulence model) on any reasonably fine computational grid. Therefore, when comparing the present experimental and numerical data from a phenomenological point of view, simplifications in the thermodynamic modeling, such as neglecting multiphase phenomena, appear to be of much greater relevance. Some of the states obtained in the LES lie well within the two-phase region, see Fig. 5. Assuming the validity of classical thermodynamic fundamentals, in particular the two-phase theory with vapor-liquid equilibrium relations, the use of a single homogeneous phase model as done for the present LES becomes questionable.

6. Transcritical two-phase phenomena

6.1. Phase equilibrium and isenthalpic-isobaric flash calculations

The thermodynamic model introduced in Sec. 2 assumes that the binary mixture exists as a single phase. In multicomponent systems, however, this may be false even though the operating pressure (here 4 MPa) is above the critical pressure of the pure components (\(p_{c,N_2} = 3.34\) MPa, \(p_{c,H_2} = 1.29\) MPa). It is well known that the critical pressure of a mixture can be much higher than the critical pressure of the pure components and two phases can coexist at pressures that exceed the critical pressure of either component. To address the question whether two-phase phenomena may occur for the present application or not, vapor-liquid equilibria (VLE) are calculated for binary \(H_2 - N_2\) mixtures at 4 MPa. A necessary condition of equilibrium is that the chemical potential, or equivalently, that the fugacity of each component is the same in the two phases:

\[ f_i^l(T, p, x) = f_i^v(T, p, y) \quad \text{for} \quad i = 1, 2 \ldots N_c. \]  

(6.1)

Liquid (\(l\)) and vapor (\(v\)) phase mole fractions are denoted by \(x = \{x_{H_2}, x_{N_2}\}\) and \(y = \{y_{H_2}, y_{N_2}\}\), respectively. Analytical expressions for the fugacity \(f\) of each component \(i\) can be found in literature, see, e.g., [38] for the PR EOS. Bubble-point and dew-point lines can be calculated by solving Eq. (6.1) for the unknown mixture mole fractions in the liquid (\(x\)) and vapor (\(y\)) phases, provided pressure \(p\) and temperature \(T\) are specified.

Figure 7 shows an enlarged view of the binary phase diagram that was already indicated in Fig. 5(a) for the nominal operating conditions of case E4 \(\left(T_{N_2} = 118\right)\) K. Again, the scattered gray points represent the thermodynamic state of the mixture obtained from the LES. Assuming the validity of the VLE relations, mixture states that lie within the parameter space enclosed by the dew-point and bubble-point line will break up into a liquid and vapor phase. Recently, [39, 40] and [41] initiated an interesting dis-
Discussion on the transition between two-phase and single-phase interface dynamics at supercritical pressures. Their results suggest that VLE assumptions may not hold for conditions similar to those investigated herein (which means that the assumed single phase assumption holds) and only a more detailed analysis based on a Knudsen number criterion together with non-linear gradient theory and highly accurate EOS models may answer the question whether a continuous gas like interface or a molecular vapor-liquid interface exists for the experimental conditions of test case E4. Such an analysis, however, is beyond the scope of this work. Based on the assumption that the VLE relations hold we rather focus on the question how a potential phase separation within the turbulent shear layer could affect flow and temperature fields.

For this purpose we developed a post-processing tool that performs phase stability and phase splitting calculations based on an instantaneous flow field obtained from the LES. The post-processing consists mainly of two parts: Starting with the temperature $T_{LES}$, pressure $p_{LES}$, and overall composition $z_{LES} = \{z_{H_2}, z_{N_2}\}$ in a computational cell the stability of the assumed single phase is determined with the Tangent Plane Distance (TPD) function [42]. If the mixture is known to be unstable the isenthalpic-isobaric flash problem (i.e., thermodynamic equilibrium calculation with specification of pressure, enthalpy and overall composition) is solved for a new equilibrium temperature ($T = T_{EQ}$ ($\neq T_{LES}$), density ($\rho = \rho_{EQ}$ ($\neq \rho_{LES}$)) as well as liquid and vapor mole fractions $x$, $y$ such that the mixture’s Gibbs energy at specified overall composition $z_{LES}$ and pressure $p_{LES}$ is at its global minimum. For comprehensive reviews and solution methods the interested reader is referred to [43], [44] and [45]. For the present work we followed the recommendation of [46] and implemented the BFGS-quasi-Newton algorithm, see [45] and references therein. Performing this analysis for the states along the FAMT line of the present test case yields the equilibrium adiabatic mixing temperature (EAMT) shown in Fig. 7. Compare also the work of [34] who did a similar analysis in the context of high pressure diesel injection.
6.2. Results

Figure 8 shows the results of phase stability and phase splitting calculations on basis of the assumed single-phase LES result from Fig. 4. Figure 8(a) depicts a snapshot of the temperature field, color map and range are the same as in Fig. 4. Taking phase separation into account, leads to a less pronounced temperature decrease within in the turbulent mixing layer. The mixing process, however, is still endothermic and the temperature drops by about 5 K. The same phenomenon can also be seen for the adiabatic mixing temperature line in Fig 7. The line labeled ‘EAMT’ corresponds to the equilibrium temperature calculated from the analytical model. The difference between frozen and equilibrium temperature is most prominent at an overall mole fraction $z_{H_2} = 0.28$.

An isolated view on regions that are located within the parameter space spanned by the bubble-point and dew-point line is provided in Fig. 8(b), which depicts the vapor fraction $\psi_v$ on a molar basis (mol vapor/mol mixture). For reasons of clarity, all cells with $\psi_v = 0$ and $\psi_v = 1$ are blanked out. Since we do not (and cannot) resolve individual phase boundaries in the case of phase separation, we assume the two phases in thermodynamic equilibrium and homogeneously distributed within a computational cell. With the vapor fraction $\psi_v = 0$ at the bubble point line and $\psi_v = 1$ at the dew point line, a smooth transition throughout the two-phase region is facilitated between a liquid rich two-phase mixture on the nitrogen side and a vapor rich two-phase mixture on the hydrogen side.

Figure 8(c) depicts the hydrogen density $\rho_{H_2}$ (color map and range were chosen the same as in Fig. 4). Compared to the assumed single-phase results we observe a decrease of the maximum hydrogen partial density. However, it is important to note that
the hydrogen partial density still exceeds its pure component value, which was also observed experimentally.

Corresponding scatter plots for the thermodynamic states are shown in Fig. 9(a) and 9(b) for the hydrogen and nitrogen partial density. Data points for which the isenthalpic-isobaric flash is solved are colored from blue to red shades by the molar vapor fraction. Mixtures that were identified as stable are colored from dark to light shades by their corresponding temperature (which means \( T_{EQ} = T_{LES} \)). The solid red and blue lines represent vapor \( \rho_{v}^{i} \) and liquid \( \rho_{l}^{i} \) partial densities of component \( i \). The frozen partial density \( \rho_{f}^{i} \) is shown as reference. As expected, the hydrogen partial density in the vapor phase \( \rho_{v}^{H_{2}} \) is higher than in the liquid phase \( \rho_{l}^{H_{2}} \). However, it is interesting to see that liquid and vapor phase partial densities are not too different from each other. In contrast, the nitrogen partial density in the liquid phase \( \rho_{l}^{N_{2}} \) is much higher compared to its density in the vapor phase \( \rho_{v}^{N_{2}} \), see Fig. 9(b). Moreover, while the overall partial nitrogen density \( \rho_{N_{2}}^{(T_{EQ})} \) decreases continuously across the mixing layer (left: 608.78 kg/m\(^3\), pure nitrogen; right: 0 kg/m\(^3\), pure hydrogen), the nitrogen density in the liquid phase \( \rho_{l}^{N_{2}} \) increases with increasing \( z_{H_{2}} \). This raises an interesting question: which partial density is actually being measured by Raman spectroscopy in case of phase separation within the turbulent shear layer and the existence of liquid and vapor phases with so different partial densities?

To give an answer to the question whether such two-phase phenomena are capable of affecting the flow field (e.g. jet break-up location, spreading angle) or not, consider Fig. 8(d) showing the relative difference in (overall) density prediction between the assumed single-phase \( (\rho_{F}, \text{frozen density}) \) and two-phase approach \( (\rho_{EQ}, \text{equilibrium density}) \). The density prediction of the single-phase approach is by about 25% higher in large parts of the shear layer compared to the two-phase approach. We may expect that such a change in density as well as the presence of phase boundaries in the turbulent shear layer will affect jet break-up dynamics.
7. Conclusion

This report has summarized recent results of large-eddy simulations (LES) of binary mixtures in shear coaxial injection at supercritical pressures with a particular emphasis on transcritical two-phase phenomena. We selected an operating point from the series of experiments of [14] for which quantitative density measurements in a coaxial liquid nitrogen (LN2) and gaseous hydrogen (GH2) jet at supercritical pressures (with respect to the critical pressure of the pure components) are available. This operating point resembles typical main-stage LOX/GH2 rocket engines, however, by using nitrogen instead of oxygen, mixing and atomization can be studied without introducing the complexities of combustion. Instantaneous LES data showed interesting thermodynamic phenomena such as endothermic mixing and partial hydrogen densities exceeding the inflow value within the turbulent shear layer. The latter was recorded also experimentally for the nominal operating conditions. A simple thermodynamic model showed that both the temperature decrease and exceeding hydrogen partial densities in the mixing layer can be attributed to real gas mixing effects, i.e., non-linear interaction between molecules introduced via mixing rules, and not, as one could also assume, to heat transfer and diffusion mechanisms or compressibility effects.

We found that the chosen inflow temperature plays a crucial role for the reproduction of the experimental results. Based on the observation that the definition of inflow boundary conditions in terms of temperature and pressure must yield a nitrogen density in the jet core much higher than what was measured experimentally, we defined a new test case for which we assumed a correct density and mass flow rate measurement and a faulty temperature measurement. For this fitted boundary condition we observed quantitatively a very good agreement between experimental and numerical data with respect to the nitrogen density. However, experimental findings of exceeding hydrogen partial densities were not reproduced anymore. With real-gas mixing effects being less pronounced at higher nitrogen injection temperatures, this result was to be expected also on basis of the analytical FAMT mixing model.

By analyzing vapor-liquid equilibria (VLE) data it was shown that some states obtained in the LES lie well within the two-phase region. In order to perform VLE calculations with respect to the local thermodynamic state within the turbulent shear layer, i.e., local pressure, composition and enthalpy, a novel post-processing of LES data based on fundamental thermodynamic principles was introduced. Results of phase stability and phase splitting calculations on basis of the assumed single-phase LES result showed that taking two-phase phenomena into account leads to a less pronounced temperature decrease and hydrogen partial density increase within in the turbulent mixing layer. While we observed hydrogen partial densities in the liquid and vapor phase not too different from each other, the partial density of nitrogen showed considerable differences in the two phases. This raised the question which density was actually measured by Raman spectroscopy in a two-phase region. With a density prediction up to 25% higher in large parts of the shear layer for the single-phase approach compared to the two-phase approach, we may expect jet break-up dynamics and consequently integral quantities such as the dark core length or spreading rate to be affected by such transcritical two-phase phenomena. In order to address this aspect in a greater depth our current research aims at performing VLE calculations during run time of the CFD simulation.
Acknowledgments

Financial support has been provided by the German Research Foundation (Deutsche Forschungsgemeinschaft – DFG) in the framework of the Sonderforschungsbereich Transregio 40.

References


---

*Large-eddy simulation of cryogenic jet injection at supercritical pressures* 147


Large-eddy simulation of cryogenic jet injection at supercritical pressures

Based on Mixing-Limited Vaporization. SAE technical paper 1999-01-0528.


