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Numerical analysis of turbulent flow dynamics and heat transport in a round jet at supercritical conditions

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ABSTRACT

Using a direct numerical simulation (DNS), a round jet of cryogenic nitrogen, which mimics the experiment by Mayer et. al. (2003) in terms of geometry, thermodynamics, and hydrodynamics, but at reduced Reynolds-Number ($Re = 5300$ based on the injection diameter), is investigated. The objectives of the present paper are: (1) to reliably predict the turbulence statistics in order to investigate the physical mechanisms, that dominate the flow dynamics, and to investigate the fuel disintegration and mixture formation, (2) to analyze the characteristics of heat transport phenomena of supercritical flows in order to determine parameter regimes advantageous to mixing, and (3) to provide a database for model development and validation that is difficult to obtain experimentally at such extreme thermodynamic conditions.

The correctness of the results has been established at two levels. First, a grid-sensitivity study has been carried out to determine the resolution, which provides grid-independent turbulence statistics. This ensures, that the quantities of interest depend only on the physics and are not affected by the numerical methods. Secondly, numerical results have been compared to available experimental data of sub- and supercritical jets. Assuming self-similarity, several characteristics of the jet, like spreading rate, density variations and thermodynamic properties have been assessed.

Finally, a comprehensive database including instantaneous flow and temperature fields, mean flow characteristics, turbulence properties along with turbulent kinetic energy budget, and heat flux has been made available. A link to heat flux transport modeling has been established to evaluate the suitability of some existing heat flux models as employed in such supercritical fluid flow.

1. Introduction

Currently, there is a great interest in processes occurring under supercritical thermodynamic conditions, like in propulsion applications including rocket engines, gas turbines or diesel engines (Messerschmid and Fasoulas, 2011; Knez et al., 2014; Ahn et al., 2015). Thereby, a clear trend to operate at higher combustion chamber pressure is observed in order to favor the production of higher specific energy conversion rates along with the improvement of thermodynamic performance. This is mainly achieved at pressures exceeding the critical pressures.

Under subcritical conditions, the injected fuel disintegrates due to the action of surface tension, which induces ligament formation, atomization and evaporating droplet with sharp interfaces. Once supercritical condition is reached, the breakup is replaced by mixing, including turbulent mixing and diffusion, as surface tension vanishes. As pointed out in Banuti et al. (2017), this leads researchers to consider continuous Eulerian mixing models instead of Lagrangian droplet tracking methods to deal with supercritical fluid flow.

In this respect, it is worth mentioning that the transition between supercritical liquid-like and gas-like states resembles subcritical vaporization. However, as pointed out in Banuti (2015), the isothermal vaporization is replaced by a continuous non-equilibrium process at supercritical pressures. High pressure real fluid effects merely distribute the latent heat over a finite temperature interval and the thermal energy supplied is used to increase the temperature and overcome molecular forces simultaneously. In the literature, this process is known as pseudo-boiling (Oschwald and Schik, 1999; Banuti, 2015). Thereby, the coexistence line between the liquid and gaseous phases is extended beyond the critical point by the so-called Widom line, a line which divides the liquid-like and gas-like supercritical states. Along the Widom line, the isothermal compressibility and the density gradient with re-

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spect to temperature and the specific heat capacity along with further thermodynamic properties exhibit maximal values. For such extremely complex phenomena, a satisfactory understanding is still needed, even though significant progress has been reported in the literature either in experiments (Mayer and Tamura, 1996; Oschwald et al., 2006; Candel et al., 2006; Habiballah et al., 2007) or in the context of numerical modeling (Oefelein and Yang, 1998; Oefelein, 2006; Bellan, 2006; Zong and Yang, 2006).

Several researchers applied RANS (Mayer et al., 2003; Sierra-Pallares et al., 2016; Kim et al., 2011) or LES (Oefelein and Yang, 1998; Petit et al., 2013; Schmitt et al., 2010; Müller et al., 2016) to gain more reliable predictions for practical applications. The main objective of these contributions was to evaluate the impact of selected SGS models and real gas equations of state on the mixing prediction. The effect on the subsequent combustion has also been addressed in Oefelein (2006), Mari et al. (2012), Huo and Yang (2017) and Tramecourt et al. (2004). Especially the effects of equations of state for turbulent flows under supercritical thermodynamic conditions and their impact on modeling strategy have been addressed in Selle and Ribert (2008) and Selle and Schmitt (2010). Okong'o and Bellan (2000) and others (Miller et al., 2001; Okong'o and Bellan, 2002; Selle et al., 2007; Foster and Miller, 2012; Taskinoglu and Bellan, 2010) considered the supercritical issues in LES modeling using DNS. Such three dimensional DNS contributions as reported in the literature all reduced the Reynolds number owing to limited computational resources.

Recently, Ruiz et al. (2016) used a two-dimensional DNS to provide a numerical benchmark for high-Reynolds-number supercritical flows with large density gradients in simple configurations containing the essential features of real devices (geometry, thermodynamics, and hydrodynamics). This DNS refers to a mixing layer forming downstream of an injector lip separating a stream of dense oxygen from a stream of light hydrogen, mimicking one experiment by Chehroudi et al. (2002). The authors provided mean and rms velocity, temperature profiles, power spectrum density of the square of transverse velocity, dense core lengths, mixing layer thickness, etc.

Focusing essentially on flow and mixing process, the so-called Mayer et al. (2003) configuration and the Mascotte benchmark test (Candel et al., 1998; Haidn and Habiballah, 2003) have been widely investigated by means of LES (e.g. Petit et al., 2013; Schmitt et al., 2010; Müller et al., 2016; Guezennec et al., 2012) with the main objective to evaluate the impact of selected SGS models known in subcritical environments and of the real gas equations of state on the mixing prediction. However, impeded by the lack of comprehensive and reliable validation data, the appraisal of the results and models used remains inconclusive.

A three dimensional DNS of such configurations appears therefore particularly important. Using a highly-resolved numerical simulation technique, a round jet of nitrogen, which mimics the experiment by Mayer et al. (2003) in terms of geometry, thermodynamics, and hydrodynamics but at reduced Reynolds-Number is simulated in the present work. Thereby, the original Reynolds number of the experiment is reduced from $Re = 1.62 \times 10^5$ (based on the injection diameter) to $Re = 5300$ in the numerical study. A grid-sensitivity study has been carried out to prove the reliability of the results and to ensure that the quantities of interest depend only on the physics and not on the numerical approach.

The aims of the present study are: (1) to reliably predict the turbulence statistics in order to investigate the physical mechanisms that dominate the flow dynamics, and to investigate the fuel disintegration and mixture formation, (2) to analyze the characteristics of heat transport phenomena of supercritical flows in order to determine parameter regimes advantageous to mixing, and (3) to provide a database for model development and validation that is very difficult to obtain experimentally at such extreme thermodynamic conditions.

Section 2 introduces the theoretical framework, which includes governing equations and appropriate conservation laws, real fluid thermodynamics and transport properties over the entire temperature and pressure regime under consideration. Subsequently, the numerical procedure is outlined. Section 3 describes the test case under investigation along with the operating conditions and the initial and boundary conditions. The results are presented and discussed in Section 4. With respect to the objectives, the results are provided in terms of instantaneous flow and temperature fields, mean flow characteristics, turbulence properties along with turbulent kinetic energy budget, and heat flux. These data are used to evaluate the suitability of some existing heat flux models as applied in such supercritical fluids.

2. Methods

In this section, governing equations, thermodynamic models and numerical methods used to simulate supercritical fluid flows are presented. A low Mach-number approach is employed, suitable for flows under incompressible conditions ($\mathrm{Ma} \ll 0.3$) and variable physical properties. In contrast to a fully compressible formulation, the pressure and density are formally decoupled by defining the density through an equation of state expressed in terms of local temperature T and thermodynamic pressure p^{th}. Thereby acoustic and compressibility effects are neglected (Bae and Yoo, 2005).

2.1. Governing equations

In the case of incompressible fluid flow with variable physical properties and no gravity force, the employed governing equations of continuity, momentum and enthalpy are

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_i)}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial (\rho U_i)}{\partial t} + \frac{\partial \left(\rho U_i U_j\right)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}, \tag{2}$$

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho U_i h)}{\partial x_j} = -\frac{\partial q_i}{\partial x_i} + \tau_{ij}\frac{\partial U_i}{\partial x_j}, \tag{3}$$

where ρ is the density, U_i the velocity, p the pressure, τ_{ij} the viscous stress tensor, h the sensible enthalpy, and q_i the heat flux. Assuming Newtonian fluid flow, the viscous stress tensor is modeled as

$$\tau_{ij} = \mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij}\right), \tag{4}$$

where μ is the molecular viscosity. The heat flux is expressed by Fourier's law assuming incompressible fluid flow

$$q_i = -\lambda \frac{\partial T}{\partial x_i} = -\frac{\lambda}{c_p}\frac{\partial h}{\partial x_i}, \tag{5}$$

where λ is the thermal conductivity and c_p the heat capacity of the fluid.

2.2. Thermodynamic models

To account for non-ideal gas behavior at supercritical conditions, the commonly used Peng–Robinson equation of state (Peng and Robinson, 1976) (PR-EOS) is applied in the present study. The PR-EOS is represented as

$$p^{th} = \frac{RT}{v_{PR} - b} - \frac{a(T)}{v_{PR}(v_{PR} + b) + b(v_{PR} - b)}, \tag{6}$$