J. of Supercritical Fluids 115 (2016) 86–98

Contents lists available at ScienceDirect

The Journal of Supercritical Fluids

journal homepage: www.elsevier.com/locate/supflu

Numerical study of supercritical and transcritical injection using different turbulent Prandtl numbers: A second law analysis

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ARTICLE INFO

Article history:
Received 27 January 2016
Received in revised form 4 May 2016
Accepted 4 May 2016
Available online 6 May 2016

Keywords:
Entropy
CFD
Supercritical
Transcritical injection
Cryogenics

ABSTRACT

The purpose of this investigation is to study the supercritical and transcritical injection of cryogenic fluids by means of a Computational Fluid Dynamics analysis using a RANS approach and different turbulent Prandtl number models. Besides, with the aid of the differential equation for entropy, the local entropy generation is pursued. Using this method, the areas where the irreversibilities occur are detected, and the mechanisms concerning entropy generation identified. The novelty of the numerical procedure presented herein is the use of two different turbulent Prandtl number (Pr^T) models that affect strongly the result produced: a constant Pr^T and a molecular dependent Pr^T. The main results show that the constant Pr^T predicts better the flow structure when compared to experimental data, being $Pr^T = 0.5$ the optimum one. This result suggest that supercritical and transcritical fluid injection are more dissipative processes than normal pressure injection, where $Pr^T \approx 1$.

1. Introduction

There is much interest in high pressure combustion for the improvement of the thermodynamic performance, production of high specific energy conversion and thrust. By a simple thermodynamic analysis of a liquid rocket engine thrust chamber, it can be shown that higher chamber pressures allow a higher specific impulse for the engine to be produced. Higher chamber pressures similarly increase the power output and efficiency of gas turbines and diesel engines. This has motivated a general trend towards increasingly higher chamber pressures in propulsion applications.

In the particular case of rocket engines, these high pressures often exceed the critical pressures of the injected fuel and/or oxidizer. Understanding the complex environment of the combustion chamber in order to get the most power out of it requires a good understanding of the injection phenomena [1]. Although liquid propellant rocket engines are operational and have been studied for decades, cryogenic injection at supercritical pressures is still considered essentially not understood [2]. Understanding the complex environment of rocket chambers gives the designer the ability to design a higher performance engine.

Several studies have addressed the problem of cryogenic injection at supercritical pressures from both experimental and theoretical approaches. For single round jets of cryogenic nitrogen injected into room temperature gaseous nitrogen [3], the visual appearance of the jet undergoes a drastic change as the pressure is increased from a subcritical to a supercritical value. The subcritical jet has the appearance of a conventional spray, but the supercritical jet has a more gas-like appearance. Segal and Polykov [4] report that the liquid break-up and atomization mechanisms, which prevail at subcritical pressure, are no longer observable because surface tension and latent heat of vaporization vanish at supercritical pressures. Furthermore, given the vanishing of latent heat of vaporization and surface tension, a phase transition no longer occurs. Some authors claim that under these conditions, a process of pseudoboiling takes place, understanding pseudoboiling a continuous, nonlinear, transcritical (i.e. starts at subcritical temperature and ends at both supercritical temperature and pressure) process resembling subcritical boiling. It occurs when the Widom- or pseudoboiling-line is crossed. The associated massive reduction in density and a high specific heat capacity strongly resemble classical subcritical vaporization [5].

On the modelling side, the problem has been tackled using a variety of computational approaches, from zero-dimensional, pure thermodynamics models to very complex Computational Fluid Dynamics (CFD) models. Qiu and Reitz [6] performed a thermodynamic analysis of fuel injection in diesel engines using a highly

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http://dx.doi.org/10.1016/j.supflu.2016.05.001
0896-8446/

Nomenclature

e	total energy
C_p	heat capacity
p	pressure
Pr	Prandtl number
s	entropy
T	temperature
u	velocity component in the x direction
v	velocity component in the y direction
w	velocity component in the z direction
$\mathbf{q}$	heat flux
$\mathbf{v}$	velocity vector
D	diameter of the nozzle

Greek symbols

α	thermal diffusivity
ϵ	dimensionless performance parameter
ε	turbulent dissipation rate
κ	conductivity
μ	viscosity
ρ	density
σ	entropy flux
τ	stress tensor
ζ	non-dimensional length
ξ	non-dimensional length

Subscripts

g	generated entropy
h	heat transfer term
i	injection conditions
μ	viscous dissipation term
τ	indicates friction velocity
mean	mean terms contribution to entropy
fluc	fluctuating terms contribution to entropy
pro	production rate
eff	effective
R	reservoir conditions

Superscripts

$\tilde{}$	mean term (Favre averaged)
$\overline{}$	mean term
$''$	fluctuating term
T	turbulent
+	indicates wall coordinate
$'$	per unit area

Acronyms

AAD	Average Absolute Deviation
CFD	Computational Fluid Dynamics

efficient phase equilibrium solver developed by them in a former publication [7]. In that research, fundamental thermodynamics analysis is applied to examine the thermodynamic states of mixtures during high-pressure fuel injection processes, with a special focus on exploring whether two phases can be present. Other different way to attack the problem has been suggested by Dahms and Oefelein [8], who employed a linear gradient theory to face the problem of interface identification of fuel mixtures at supercritical pressures, with application to rocket engines and diesel engines. Gradient theory provides a widely accepted methodology to calculate detailed interface structures between gases and liquids, and the authors found a valuable tool to distinguish the existence of droplets under supercritical pressure conditions.

CFD models found in the literature range from Direct Numerical Simulation (DNS) approaches to LES (Large Eddy Simulation) and RANS (Reynolds Averaged Navier Stokes) models. Bellan and her co-workers [9] develop DNS models of supercritical mixing layers, with the objective of creating a database detailed enough to derive supercritical pressure LES models from it [10]. These models are the most complete up to date, with an exhaustive treatment of transport processes at the molecular level, and high pressure thermodynamics. This is necessary since supercritical transport phenomena is quite different from subcritical one.

Other different computational approach is the use of a subcritical closure to tackle a supercritical pressure problem. This can be performed for both LES and RANS models. The only difference with normal pressure models in this case is the addition of an adequate equation of state to capture the thermodynamic non idealities of the processes under study. In this regard, the pioneering work of Oefelein and Yang [11] is remarkable. The authors employed an equation of state and the classical Smagorinsky closure for LES to the study of near critical mixing and combustion. Following their steps, other groups have performed similar computation for the analysis of cryogenic round jets of nitrogen [12,13].

DNS and LES have in common a very detailed description of flow structures, with a heavy load of computation (much larger for DNS than for LES). Without any doubt, these very detailed studies helped to understand elementary physical processes in cryogenic high pressure injection. However, going one step up to study not mixing processes but system level phenomena, high fidelity methods have not yet proven their superiority [14]. Besides, there is not necessarily a monotonous relation between model complexity and quality of the result. Excellent results can be achieved using RANS models, see for example Mayer et al. [1] and Sierra-Pallares et al. [15]. With these modelling approach, the computational load is much lower. However, challenges still remain, since prediction offered by this modelling approaches show a heterogeneous behaviour between different cases under analysis. Sometimes the prediction is very good, but is much worse in others [16]. Besides, most of the studies thus far using the RANS approach have been limited to the application of classical turbulence models, without modification, to the study of round jets of cryogenic fluids. An exception to this fact is the study of transcritical water flows of Schuler et al. [17]. In that work, a modification of the turbulent Prandtl number expression was performed to obtain a closer description of the experimental temperature profile of a round jet. However, the choice of such a model still depends on the availability of experimental data.

The main contributions of the paper are the following:

- We perform an evaluation of different alternatives found in the literature for the turbulent Prandlt number.
- For each alternative, we tackle a fundamental analysis of mass, energy, momentum and entropy production in order to obtain additional information on cryogenic injection. To the best of our knowledge, this is the first time a second-law analysis is made for supercritical and transcritical jets with a RANS approach. Such an analysis would help in the construction of much better RANS approaches to supercritical flow and combustion [10].
- We validate our methodology using experimental data taken from the literature.

Our aim is to improve the literature concerning RANS models with additional tools to develop a better understanding of the phenomenon.

The paper is organized as follows: first the model equations are presented, along with a detailed description of the entropy production calculation followed by the turbulent Prandtl number models employed. Then, the test case is described and evaluated