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Numerical Investigation of Real Gas Effects in an Impinging Supercritical CO2 Jet

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ABSTRACT

Supercritical carbon dioxide (S-CO2) fluid is characterized by low viscosity like gas, high density like liquid and thermo-physical properties variation by several orders of magnitude. Considering these variations is difficult and there are no de facto standard for the real gas models to be used in numerical simulations. In this paper, numerical study of S-CO2 free-jet through an orifice and its impaction on a flat plate is presented. The simulation uses RANS equations together with the standard k-□ turbulence model. Pressure boundary conditions were applied to the inlet and outlet boundaries. The cases simulated showed reasonably good qualitative agreements with the experimental data. The internal shock-structure has been studied extensively, in order to determine the impact of real gas behavior on S-CO2 jets and several interesting results have been found.

INTRODUCTION

Supercritical fluids (SCF) are very popular in a number of industrial applications because of their special thermal properties. Recently, carbon dioxide has been used frequently because of its lower critical pressure and temperature. Several reviews [Arai,2001 and Sun,2002] are available which describe the properties and uses of SCF. Recently, there has been considerable interest in the supersonic free-jet expansion of supercritical fluids because of its importance in several engineering and scientific fields, such as decompression of high-pressure SCF tanks, fabrication of nanoscale particles and to grow thin films etc. Hence, a comprehensive understanding of the flow and heat transfer characteristic of supercritical fluid is essential.

These free-jet expansions have been well studied for ideal gases whereas for SCF there are only a few experimental studies. There are large variations in the S-CO2 properties near the critical point (7.38 MPa, 304.25 K). When the temperature is higher than 304.25 K and pressure is higher than 7.38MPa, the state of carbon dioxide changes into supercritical (S-CO2). Hyungrae et al. and Liao et al. experimentally studied the heat transfer of S-CO2 flowing through tubes. Whereas Imane et al. theoretically and experimentally examine the structure of the free-jet expansion for a SCF. At the same time, SCF is studied by using computational fluid dynamics (CFD) for a better understanding of the flow physics. Sharabi et al. investigated the effect of different turbulent models on the flow of S-CO2 in triangular and square shaped channels.

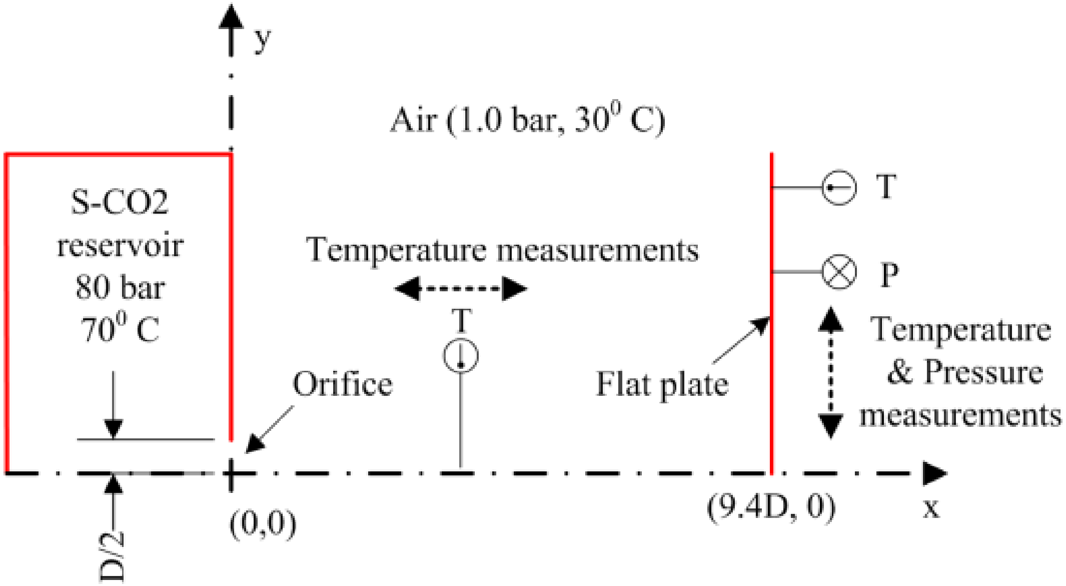

Figure 1. S-CO2 free-jet expansion into air with a flat-plate.

Imane et al. investigated the interactions of *an* S-CO2 Jet with a flat surface, where the upstream reservoir conditions are held near the critical point to impart maximum property changes. They reported experimental data for free-jet expansions of S-CO2 from an orifice, with diameter (D) 100 µm, stagnation conditions of 700C and 8.0 MPa, and impacting on a flat plate at a distance (x) 9.4D from the orifice. The data include optical shadowgraph measurements of the jet and shock wave structure, and impact pressure and temperature measurements along the plate [5]. Hence, their experimental work is taken as the test case for the present numerical study. Schematic representation of the S-CO2 injection into still air, which is investigated in this *study,* is shown in Fig. 1.

Although a number of experimental and numerical studies on S-CO2 have been carried out by various authors, still the flow property variations when passing through a shockwave is seldom looked upon. Hence, the objective of this study is to figure out the distinctive characteristics of S-CO2 free-jet and the impact of real gas behavior on the flow properties and the shock-structure.

CFD Model

The S-CO2 flow through the orifice is assumed axisymmetric. The computational geometry along with the boundary conditions are shown in Fig. 2. The diameter of the orifice (D) is 100µm. CFD code Fluent was employed in all the simulation works. The simulation uses the RANS equations together with the standard k-ω turbulence model. Pressure boundary conditions were applied to the inlet and outlet boundary. The properties of carbon dioxide and air were described by user-defined functions (UDF). The computational mesh is structured with around 80000 quadrilateral cells and the grid points are clustered towards the wall. Such a mesh is required in order to capture the steep macroscopic gradients close to the walls and maintain a reasonable computational resolution. The maximum wall y+ value was around 40 and for most of the wall regions y+ was around 1.0.

The numerical boundary conditions used are total pressure, P_0 (8.0 MPa) and total temperature, T_0 (343 K) at the inlet and static pressure, p_b (1 bar) at the outlet. S-CO2 discharging into quiescent ambient air is considered as the working fluid pair and Sutherland law is used to calculate viscosity. A non-uniform distribution of S-CO2 and air phases is specified (shown as the shaded region in Fig. 2). In addition to the conventional ideal gas equation of state (EOS), we also used Redlich-Kwong, Peng-Robinson, Aungier-Redlich-Kwong and Soave-Redlich-Kwong equations of states.

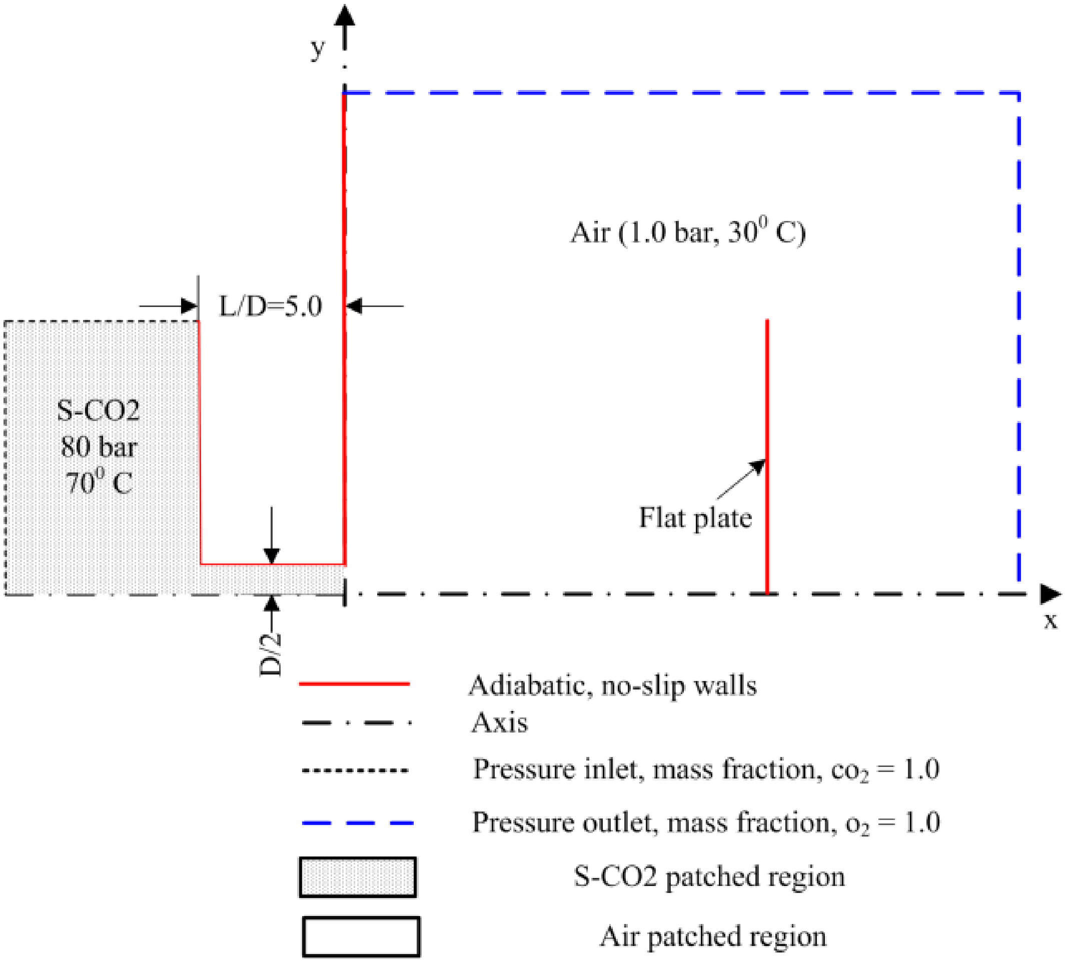

Figure 2. Numerical setup for simulations.

RESULTS AND DISCUSSION

Figure 3a shows the experimental shadowgraph [Imane et al.], of S- CO2 expansion from an orifice and the free-jet impaction on a flat plate. Figure 3b is the corresponding numerical shadowgraph. The fluid flows from a reservoir kept above the critical point of CO2. Cunningham first drew attention to the fact that choked flow (Mach number M=1), will not occur across a standard, thin, square-edged orifice. Hence, for achieving choked flow for the present work the length of the orifice plate (L) was assumed 5.0 D. The supersonic free-jet expansion rapidly adjusts to the ambient conditions by a Mach disk as shown in Fig. 3 and becomes subsonic. The barrel shock, Mach disc and the slip regions are captured well by the present code.

Fig. 4 shows the pressure distribution along the flat plate. In all the cases, the CFD code under predicts the impact pressure (near the core) and reasonable agreement is obtained away from the jet-core. Surprisingly, the ideal gas calculation appears to be more accurate in reproducing the impact pressure near the jet-core.

The difference between real and the ideal EOS becomes evident in Fig. 5. The ideal gas EOS over predicts the temperature distribution along the plate, whereas the real gas EOS appears to be reasonable. The Redlich-Kwong EOS seems to agree well with the experiments. Hence, the Redlich-Kwong EOS do well, but the ideal gas EOS is not acceptable, for the S-CO2 free jet expansion.

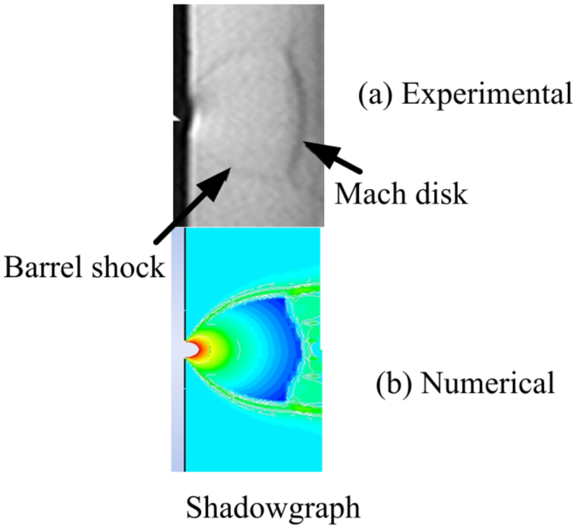

Figure 3. Supersonic S-CO2 Jet Shadowgraph.

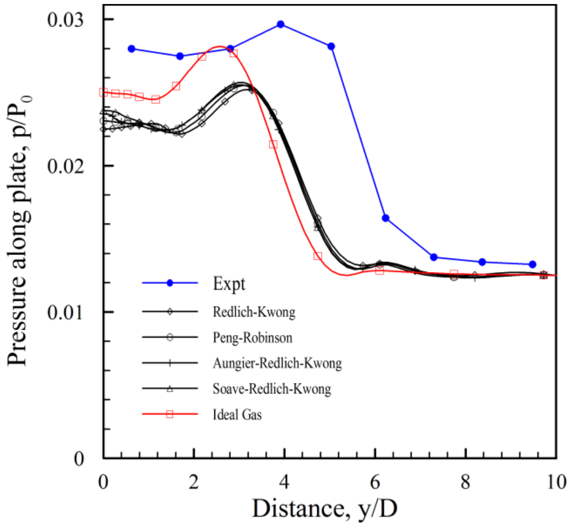

Figure 4. Comparisons of predicted and experimental [Imane et al.] static pressure-profiles along the flat plate.

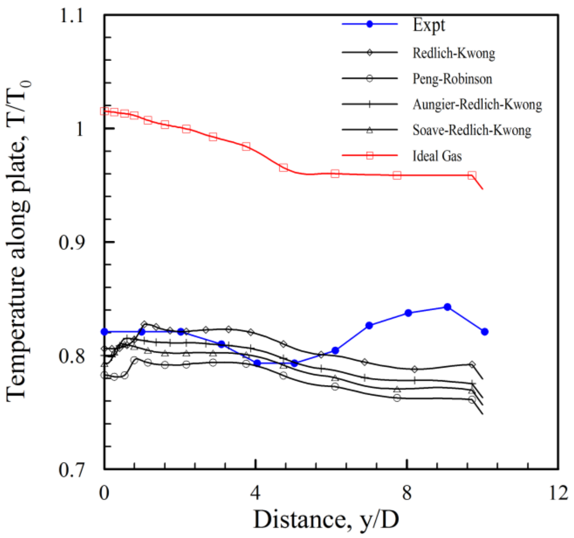

Figure 5. Comparisons of predicted and experimental [Imane et al.] static temperature along the flat plate.

Table 1. Characteristics of different EOS on the shock structure

Along the shock	**EOS**	**Orifice exit**	**Before shock**	**After shock**
p/P0	Ideal gas	0.42	0.002	0.024
	Redlich-Kwong	0.425	0.002	0.019
	Peng-Robinson	0.416	0.001	0.021
	Aungier-Redlich-Kwong	0.417	0.002	0.022
	Soave-Redlich-Kwong	0.409	0.001	0.022
T/T0	Ideal gas	0.824	0.222	0.983
	Redlich-Kwong	0.806	0.197	0.791
	Peng-Robinson	0.796	0.192	0.773
	Aungier-Redlich-Kwong	0.806	0.202	0.773
	Soave-Redlich-Kwong	0.793	0.197	0.765

Table 1 shows the characteristics of different EOS on the shock structure. In all the cases supersonic flow is produced at the orifice exit (throat), as indicated by the low-pressure ratio. Not much difference can be seen in the pressure predictions obtained with different EOS along the axial direction. However, the difference becomes obvious for the temperature rise along the shock. The ideal gas EOS showed larger discrepancy after the shock.

The discrepancy may be because the supersonic free-jet passed through some intermediate two-phase regions before the shock wave. After the shock wave better agreement between the experiment and CFD (cf. Fig. 6) is an indication that no condensations occurred. Hence, we are planning to incorporate a condensation mixture model in the future work.

Fig. 6 shows the static temperature distributions with different EOS when passing through a strong Mach-disk type shock. It is reported that quantitative temperature measurements before the shockwave, are difficult because in the supersonic regime the probe induce bow shocks in front of the thermocouple probe [5]. However, after the shockwave the real gas EOS reproduces the distributions quite well. Hence, the present study showed that ideal gas EOS is not acceptable for flow property computations in the axial or radial directions of the free-jet.

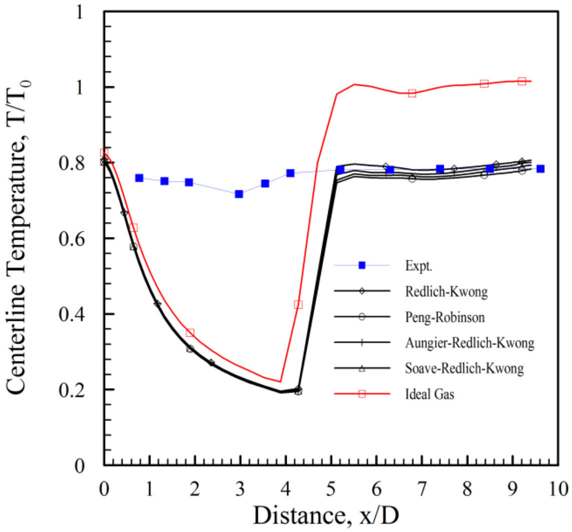

Figure 6. Axial static temperature distributions with different EOS from orifice exit (x/D = 0). Expt [Imane et al.]

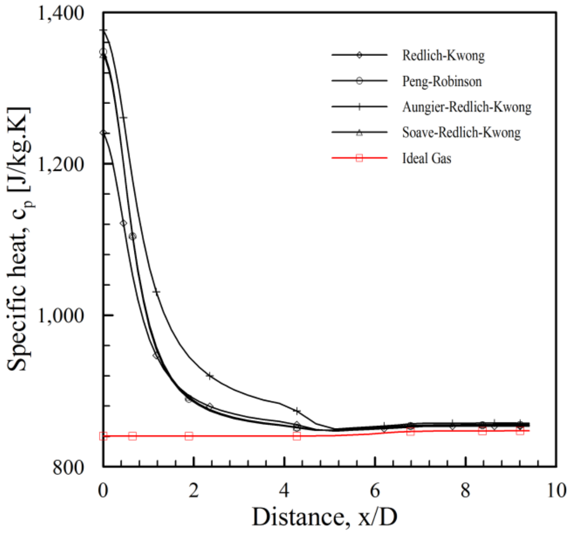

Figure 7. Variations in specific heat with different EOS from orifice exit (x/D = 0).

The large variation of the specific heat (c_p) influences heat transfer strongly and the ideal gas EOS fails to account for such changes in cp as can be seen from Fig. 7. This may be one of the reasons for the ideal gas EOS failure to predict the correct temperature distributions along the free-jet, with ideal gas EOS.

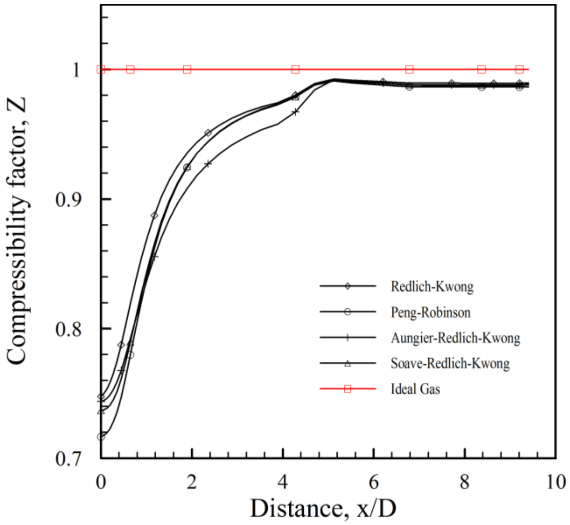

Figure 8. Compressibility factor variations with different EOS from orifice exit (x/D = 0).

From Fig. 8 it can be seen that, closer to the orifice exit, the S-CO2 gas deviates more from the ideal case. Compressibility factor, $Z < 1.0$ is an indication that the attractive forces dominate in S-CO2 jet. For accurate modeling of the S-CO2 both the specific heat and compressibility factor variations should be taken into account by means of a real EOS in the simulations.

CONCLUSIONS

This work presents a comprehensive assessment of real gas effects on the flow through orifice with CO2 at supercritical conditions. The pressure in the reservoir is slightly above the critical point hence the fluid properties changed rapidly during expansion. Higher pressure than 8.0 MPa can result in condensation, hence not considered in the present study. Different real gas models have been applied for the solution of the pressure driven orifice flow and the S-CO2 free-jet. Both the pressure and temperature profiles along the flat-plate indicate a circular core of high pressure and temperature, falling off to lower values away from the center. Also, ideal gas EOS is not acceptable for flow property computations in the axial or radial directions of the free-jet. The important characteristics of supercritical fluids from the point of heat transfer, is that their rapid variations in both specific heat and compressibility which should be accounted properly in the simulations. Future work will focus on the condensation effects on the S-CO2 jet, which may provide more quantitative agreements with the experimental data.

NOMENCLATURE

EOS = Equation of state
SCO2 = Supercritical CO_2
D = Diameter
L = Length
P = Pressure
T = Temperature
x = Axial distance
y = Radial distance

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