Numerical Investigation of Real Gas Effects in an Impinging Supercritical CO_2 Jet

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INTRODUCTION

- Supercritical fluids (SCF) are very popular in a number of industrial applications because of their lower critical pressure and temperature.

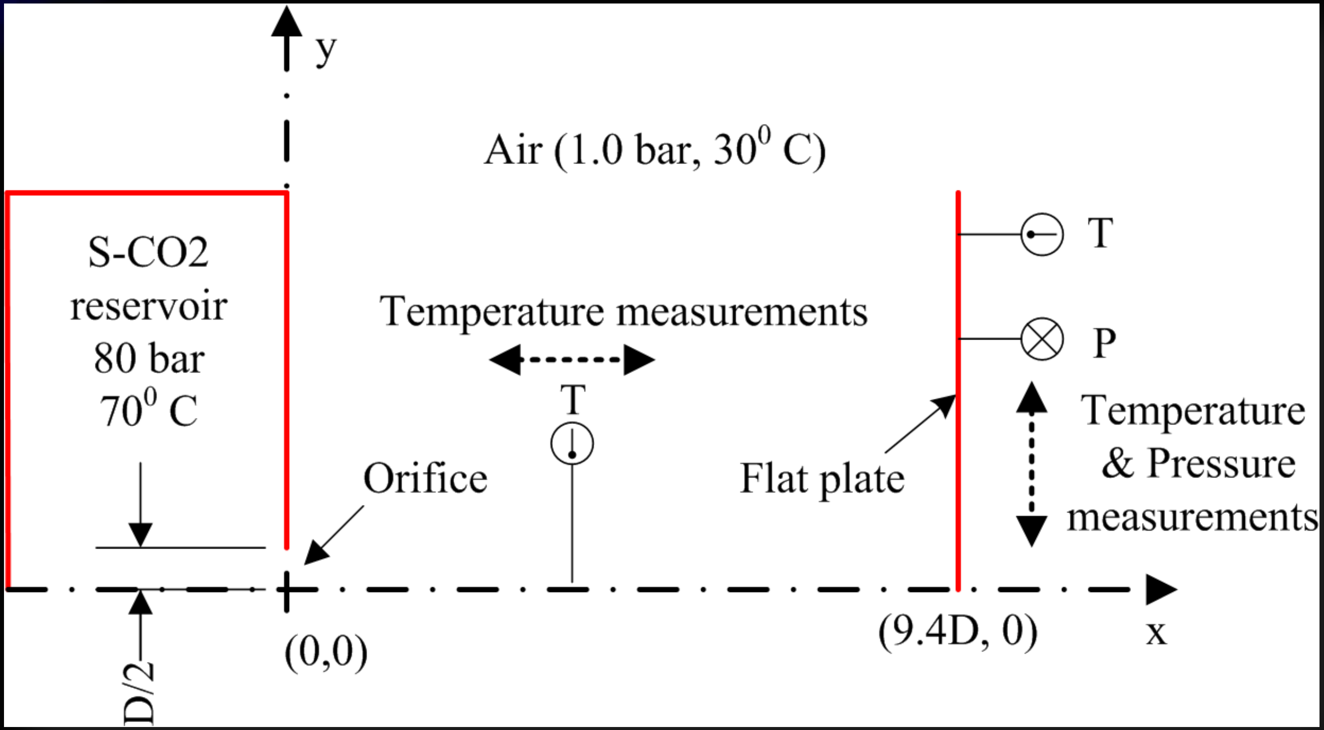
- Recently, there has been considerable interest in the supersonic free-jet expansion of supercritical fluids because of its importance in several engineering and scientific fields, such as decompression of high-pressure SCF tanks, fabrication of nanoscale particles and to grow thin films, etc.

Research Motivations

- Supersonic impinging jet involves many characteristic features of gas dynamics, such as rapid expansion, shock wave, strong shear action, stagnation flow, separation and reattachment, etc.
- During the supersonic impinging jet process, gas dynamic behaviors of S-CO2 are not well understood yet.
- Major characteristics of the supersonic S-CO2 jet should be fully understood to explore the EOS of S-CO2 appropriate.
- In the present study, the supersonic S-CO2 impinging jet has been investigated with a help of CFD method.

Several different EOSs were incorporated into the compressible Navier-Stokes equations. The present CFD results were validated with some experimental data available.

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

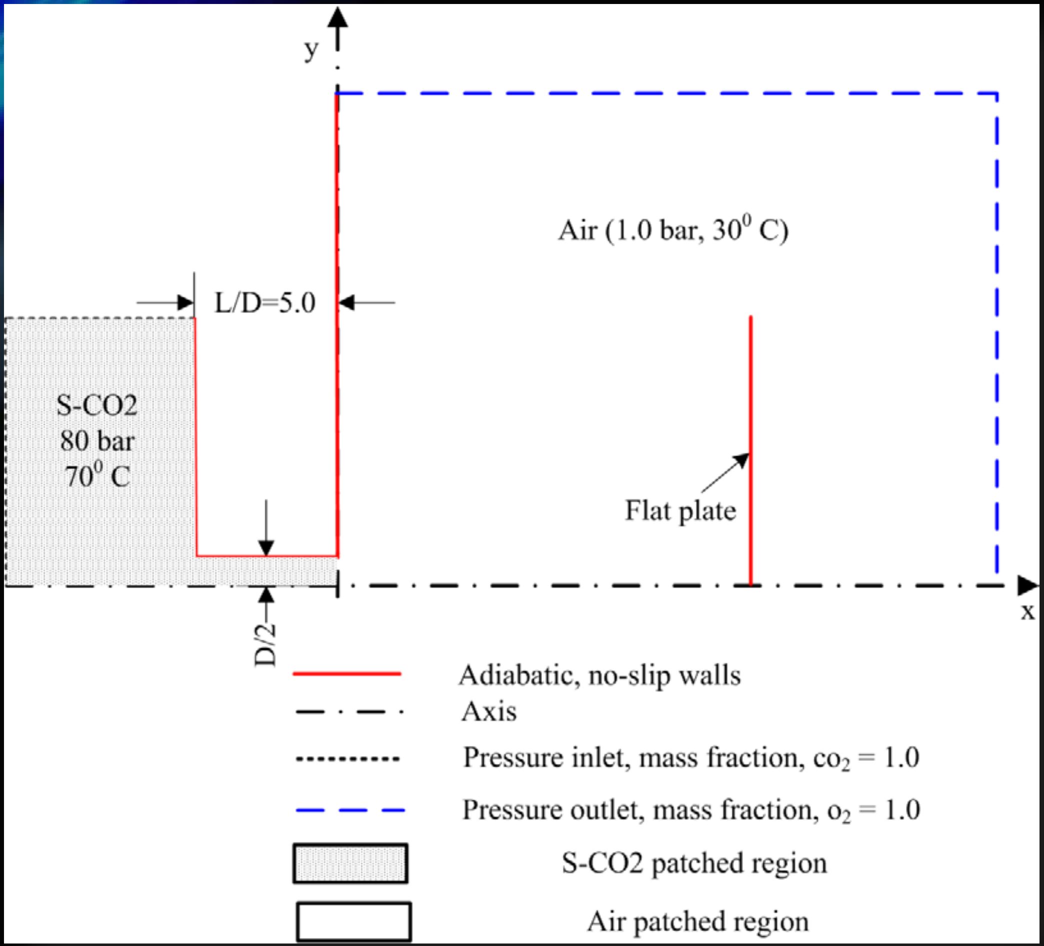


Ref: Imane, K.,David, R. M., “The Structure of Supercritical Fluid Free-Jet Expansions,” AIChE Journal November 2004 Vol. 50, No. 11, pp. 2697-2704.

CFD MODEL

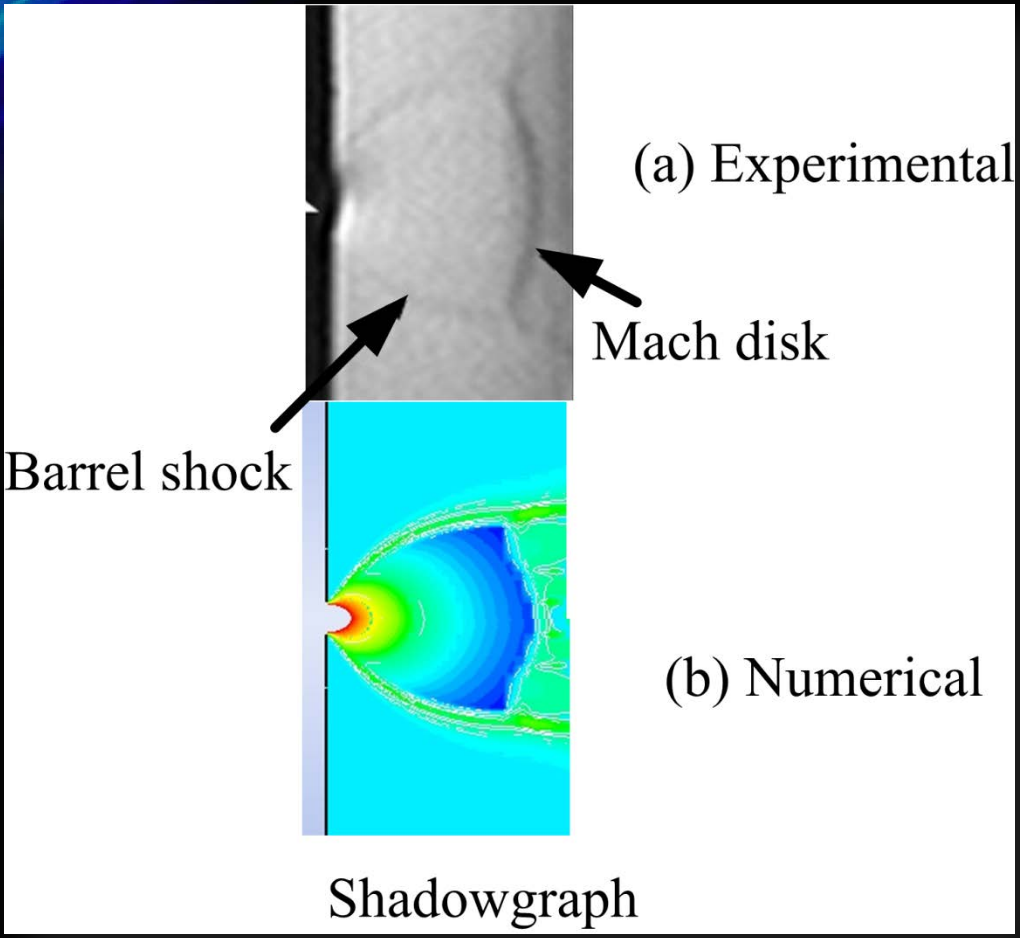
- The S-CO2 flow through the orifice is assumed axisymmetric.
- The diameter of the orifice (D) is 100µm.
- The simulation uses the RANS equations together with the standard k-ω turbulence model.
- Pressure boundary conditions were applied to the inlet and outlet boundary.
- The properties of carbon dioxide and air were described by user-defined functions (UDF).

Numerical setup for simulations



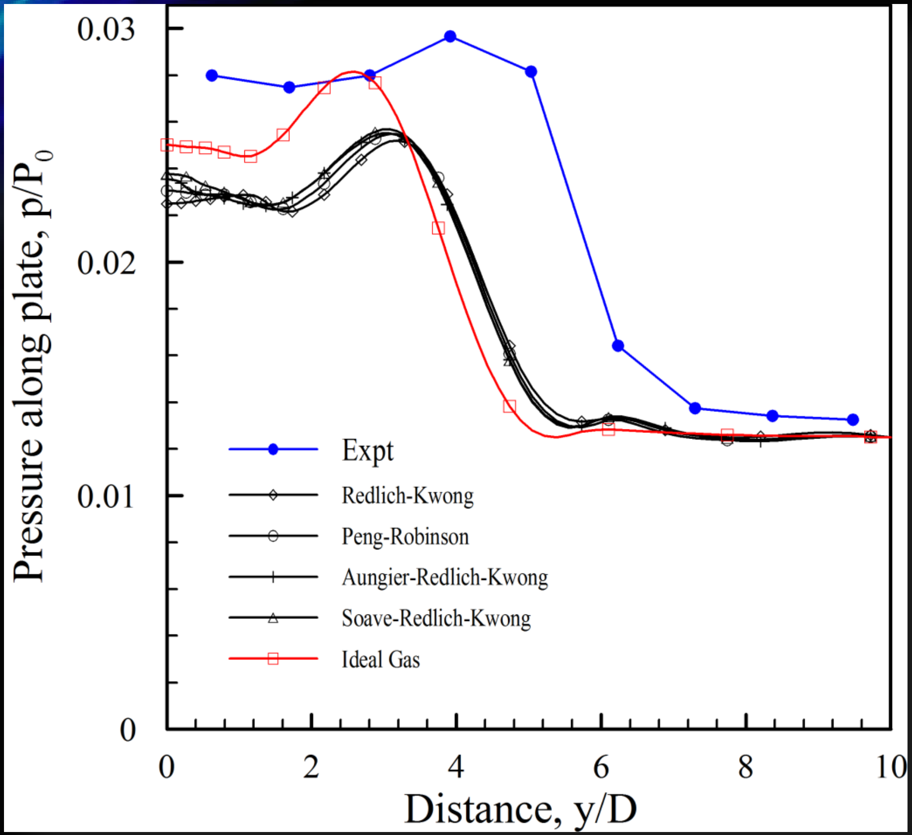
- A non-uniform distribution of S-CO2 and air phases is specified(shown as the shaded region).
- In addition to the conventional ideal gas equation of state(EOS), we also used Redlich-Kwong, Peng-Robinson, Aungier-Redlich-Kwong and Soave -Redlich-Kwong equations of states.

RESULTS AND DISCUSSION



- The supersonic free-jet expansion rapidly adjusts to the ambient conditions by a Mach disk as shown in Figure.
- The barrel shock, Mach disk and the slip regions are captured well by the present code.

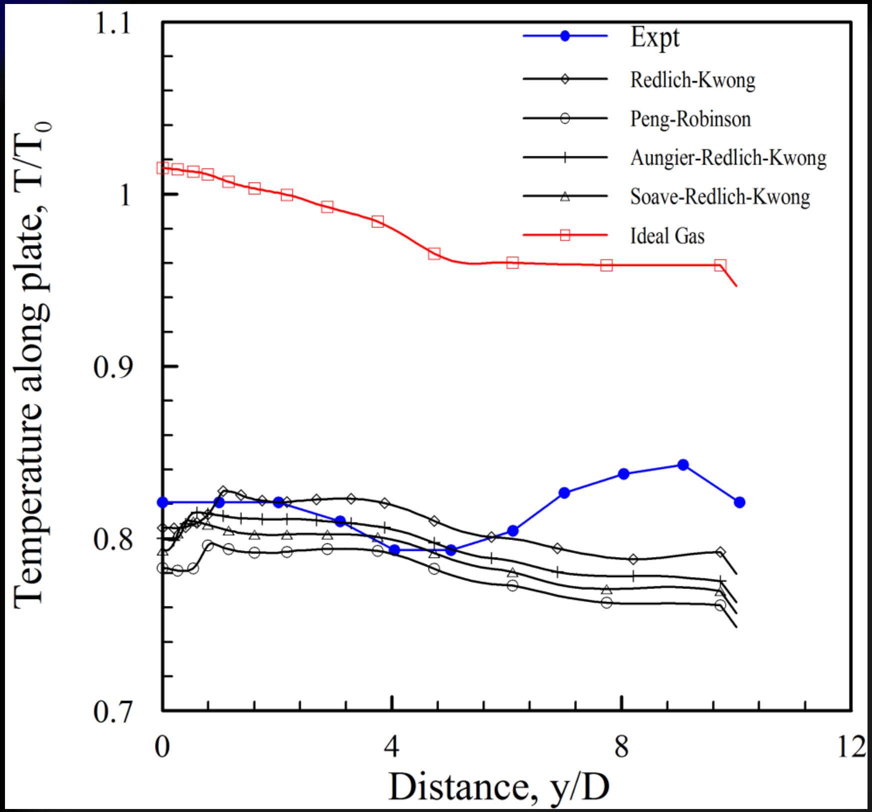
Comparisons of predicted and experimental static pressure-profiles along the flat plate.



- 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.

Comparisons of predicted and experimental static temperature along the flat plate

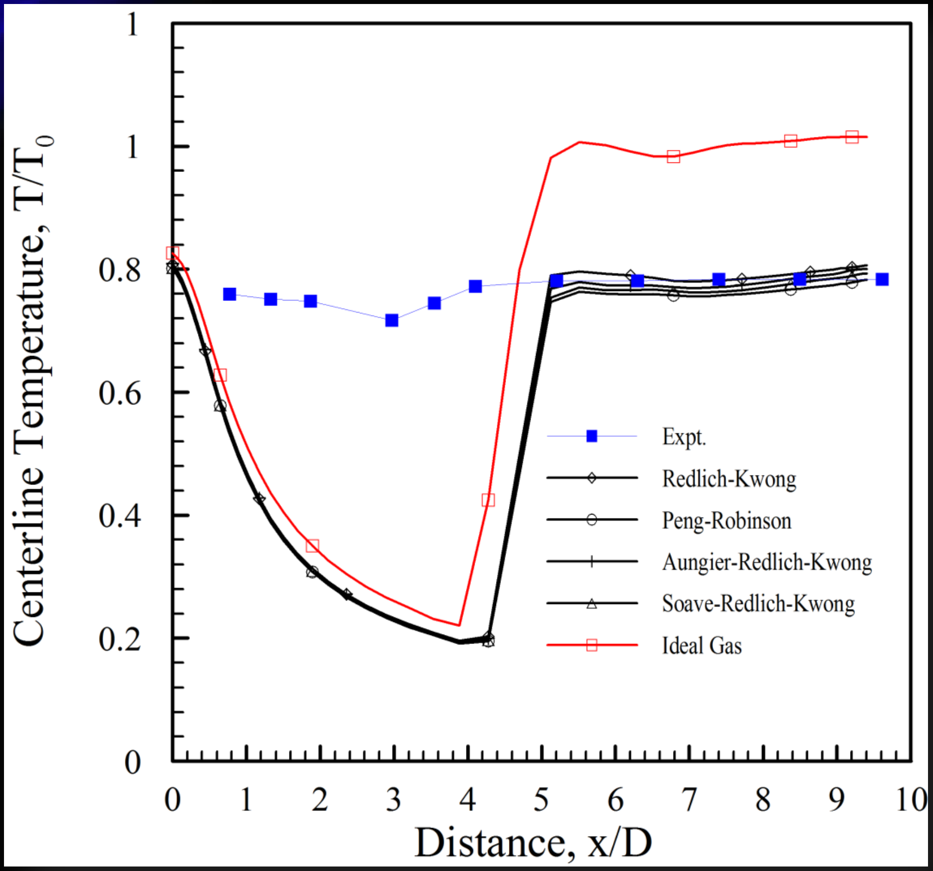


- The ideal gas EOS over predicts the temperature distribution along the plate, whereas the real gas EOS appears to be reasonable.

- 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.

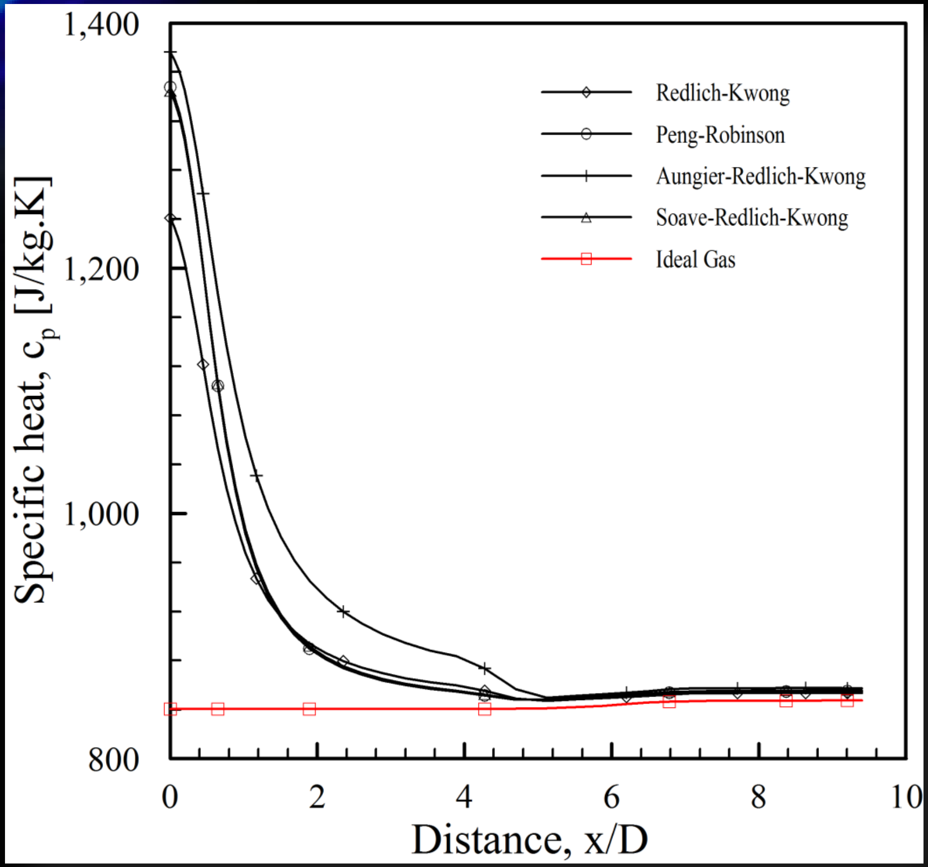
Axial static temperature distributions with different EOS



- 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.

- However, after the shockwave the real gas EOS reproduces the distributions quite well.

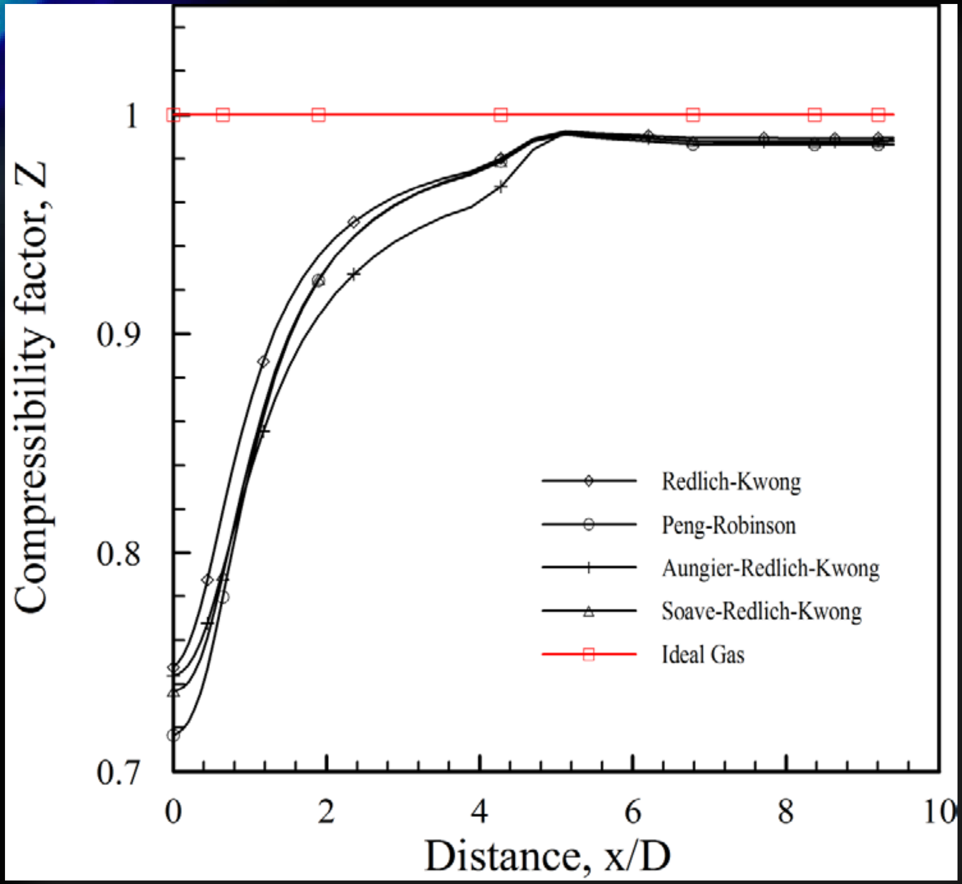
Variations in specific heat with different EOS



- 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 c_p as can be seen from Fig.

- This may be one of the reasons for the ideal gas EOS failure to predict the correct temperature distributions along the free-jet.

Compressibility factor variations with different EOS



- 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.

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

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.

Conclusions

- This work presents a comprehensive assessment of real gas effects on the flow through orifice with CO_2 at supercritical conditions.
- The pressure in the reservoir is slightly above the critical point hence the fluid properties changed rapidly during expansion.
- Different real gas models have been applied for the solution of the pressure driven orifice flow and the S-CO_2 free-jet.
- 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.
- More elaborate EOS model studies are needed to represent the super-sonic flows with the rapid expansion and strong shock wave of S-CO_2