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Solutions of supercritical CO_2 flow through a convergent-divergent nozzle with real gas effects

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ABSTRACT

Supercritical CO_2 (S-CO_2) has a density as high as that of its liquid phase while the viscosity remains closer to its gaseous phase. S-CO_2 has the potential to be used as a working fluid in compressor as it requires much less work due to its low compressibility as well as relatively small flow resistance. Besides the material properties and design calculations, the thermodynamic properties of working gases play a vital role in the design and efficiency of various machinery such as compressors, turbines, etc. Equation of state (EOS) which accounts the real gas effects is used in computational analysis to estimates the thermodynamic properties of the working fluid. Each EOS gives priority to real gas effects phenomena differently and for the analysis of the fluid dynamic machinery, as of today, there is no standard procedure for selecting a suitable equation of state (EOS). To understand the influence of real gas effects on the formation of a shock wave, S-CO_2 flow through a convergent-divergent nozzle, is theoretically analyzed. The thermophysical and transport properties calculated with the six different equation of state (EOS) are used to estimate the flow characteristics.

An in-house code based on the real gas approach which solves gas dynamics equations with variable gas properties is used to analytically analyze the compressible flow of S-CO_2 through nozzle. The solution for the shock strength, total pressure loss, and location of the normal shock wave at different back pressure conditions is obtained. Using Becker's solutions with varying viscosity and thermal conductivity estimated from each EOS, the properties inside the normal shock wave are calculated. Numerical results of supersonic S-CO_2 flow varies with different EOS candidates and the formation of shock wave is found to be significantly influenced by the real gas effects.

1. Introduction

Carbon dioxide above its critical point attains a supercritical state and exhibits certain peculiar properties such as higher density as a liquid but with a lower viscosity comparable to a gas. This supercritical carbon dioxide (S-CO_2) has a range of engineering applications such as enhanced oil recovery, caffeine extraction, drying aerogels, textile dying, dry cleaning, etc. S-CO_2 has become a subject of vital research interest for investigators all over the world mainly due to its interesting characteristics as well as its potential applications [1]. In thermodynamic power cycles, the high-density property of S-CO_2 is utilized to design compact machines with less required compressor work, thereby augmenting the effective power output [2]. Application of S-CO_2 as a working fluid increases the efficiency of the refrigeration cycles [3]. Naturally, CO_2 has two main advantages. Firstly, easy availability of CO_2 makes it cheaper to procure and secondly, it can attain supercritical state relatively close to the standard ambient temperature, without employing any powerful heating systems. Hence, the research on the power cycles based on S-CO_2 as a working fluid has substantially increased in last few years [4].

The thermodynamic properties of S-CO_2 such as density, local speed of sound and specific heat capacity vary significantly for slight change in temperature and pressure due to real gas effects. Equation of state (EOS) which account these real gas effects is used to calculate the thermodynamic properties of S-CO_2. Till date, a number of EOSs has been developed but still researchers are interested to develop a new method to calculate the thermodynamic properties [5]. The design and efficiency of machinery mainly depends on the physical properties like specific heat capacity and density [6,7]. But only a limited attention has been devoted for the assessment of EOS and its influence of simulations [8]. Zhoa et al. [9] analyzed the significance of thermodynamic model in the S-CO_2 cycle design and stated that impact of EOS on turbomachinery is important. Baltadjiev et al. [10] investigated the real gas

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Nomenclature

A	cross sectional area, m^2
κ	isentropic exponent
M	Mach number
P	pressure, N/m^2
T	temperature, K
ρ	density, kg/m^3
v	specific volume, m^3/kg
u	velocity, m/s
x	distance coordinate along the nozzle axis from throat, mm
C_p	specific heat constant at constant pressure, J/kg K
$\dot{m}$	mass flow rate, kg/s
R	specific gas constant, J/kg K
h	enthalpy, J/kg
S	entropy, J/kg
Z	compressibility factor
ξ	dimensionless distance coordinate
V	dimensionless velocity
ω	acentric factor
λ	thermal conductivity, W/(m K)
μ	dynamic viscosity, N m/s

Subscript

t	total state
s	static state
$1, 2$	upstream and downstream state of the shock wave respectively
in	nozzle inlet
th	throat section of nozzle
e	exit section of nozzle
r	reduced property i.e., ratio of the property value and its value at the critical point
0	stagnation condition at inlet
cr	ratio for the choked nozzle
$super$	entire flow in the divergent section is supersonic
sub	entire flow in the divergent section is subsonic

Coefficients used in EOS

a,b,c,d, A_0, B_0, C_0, D_0, B, C, D, α, β, γ, c_4

effects on S-CO_2 centrifugal compressor and stated that the local acceleration due to negative incidence at leading edge of impeller results in supersonic flow region. In this region, the static pressure and temperature of the S-CO_2 significantly decreases and influences the performance of the compressor. At these conditions, computational tools have uncertainty in accurately predicting the thermodynamic properties of S-CO_2 due to lack of proven method for selecting a suitable EOS.

In underground applications, S-CO_2 improve the efficiency of rock breaking mechanisms as well as enhance the oil recovery. For understating these applications, researchers conducted experiments and numerical investigations on supersonic S-CO_2 jet impingement, and found significant differences between both results [11,12]. Numerical results show that the structure and position of the shock wave which forms during jet impingement varies on implementing different EOSs. These differences in results directly highlights influence of various EOSs in the supersonic S-CO_2 flow modeling. Much attention has been devoted to the investigation of different turbulent models in S-CO_2 modeling in earlier studies [13,14]. Even though variety of EOS are available, much of them were neither tested nor explored for their applicability to S-CO_2 flows. Hence, the assessment of the different EOSs in numerical modeling of S-CO_2 is necessary.

The turbine inlet temperature approximately varies from the range of 700 K to 1100 K for the S-CO_2 based power cycles [1]. Practical difficulties arise while demonstrating experiments at such very high pressure and temperature with high speed. Hence, for S-CO_2 is concern, numerical analysis is not only cost-effective but also safer research tool. This further demands for the assessment of different thermodynamic models on the supercritical CO_2 compressible flow modeling. The present work investigates the influence of the different thermodynamic models on S-CO_2 flow through a critical nozzle. The EOS developed by Aungier (ARK) [15], Peng and Robinson (PR) [16], Boston and Mathias (PRBM) [17], Plöcker (LKP) [18], Benedict-Webb-Rubin (BWR) [19] and Span and Wagner (SW) [20] are considered. The National Institute of Standards and Technology (NIST) developed a program REFPROP (REFerence fluid PROPerties) to calculate the thermodynamic and transport properties of the fluids accurately. NIST utilizes SW EOS for the calculation of thermodynamic properties of CO_2, and hence throughout this work, SW EOS is represented as NIST. Detailed study on the flow properties inside shock wave using Becker's solution [21,22] with variable properties has also been presented in this context. The real gas effects in the shock front of S-CO_2 at different upstream Mach numbers are studied with varying pressure ratio.

The current analytical study has been conducted using an in-house code based on real gas approach [23,24] written in Scilab V5.5.2 programming language. Thermodynamic properties are calculated from each EOS using separate functions [25]. The solutions of S-CO_2 is compared with gaseous CO_2 (G-CO_2) for the same pressure ratio. Since different thermodynamic models predicts real gas properties differently, the flow properties calculated with each EOS is also different.

2. Theoretical analysis

2.1. Real gas equation of state

At standard atmospheric pressure and temperature, the CO_2 behaves as an ideal gas, and its compressibility factor equals to unity. However, at high temperature and pressure, the compressibility factor varies from unity, due to real gas effects. In order to predict this real gas effect, six different EOSs are considered for analysis of the real gas effect in the compressible S-CO_2 flow. The Table 1 shows the summary of the various EOSs that are adopted for this study, along with their critical fluid properties.

2.2. Governing equations

The supersonic flow of supercritical CO_2 at high pressure and temperature is analyzed theoretically based on the equation derived with the assumption of quasi-one-dimensional, inviscid, isentropic flow and ideal gas equation of state. The equations are summarized in expressions (1)–(3). S-CO_2 is at high temperature and pressure and hence it is highly compressed and its compressibility factor deviates much from unity. At this point, the assumption of perfect gas behavior losses its basis and instead the qualities of real gas must be assumed. Therefore, in order to approximate the behavior of real gas, all the properties (isentropic exponent,