Proceedings of Global Power and Propulsion Society
ISSN-Nr: 2504-4400
GPPS Xi'an21
18th – 20th October, 2021
www.gpps.global

GPPS-TC-2021-0247

Effects of Different CO_2 equations of state on Condensation Position in Numerical Investigation

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ABSTRACT

Supercritical CO_2 power generation system have been gaining interest in the field of thermal power conversion due to its high efficiency and compactness. The low power consumption of the near-critical compressor is the key factor for its high efficiency. However, when CO_2 is pressurized from a near-critical state to supercritical state, condensation may occur locally due to the high nonlinear behavior of the flow properties in the compressor. In the numerical simulation of compressor, sharp change of CO_2 fluid properties near critical point also brings difficulties in capturing the condensation phenomenon. In order to explore the influence of fluid properties on the condensation phenomenon, this article first discussed the difference among the RK equation of state, the PENG-ROB equation of state, and the CO_2 real fluid properties from the NIST REFPROP database. Then a numerical three-dimensional simulation was done using a de Laval nozzle model and the results were used to study the influence of fluid properties calculated from different equations of state in CO_2 numerical simulation on the condensation position.

Key words: supercritical carbon dioxide, equation of state, thermodynamic property, condensation, de Laval nozzle

Nomenclature

P	Pressure (MPa)
R	Gas constant
T	Temperature (K)
Tr	T/Tc
υ	specific volume (m^3/kg)
S-CO_2	Supercritical CO_2

INTRODUCTION

There is increasing interest in supercritical CO_2(S-CO_2) Brayton cycle, due to its high power generation efficiency over a moderate range of heat source temperatures and compact size. The critical pressure and temperature of CO_2 is 7.3773MPa and 304.128 K respectively, and it has abundant reserves in nature and good stability. CO_2 in the supercritical state is not a liquid nor a gas, and it has a higher density and a lower viscosity. This feature allows the size of the compressor to be greatly reduced, while the volume of entire circulation system is also smaller(Wright et al., 2011). The compact S-

CO_2 Brayton cycle system can play an important role in many small space occasions, such as shipbuilding, aerospace and other industries, so it has good development prospects and research value.

In the S-CO_2 Brayton cycle, compressor is the core component. Since CO_2 has a larger isobaric specific heat capacity easier to be compressed near the critical point, the compressor inlet parameters in the S-CO_2 Brayton cycle are often designed to be as close as possible to CO_2 critical point to obtain higher efficiency. However, when the CO_2 parameter at the compressor inlet is close to the critical point, due to the complex flow inside the compressor, the parameters of CO_2 will inevitably fall below the critical point, leading to possible local condensation, such as the local flow acceleration of the working fluid near the front edge of the impeller (Rinaldi et al., 2013; Baltadjiev et al., 2014). When the operating conditions change, the compressor inlet parameters may drop below the critical point, which may produce a larger two-phase area. Accordingly, it is very necessary to study the influence of CO_2 thermodynamic property near the critical point on condensation prediction and condensation zone which coule be helpful in studying the internal flow characteristics and losses of the compressor.

Lettieri found that in the immediate vicinity of the critical point, two-phase effects are expected to become more prominent due to larger residence times (Lettieri et al., 2015). They also report flow visualization and pressure measurements for a series of supercritical CO_2 blowdown tests, providing a valuable data set for condensation model assessment. High-speed imaging shows the onset of condensation at nozzle throat as "white fog" (Lettieri et al., 2017). Kevin W. Brinckman proposed a method for predicting condensation in supercritical CO_2 compressors(Brinckman et al., 2019). The results indicate that there is sufficient residence time to form local nucleation points under the analyzed conditions, however, the droplets are expected to be short-lived because the model predicts that they will evaporate quickly. Due to the non-ideal gas characteristics of CO_2, both the study of the circulation system and the study of the internal flow of the compressor require accurate equations of state to describe the physical properties of CO_2.

Alireza Ameli and others discussed the accuracy of the thermodynamic properties lookup table, and found that the increase in table resolution makes the calculated compressor efficiency closer to the experimental value (Alireza et al., 2017). However, higher table resolution will bring greater instability to the calculation, which requires a better balance between accuracy and calculation convergence. Ameli, Alireza also developed a set of averaging procedures to predict the performance of compressors operating near the critical point(Alireza et al., 2019). The results show that if the fluid properties are calculated accurately, the program can get results with acceptable accuracy even near the critical point.Yongju Jeong evaluated five similitude models, found that if the thermodynamic property and the error distribution have a similar trend, it can be used to improve the similitude models(Yongju et al., 2020). Therefore, density could be a potential candidate for improving the model, and the external loss effect is also related to density. Considering the SW EOS cannot accurately predict the changes in physical properties in the near-critical region due to the non-linear variation of CO_2 thermodynamic property, the results obtained from SW EOS may not accurate enough in predicting the condensation region of CO_2 near the critical point. The influence of other state equations such as RK EOSand PR EOS on the prediction of condensation position has not been fully studied. In this paper, the influence of different state equations on the condensation zone is compared and discussed through physical property comparison and simulation calculation.

The structure of this paper is as follows. First, the difference in physical properties calculated from the same equation of state is compared. Second, the effect of different equations of state on the condensation position of S-CO_2 in the Laval nozzle is studied by numerical simulation. The simulation results and the reliability of using a simpler equation of state to predict the location of CO_2 condensation is discussed.

METHODOLOGY

1 Comparison of different equation of state

In the current numerical simulation, the accuracy of the physical properties near the critical point of CO_2 is not very satisfactory, and the use of the high-precision SW EOS will bring stability problems. This research aims to compare the effects of different equations of state on the condensation position of S-CO_2, so as to find a more ideal equation of state, which can quickly obtain a relatively accurate prediction of the CO_2 condensation area, and qualitatively analyze its generation area and possible impact.

When calculating the thermodynamic properties of a pure substance, the equation of state describing its P-V-T relationship directly affects the accuracy of the thermodynamic properties calculation, thereby affecting the accuracy of the simulation results. This paper selects the PR EOS, the SRK EOS and the SW EOS. The SW EOS is formed by Span and Wagner, which is intergrated in the NIST database. this paper mainly compares the differences in temperature, pressure and density of different state equations (Span and Wagner, 1996). As a cubic EOS, the PR EOS and the SRK EOS are derived from the pioneering van der Waals theory. Among of them with few parameters, simple form, high calculation accuracy, and high reliability in predicting real fluid behavior (Soave, 1972; Ding-Yu Peng and Donald B. Robinson, 1976).

In order to evaluate the influence of different equations of state on the S-CO_2 condensation , the process of S-CO_2 in the nozzle was simulated. As shown in the Fig.1, the CO_2 at the inlet of the nozzle is in a supercritical state. When CO_2 flows to the throat, due to the reduction of the flow area and the acceleration of the flow, the pressure and temperature will decrease, leading to the condensation. This is similar to the process when the airflow in the compressor flows through the leading edge of the blade, where the condensation of S-CO_2 mainly occurs. The nozzle used in the study refers to Lettieri's experimental data.

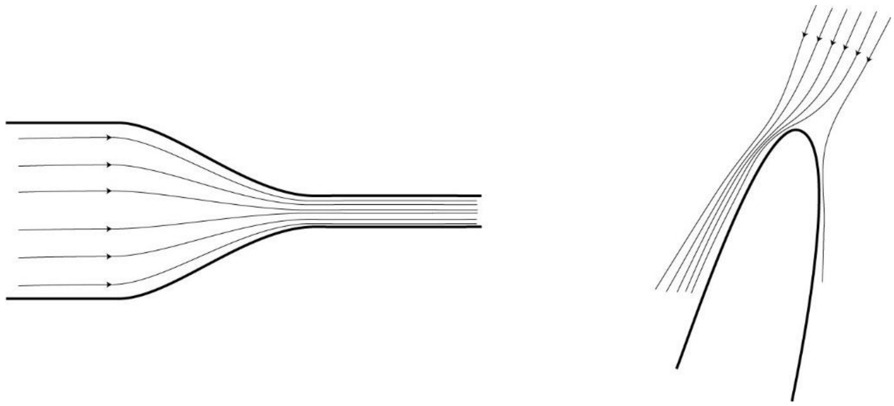

Figure 1 Flow acceleration of the nozzle and the leading edge of the blade

1.1 SRK EOS

The SRK EOS of state is improved from the RK equation, which includes three parameters. It is assumed that *a* is related to temperature. It is applicable to all non-polar compounds, but the calculation result of CO_2 is not very accurate. The basic equation is as follows:

$$P=\frac{RT}{\upsilon-b}-\frac{a}{\upsilon(\upsilon+b)} \quad (1)$$

where:

$$a=0.42747\frac{R^2T_c^2}{P_c}\alpha(T) \quad (2)$$

$$b=0.08664\frac{RT_c}{P_c} \quad (3)$$

$$\alpha(T)=\left[1+m(1-T_r^{0.5})\right]^2 \quad (4)$$

$$m=0.48508+1.55171\omega-0.15613\omega^2 \quad (5)$$

1.2 PR EOS

The RK and SRK EOSs have a common shortcoming. The accuracy in predicting the molar volume of the liquid phase is quite poor. In order to make up for this shortcoming, Peng and Robinson proposed a new equation of state, the PR EOS, in 1976. Its critical compressibility factor Z_C is 0.307, which is a significant improvement over the 0.333 of the RK EOS, but it still deviates from the value of the real fluid. The accuracy of saturated vapor pressure, saturated liquid density and gas-liquid balance calculated by PR EOS is higher than that of SRK EOS.

$$P=\frac{RT}{\upsilon-b}-\frac{a}{\upsilon(\upsilon+b)+b(v-b)} \quad (6)$$

where:

$$a=0.45724\frac{R^2T_c^2}{P_c}\alpha(T) \quad (7)$$

$$b=0.07780\frac{RT_c}{P_c} \quad (8)$$

$$\alpha(T)=\left[1+m(1-T_r^{0.5})\right]^2 \quad (9)$$

$$m=0.37464+1.54226\omega-0.26992\omega^2 \quad (10)$$

$$T_r \le 1: \quad \alpha(T) \text{ given by eq (4)}$$

$$T_r \ge 1: \quad \alpha(T) = \left[\exp\left[c(1-T_r^d)\right]\right]^2 \quad (11)$$

$$d = 1 + (\frac{m}{2}) \quad (12)$$

$$c = 1 - \frac{1}{d} \quad (13)$$

1.3 SW EOS

The SW EOS is a set of multi-parameter physical property equations established from the measured real gas parameters. Its main advantage is that it is very consistent with the actual gas properties of CO_2, but it still cannot precisely predict the changes in physical properties in the critical point area. The physical property data of the SW EOS in this paper are derived from the NIST database.

2 De laval nozzle simulation

The model is established by Lettieri's experimental parameters. The whole fluid domain is divided into structural grids, and the equilibrium condensation model in CFX is used. This model ignores the time required for condensation to occur, and is suitable for rapid heat transfer and mist condensation with a small droplet diameter.thus it is suitable for the calculations in this article. The turbulence model adopts the SST k-ω model, and the setting of boundary conditions refers to the experimental data.

RESULTS AND DISCUSSION

1 Comparison of different EOS

For the physical properties of CO_2, this paper compares the CO_2 density calculated by different equations. Three temperature ranges under different pressures are selected. When the pressure is 7MPa, the temperature range is 250K to 330K, and when pressure is 15MPa temperature range is 250K to 550K, and the near critical state. In different ranges, the density is calculated and compared.

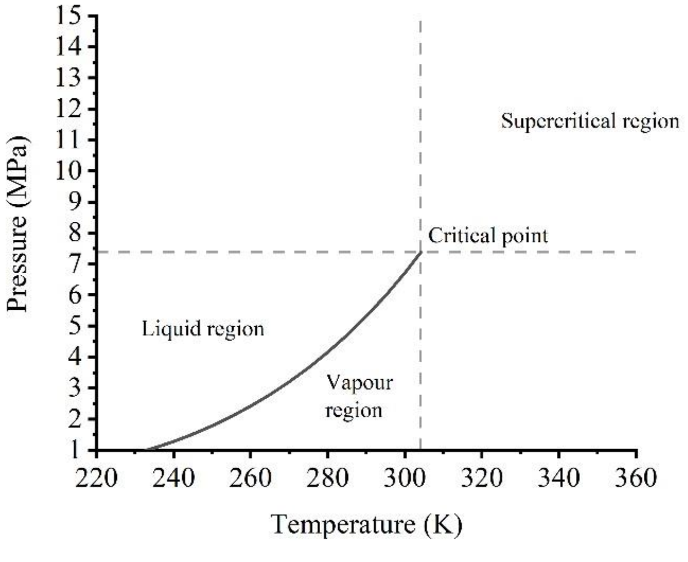

Figure 2 CO_2 P-T phase diagram

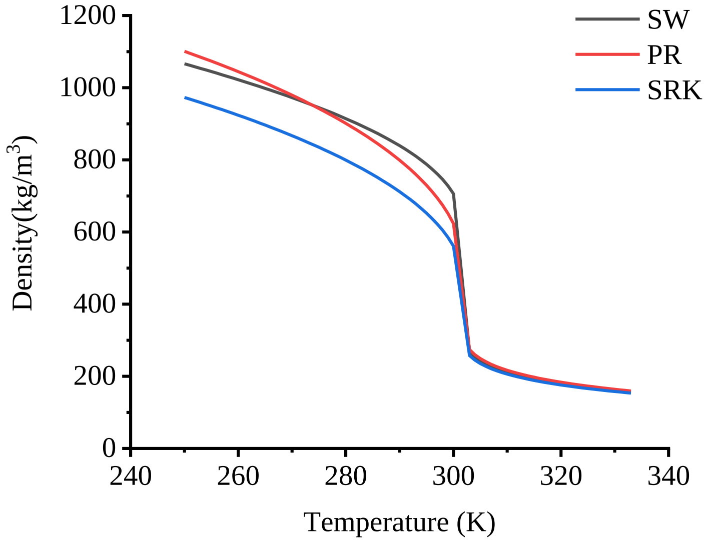

Figure 3 density at different temperatures under 7MPa pressure

As shown in Fig. 3, when the temperature is in supercritical state, the density prediction results of PR EOS, SRK EOS, and SW EOS are very close, relative error is below 5%. However, for the density prediction of the subcritical state, the calculation result of the PR EOS is relatively close to that of the SW EOS, while the SRK EOS shows a larger deviation. The density prediction of the SRK EOS in the subcritical region is smaller than that of the PR EOS and the SW EOS.

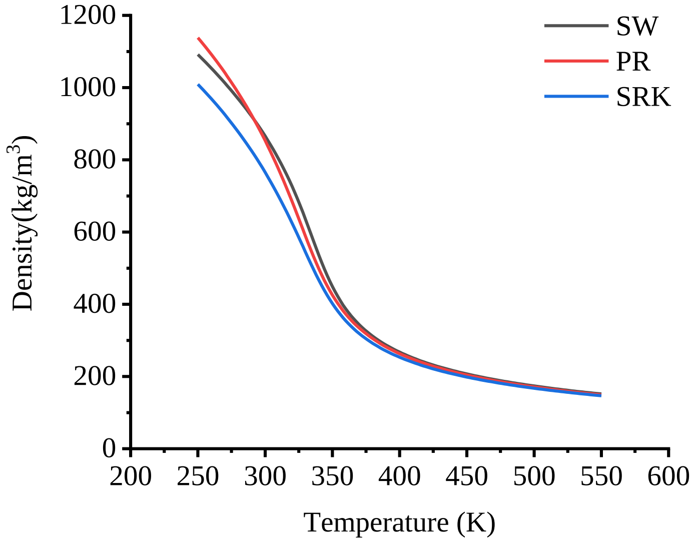

Figure 4 density at different temperatures under 15MPa pressure

When the pressure is in supercritical state, the results of different state equations are relatively close. Meanwhile the gap between the calculation results of the different equations gradually decreases with the increase of temperature, which is the same as the calculation result when the pressure is 7MPa. In the near-critical and supercritical regions, both the PR EOS and the SRK EOS can obtain almost the same density predictions as the SW EOS. In the S-CO_2 Brayton cycle, S-CO_2 is always in a supercritical state during the compression process in the compressor. Therefore, a relatively accurate result may be obtained by using the PR EOS. For the condensation that may occur near the leading edge of the blade, further research is needed on the physical properties of the critical point. Thus, the density calculated by different equations when the temperature is near the critical point under the critical pressure is compared.

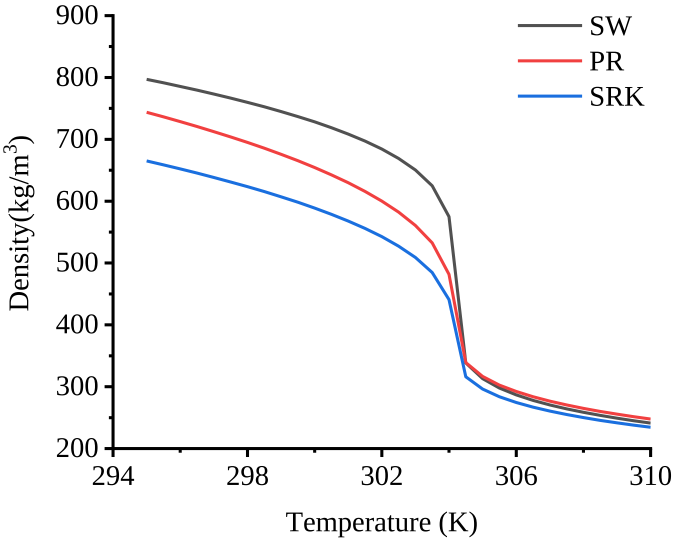

Figure 5 density near the critical point

Fig.5 shows that the trend of the density difference is the same as that of Figures 3 and 4. When the pressure is the critical pressure and the temperature is above the critical point, the difference between the calculation results of the three equations is small. When the temperature drops to 304K, the difference of different equation increased gradually. The density calculated by the SW EOS is greater than that of the PR EOS and the SRK EOS, and the result of PR EOS is greater than that of the SRK EOS. From the Fig.5, the density calculated by the PR EOS is closer to the SW EOS, and the decreasing trend of the density near the critical point is very close to the SW EOS.

2 Comparison of simulation results

With reference to Lettieri's experimental data, the nozzle inlet pressure is set to 8MPa and the temperature is 314K. The pressure and density data on the centerline of the nozzle are extracted for comparison. Lettieri observed the formation of misty white droplets from the throat in the experiment. Fig.6 shows the calculation results of three different equations of state compared with the experimental data. Under the same inlet conditions, P/P_0 curves along the flow direction showed similar trend to the experiment data. The three state equations show considerable accurate prediction results at the position of the nozzle throat.

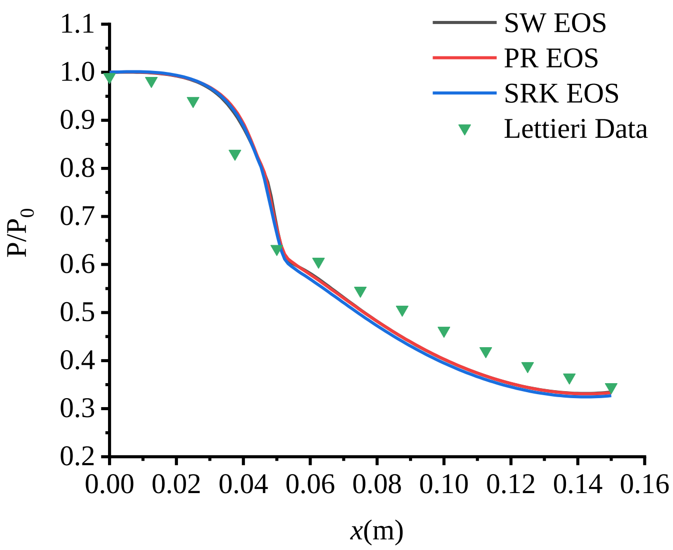

Figure 6 P/P_0 on the centerline of the nozzle

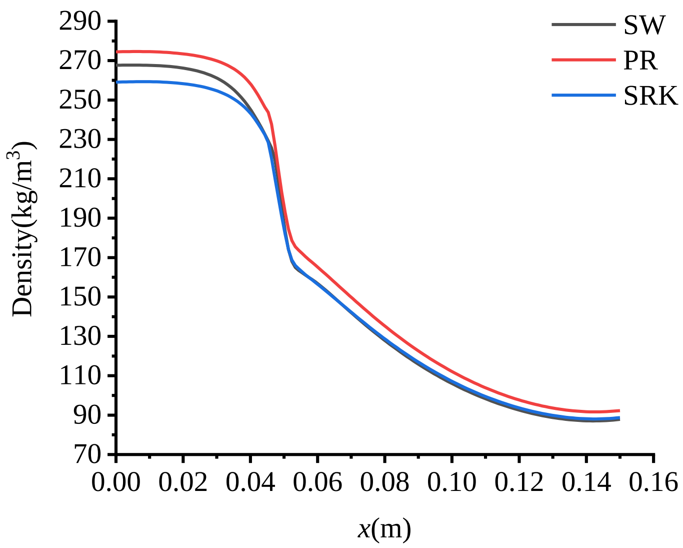

Figure 7 Density results along the nozzle direction

As shown in the Fig.7, the difference between pressure simulation results of the three different equations along nozzle direction is very small. Meanwhile, there is a sudden drop in the throat pressure, where the condensation starts. It can also be seen in Lettieri's experimental results that white fog began to appear at the throat, indicating that small droplets of CO_2 began to form. Figure 7 shows the density results calculated by different equations, which are similar to the previously compared density data. In the simulation, the density obtained by the PR EOS and the SRK EOS is smaller than that of the SW EOS. In addition, at the position of the nozzle throat, the position of the sudden density drop predicted by different equations is very close. That is to say, the CO_2 condensation position predicted by the PR EOS and the SRK EOS are in good agreement with the results of the SW EOS.

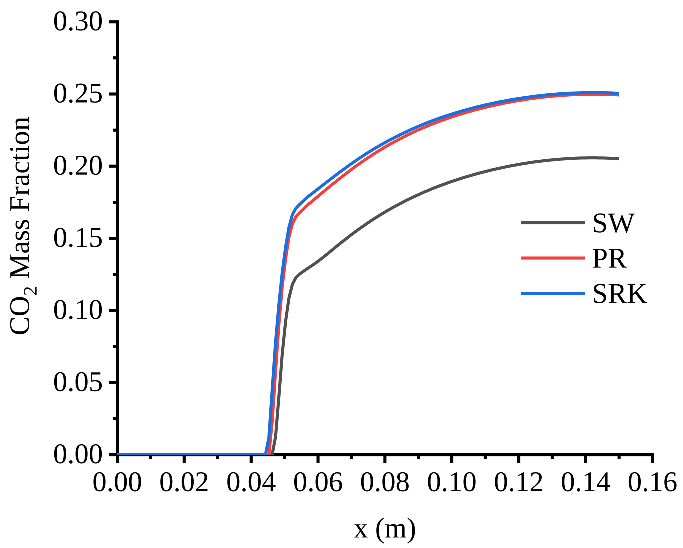

Figure 8 CO_2 mass fractio along the nozzle direction

Figure 8 visually shows the CO_2 mass fraction change trend along the nozzle direction. It can be seen that there is a sudden increase in the CO_2 liquid phase mass fraction at the nozzle throat, and then gradually flatten out in the expansion section of the nozzle. In Figure 8, the CO_2 condensation position predicted by the SRK EOS is higher than that of the SW EOS, while the PR EOS is between the two. The results of the three equations for predicting the start position of CO_2 condensation are not very different. In the expansion section of the nozzle, the mass fraction of CO_2 liquid phase calculated by PR EOS and SRK EOS is obviously greater than that of SW EOS. The possible reason is that in the expansion section of the nozzle, the pressure decreases and the CO_2 state is subcritical.Meanwhile, from the above comparison, it can be known that there are still some gap that cannot be ignored in the results of the three EOS.especially in the subcritical zone, because its lead to differences in the results of the nozzle expansion section.

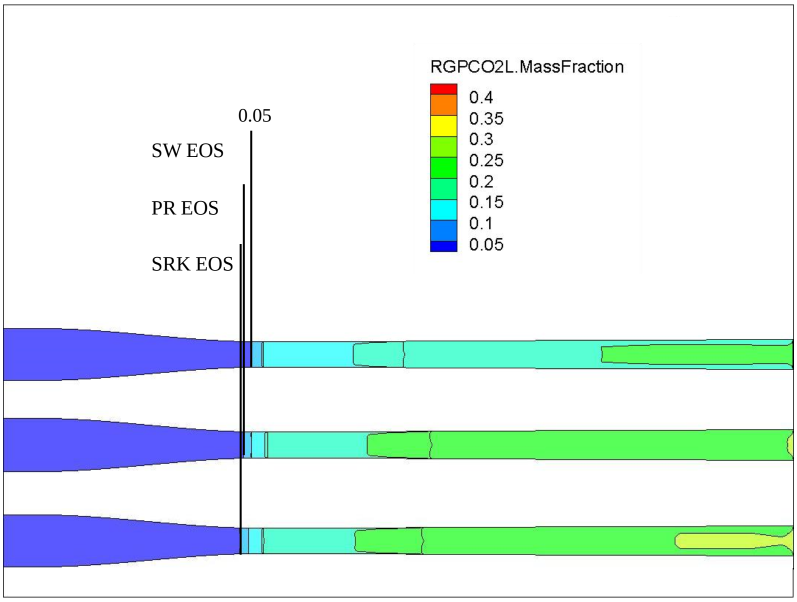

Figure 9 CO_2 mass fraction along the nozzle direction

Taking the CO_2 liquid phase mass fraction of 5% as the condensation starting point, it can be clearly seen from the above figure that the condensation starting point calculated by the SW EOS is lower, and the result of the SRK EOS is higher. The result of the PR EOS is close to that of the SRK EOS, and lies somewhere in between. In the nozzle expansion section, both the SRK EOS and the PR EOS for the prediction of condensation show a larger prediction area.

CONCLUSIONS

This paper compares the calculation results of SW EOS, PR EOS and SRK EOS for CO_2 temperature, pressure and density. The three equations of state are used to simulate and compare the flow of S-CO_2 in the nozzle, and the effects of different equations of state on the location and area of CO_2 condensation are discussed.

(1) The study found that there is still a large gap in calculating density in subcritical region between SRK EOS, PR EOS and SW EOS, but the results of PR EOS and SW EOS are closer. When the temperature is near the critical point and the far critical region, the density calculation results of the three equations are very close.

(2) The previous comparison results also be verified in the simulation comparison. The physical property predictions of PR EOS and SRK EOS in the subcritical region have a larger gap with SW EOS, but in the S-CO_2 Brayton cycle system, this gap may not have much impact on the efficiency prediction.

(3) For the prediction of the condensation start position, the calculation result of SRK is more advanced, which may indicate that in the compressor simulation, the prediction of the condensation area by the SRK EOS and the PR EOS will be larger than that of the SW EOS, and the predicted mass fraction will also be greater.

ACKNOWLEDGMENTS

The authors would like to thank Dr.Zhang, and Dr. Sun for their support during the writing of the paper.

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