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A Method for Predicting the Phase Characteristics and Physical Properties of Carbon Dioxide Containing Impurities under Various Transport Conditions

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ABSTRACT

Based on the cubic equation of state, the effect of impurities such as nitrogen, methane, hydrogen and oxygen on the characteristics of phase behavior of carbon dioxide (CO_2) was discussed in this study. A prediction model of the phase characteristics of CO_2 system containing impurities was established by correlating phase equilibrium and critical state prediction. Additionally, a mathematical model for the calculation of physical properties of the multi-component system was established. The changing rules of the physical properties including density, viscosity, Joule-Thomson coefficient, and specific heat capacity at constant pressure were analyzed. Based on the constructed prediction model, the analysis of phase properties and physical properties of impurity-containing CO_2 streams under various transport conditions was carried out. The comparison of the prediction results with the experimental results shows that the prediction accuracy was improved under certain conditions, which provides a certain theoretical basis for the analysis of pipeline transmission chain in the CCUS engineering practice.

Keywords: Impurity-containing CO_2, CO_2 physical properties, CO_2 phase properties

1. INTRODUCTION

The issue of global warming has been a significant and pressing concern, with growing international attention being drawn towards it. Carbon dioxide is the most significant greenhouse gas generated by human activities, and its production is primarily associated with the burning of fossil fuels. Since the onset of the industrial revolution, there has been an exponential increase in the exploitation of fossil fuels, leading to a dramatic escalation in carbon dioxide emissions into the atmosphere[1]. Consequently, there has been a significant rise in the concentration of carbon dioxide in the atmosphere, posing a critical threat to the planet. Over the last three decades, CO_2 emissions have increased alarmingly, indicating that reducing CO_2 emissions has become a global issue that cannot be delayed[2].

Carbon capture, utilization, and storage (CCUS) has emerged as an effective and integrated technology for mitigating CO_2 emissions. The CO_2 emitted from each carbon emission source will be transported to the sequestration point or utilization point after the capture process, thus achieving the goal of CO_2 reduction[3]. However, impurities, such as nitrogen, methane, hydrogen, and oxygen, are inevitably entrained in the CO_2 stream in small amounts throughout the process. These impurities have been shown to influence the phase properties of the CO_2 system, which can alter the critical point and affect phase equilibrium properties. As a result, it has implications for the operating conditions of the various stages of the CCUS project. Accurate identification of the phase characteristics and physical properties of the CO_2 flow is a prerequisite for the safe and efficient operation of CCUS technology, as well as for the optimization and design of related processes[4][5].

In this paper, we aim to investigate the impact of impurities on the phase properties of CO_2 in the CCUS project. To address the complex behavior of impurities in CO_2 flow, we constructed a model to predict the phase characteristics and physical properties of

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impurity-containing CO_2, and analyzed the effects of impurities such as nitrogen, methane, hydrogen, etc.

2. THEORY

The basic properties of the substance are characterized mostly by the equation of state (EOS).There are several types of classical equations of state (EOS) that can be referenced for CO_2 systems, such as cubic equation of state, multi-parameter equation of state and deviation function-based equation of state. The most widely recognized and utilized cubic equations include RK, SRK, and PR, while BWR and BWRS stand out as the most prominent multi-parameter equations [6].

The PR equation of state can efficiently and accurately obtain the basic physical parameters of CO_2, such as density, compression factor, etc, as well as thermodynamic parameters such as enthalpy, and entropy, etc [6]. As a result, this study constructed models for calculating the phase properties and physical properties of impurity-containing CO_2 based on the PR equation of state, which have been combined other relevant theories under specific operating conditions. Consequently, in order to more accurately describe the transition process of CO_2 stream viscosity from low to high intensity states, this study incorporated free volume theory [7] to better relate CO_2 viscosity to its molecular structure. This theory expresses the viscosity as two components, the dilute gas viscosity term and the dense fluid correction term [8]. In addition, in order to achieve the prediction of the phase properties of CO_2 systems containing impurities, the FECP method was selected to estimate the critical temperature of CO_2 containing impurities[9], and the conformal solution theory[10] was applied to predict the critical pressure.

3. RESULTS AND DISCUSSIONS

3.1 Physical properties prediction

Based on the 96% CO_2+2%N_2+2%CH_4 system, the accuracy of the calculation of the physical property model constructed in this study was analyzed at the temperature of 35°C and the pressure range of 3-15 MPa. The model demonstrated good accuracy in calculating parameters such as density, Joule-Thomson coefficient, and specific heat capacity at constant pressure for CO_2 physical properties calculations, especially for the calculation of viscosity. The calculated results were found to be within acceptable error limits when compared to data provided by the REFPROP database. These results further confirm the effectiveness of the model in accurately predicting the physical properties of impurity-containing CO_2 systems.

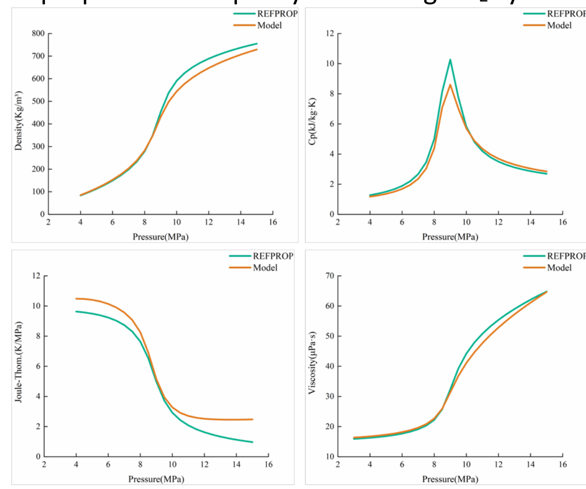

Fig. 1. Comparison of physical property prediction model results with REFPROP data

3.2 Phase properties prediction

We constructed multiple CO_2 systems containing impurities commonly encountered in real-world CCUS projects. The model predictions of critical temperature were found to be consistent with REFPROP data, while the critical pressure predictions were slightly lower, with relative errors maintained at approximately 2%. To further verify the effectiveness of the constructed model, the impurity system was enriched by introducing ethane and oxygen, results of the model show that the mixture system contains methane, ethane and nitrogen maintain a low level of relative error. However, the addition of oxygen resulted in an increased level of error, particularly in the presence of hydrogen. Despite this, the relative error remained within 5%, which meets the engineering requirements.

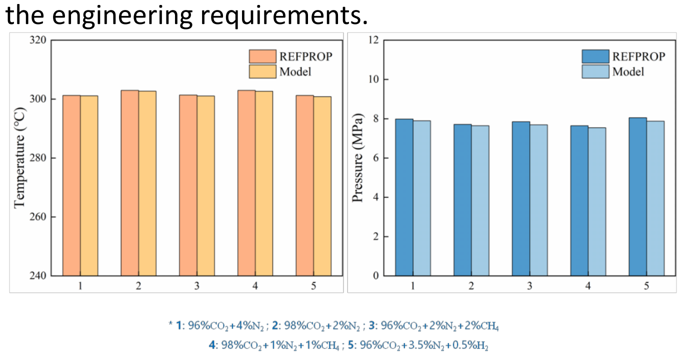

Fig. 2. Comparison of predicted results of critical parameters

4. CONCLUSIONS

In this paper, the critical point prediction was performed using the FECP method and conformal solution theory, while the free volume theory and deviation function concepts were employed for calculating basic and thermal properties. The proposed model's computational accuracy was validated by constructing multiple impurity-containing CO_2 systems. Comparing the predicted critical parameters of each impurity system with the data provided by REFPROP database, it can be found that when the impurity system contains N_2, CH_4 and C_2H_6, which are common impurities in actual pipeline projects, the relative errors of the results are within 5%, and when the impurity system becomes complex and has O_2 and H_2, the relative errors of the results have a tendency to increase, but still meet the engineering requirements.

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