Simple and accurate calculation model of viscosity for supercritical CO₂

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Abstract: The high-precision calculation method suitable for the viscosity of supercritical CO₂ is reported. The modified LBC model, modified DS model and Ehsan empirical formula are selected to calculate viscosity. The error analysis result shows that the average absolute error of the modified DS model is the lowest, which can be applied to the engineering calculation. The LBC model is suitable at 7.5–25MPa and the Ehsan empirical formula has high accuracy at 25–60MPa. Then the viscosity plate is drawn at temperature range of 310–800K and pressure range of 7.5–60MPa, which can be applied in carbon dioxide resources recovery and utilization of technology.

1. Introduction

Increasing CO₂ emissions pose a direct threat to the global climate change⁴. On the other hand, the recovery and utilization of CO₂ resources has broad application prospects, which can be used as a fracturing fluid, solvent, refrigerant fluid, etc.²⁴. The viscosity calculating method of CO₂ has been researched. Najafi et al.⁵ built a new viscosity model based on modified Enskog theory. Lohrenz et al.⁶ proposed a LBC model for calculating the viscosity of high-pressure gases. David E. Dean et al.⁷ proposed a DS model for calculating the viscosity of nonpolar gases. On the basis of the viscosity data of supercritical CO₂ measured by Pensado et al.⁸, Ehsan et al.⁹ proposed the Ehsan empirical formula for calculating the viscosity of supercritical CO₂. Compared with the experimental data, these viscosity calculation models have large errors¹⁰¹¹, which can not be directly applied to engineering calculation, and the scope of application is limited. In our study, a modified LBC model and a modified DS model are proposed. The viscosity of supercritical CO₂ is calculated by using these two models and the Ehsan empirical formula at 310–800 K and 7.5–60 MPa. In comparison with the NIST data, the high-precision calculation method suitable for the viscosity of supercritical CO₂ is further described.
We find that several viscosity model which are widely used have a relatively large deviation compared with the standard data from National Institute of Standards and Technology (NIST)\(^{[12]}\). So in this paper, the viscosity model was verified and improved, the applicable scope of viscosity model - evaluated. Error analysis was adopted between the calculated results and the standard data from NIST.

| Nomenclature | Definition |
|--------------|------------|
| \( D \) | Relative error (%) |
| \( AAD \) | Absolute mean error (%) |
| \( N \) | Number of experimental data points |
| \( P \) | Pressure (MPa) |
| \( \rho \) | Density (kg/m\(^3\)) |
| \( T \) | Temperature, K |
| \( \xi \) | The correlation parameter |
| \( \mu_0 \) | The first intermediate viscosity variable (mPa \( \cdot \) s) |
| \( \mu^* \) | The second intermediate viscosity variable (mPa \( \cdot \) s) |
| \( T_r \) | Reduced temperature (K) |
| \( \rho_r \) | Reduced density (kg/m\(^3\)) |
| \( \mu \) | Viscosity of supercritical CO\(_2\) at high temperature and pressure (mPa \( \cdot \) s) |
| \( T_c \) | Critical temperature of CO\(_2\) (304 K) |
| \( p_c \) | Critical pressure (7.38 MPa) |
| \( M_{g,CO_2} \) | Molar mass of CO\(_2\) (44 g/mol) |
| \( \mu_{cal} \) | Calculated viscosity (kg/m\(^3\)) |
| \( \mu_{exp} \) | Experimental density (kg/m\(^3\)) |
| \( D \) | Relative error (%) |

2. Calculation method for the viscosity of supercritical CO\(_2\)

The modified LBC and DS models are proposed to improve the accuracy of the viscosity method. The absolute average error is expressed as:

\[
AAD = \frac{1}{N} \sum \left| \frac{\mu_{cal} - \mu_{exp}}{\mu_{exp}} \right| \times 100\% \tag{1}
\]

2.1. Modified LBC model

The viscosity of supercritical CO\(_2\) at 310–800 K and 7.5–60 MPa is calculated for the LBC model. The average absolute error is 77.53% compared with the NIST data. The modified model is as follows:

\[
\left( \mu - 5\mu_0 + 2.6 \times 10^{-5}\xi + 5 \times 10^{-4} \right)^{\frac{1}{2}} = 5 \times (0.10230 + 0.023364 \rho_r + 0.058533 \rho_r^2 - 0.0400758 \rho_r^3 + 0.0093324 \rho_r^4)
\tag{2}
\]

\[
\rho_r = \frac{\rho}{\rho_{p_c}}
\tag{3}
\]

\[
\xi = \frac{T_{p_c}}{M_{g,CO_2}}
\tag{4}
\]

\[
\mu_0 = 34.0 \times 10^{-4} T_{p_c}^{0.94}, T_{p_c} \leq 1.5
\tag{5}
\]

\[
\mu_0 = 17.78 \times 10^{-4} (4.58 T_{p_c} - 1.67)^{\frac{5}{2}}, T_{p_c} > 1.5
\tag{6}
\]

2.2. Modified DS model

The DS model is calculated, and the average absolute error is 77.77% compared with the NIST data. The modified model is as follows:
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\[
\xi = \frac{1}{\frac{T^6_c}{M^2_p P^3_c}} \tag{7}
\]

\[
\mu_0 \xi = 34.0 \times 10^4 T^{7.5} \leq 1.5 \tag{8}
\]

\[
\mu_0 \xi = 166.8 \times 10^4 (0.1338 T^{0.932} - 0.932) T \geq 1.5 \tag{9}
\]

\[
\mu' = 10.8 \times 10^3 \left[ \exp(1.439 \rho_s) - \exp(-1.111 \rho_s^{-0.838}) \right] / \xi \tag{10}
\]

\[
\mu = 5 \times 10^3 \times (\mu' + \mu_o) - 2.6 \tag{11}
\]

2.3. Discussion, analysis, and viscosity plate

The viscosity of supercritical CO2 at a temperature range of 310–800 K and a pressure range of 7.5–60 MPa is studied in this paper.

2.3.1. Comparison analysis

In this paper, the accuracy of the modified LBC model, the modified DS model and the Ehsan empirical formula are verified by using the absolute average error compared with NIST data. For example, the viscosity distribution curves were drawn by these three methods at 15 and 60 MPa respectively (figure 1). The LBC and DS models fit well with NIST data at 15 MPa, but the Ehsan empirical formula is better at 60 MPa, so we did error analysis to calculate the deviation.

The average absolute errors of the three calculation methods at 7.5–60 MPa were drawn (figure 2). The average absolute error of the modified DS model is the lowest at 4.86%. In order to further analyze the situation of different pressure range, The error analysis of high and low pressure was made respectively.

In figure 3, the accuracy of viscosity calculated using the modified LBC model at a low pressure (7.5–25MPa) is high with an average absolute error of 2.28%. The Ehsan empirical formula has a high accuracy in viscosity calculation at a high pressure (25–60MPa) with an average absolute error of 4.66%.
Figure 1. The viscosity distribution calculated by different methods: (a) 15 MPa, (b) 60 MPa

Figure 2. The mean absolute errors of the three calculation methods at 7.5–60 MPa

Figure 3. The mean absolute errors of three calculation methods: (a) 7.5–25 MPa, (b) 25–60 MPa
2.3.2. Viscosity plate
When the temperature range is 310–800 K, the viscosity of supercritical CO\textsubscript{2} at 7.5–25MPa is calculated using the modified LBC model, at 25–60MPa is calculated by the Ehsan empirical formula. A plate was drawn on the basis of the viscosity data (figure 4) for easy inquiry and industrial application.

![Figure 4: Viscosity calculation data plate.](image)

3. Conclusions
In this paper, the viscosity model was verified and improved, its application scope was evaluated, and the viscosity plate was drawn.

(1) The average absolute error of the modified DS model is the lowest (4.86\%) at 7.5–60MPa, which can satisfy the requirements of engineering calculation.

(2) The average absolute error of the modified LBC model is 2.28\% at 7.5–25MPa, the average absolute error of the Ehsan empirical formula is 4.66\% at 25–60MPa. Based on the above discussion, a viscosity data plate is drawn for easy inquiry and industrial applications.

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