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Unisim Software was used to Analyze the Pure CO_2 Physical Properties in the Supercritical Region

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Abstract: ***In this study, the physical properties of pure CO_2 in the supercritical region were analyzed using Unisim software. Analyzed properties include density, viscosity, specific heat, thermal conductivity, and compressibility. These findings have implications for the efficiency of CO_2 transport and contribute to the broader field of CCUS technologies for carbon capture, utilization and storage.***

Keywords: Unisim software;Supercritical; Pure CO_2; Changes in Physical Properties

Carbon dioxide, as the "black boss" of greenhouse gas emissions, accounts for 74.4% of them. As the largest carbon emitter, China needs to spend more energy and financial resources to achieve the "carbon peaking and carbon neutrality" dual carbon goals proposed in the 14th Five-Year Plan. To this end, CCUS (carbon capture, utilization and storage) technology as an indispensable technical means to cope with global climate change and reduce carbon emissions has been studied a lot in China and is widely used[1]. The transport of CO_2 is a key link in connection capture and reuse or storage, and changes in the physical properties of CO_2 are the key to affecting the efficiency of transportation.

1. Introduction to the Unisim Software

Unisim is a process design and dynamic simulation tool, mainly committed to helping users fully familiar with their own production equipment and process, master dynamic process characteristics, accumulate operation experience, improve the ability to deal with abnormal accidents, ensure the smooth production of production equipment, and maintain normal production operations. UniSim is not a steady-state process simulation in general, it is a comprehensive dynamic process simulation[2]. Based on accurate thermodynamic equations and mass transfer dynamics models, Unisim is recognized as a set of tools that can help engineers study and explore processes, conduct operating condition studies, identify process bottlenecks, find optimal operating procedures, conduct failure analysis and control strategy research, and become a training tool to help plant operators accumulate operating experience, familiarize themselves with the process, and improve their operational skills. It is related to process design, process bottleneck analysis, dynamic simulation, working condition research, operation plan demonstration, control strategy confirmation and commissioning, production optimization, device transformation and other comprehensive solutions throughout the entire plant equipment life cycle[3].

2. Physical property analysis

The physical properties that affect the phase change of CO_2 transport mainly include density, viscosity, specific heat, thermal conductivity, compression coefficient and hydrate formation conditions, so this section uses Unisim software to analyze the change of CO_2 physical properties.

2.1 Density

Density refers to the ratio of the mass to volume of a substance. CO_2 is prone to phase change due to its particularity, and the CO_2 density value in different phases is very different, so the density can directly affect the efficiency of pipeline transportation, and the change law of simulated pure CO_2 density is shown in Figure 1.

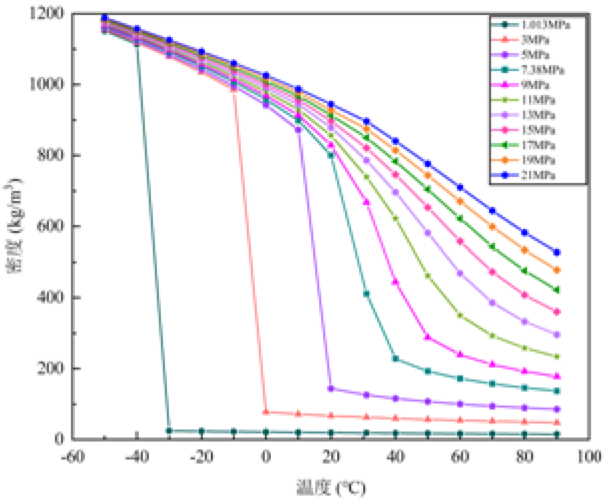

Figure 1: Density variation law of pure carbon dioxide

It can be seen from Figure 1 that when the pressure is constant, the density of pure CO_2 decreases with the increase of temperature. The density of pure CO_2 at the same temperature increases with the increase of pressure, and the specific law is as follows:

1) When the temperature is less than -40 °C, the density drop is little affected by temperature and pressure, and the CO_2 at this time is completely in the liquid phase or dense phase, and the density value at each pressure and temperature is not much different;
2) When the temperature exceeds -40 °C and the pressure

is constant, the density decreases as the temperature increases, but the reduction range is different. When the pressure does not exceed 7.38MPa, with the increase of temperature, the phase change of CO_2 from liquid phase to gas phase, and the density instantly decreases to the liquid phase and basically remains stable; when the pressure is greater than 7.38MPa, with the increase of temperature, the density gradually decreases and the reduction amplitude is smaller and smaller.

3) In the supercritical region, the overall decrease trend of density is flat, and the reduction is not large, which is closer to the density of liquid.

2.2 Viscosity

Viscosity is a physical quantity that measures the viscosity of a fluid, so the resistance of CO_2 in the pipeline transportation process can be analyzed according to the law of viscosity change, which directly affects the flow characteristics of the pipeline. The change law of simulated pure CO_2 viscosity is shown in Figure 2.

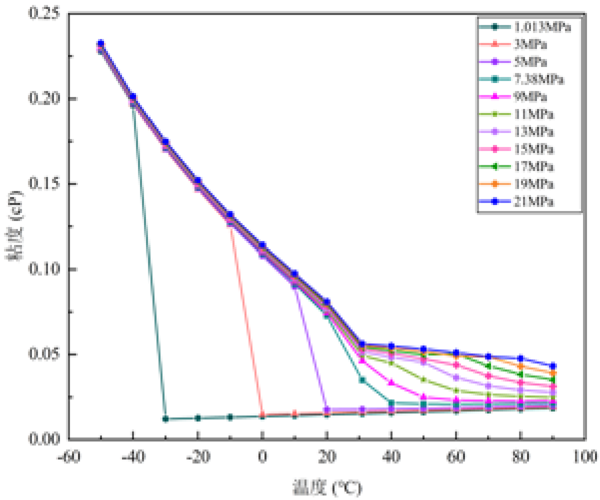

Figure 2: Viscosity variation law of pure carbon dioxide

It can be seen from Figure 2 that the viscosity of pure CO_2 decreases with the increase of temperature and pressure and then rises slightly, and the specific rules are as follows:

1) When the temperature is lower than -40 °C, the viscosity under each pressure decreases with the increase of temperature and the value is equal, and it is not affected by pressure;
2) When the temperature exceeds -40 °C and the pressure is less than 7.38MPa, with the gradual increase of temperature and pressure, the phase change of CO_2 from liquid phase to gas phase, and the viscosity decreases instantaneously, when the fluid is all in the gas phase, with the increase of temperature and the intensification of molecular movement, the viscosity rises slightly and remains basically equal; When the temperature exceeds -40°C and the pressure exceeds 7.38MPa, the viscosity gradually decreases and the amplitude becomes smaller and smaller.
3) The viscosity of the supercritical region is relatively close to that of the gas, and there is no large change.

2.3 Heat Capacity

Heat capacity is a physical quantity used to describe the ability of an object to absorb or release heat, which is closely related to thermal calculations and directly affects the temperature change of the fluid. The specific heat change law of pure CO_2 after simulation is shown in Figure 3.

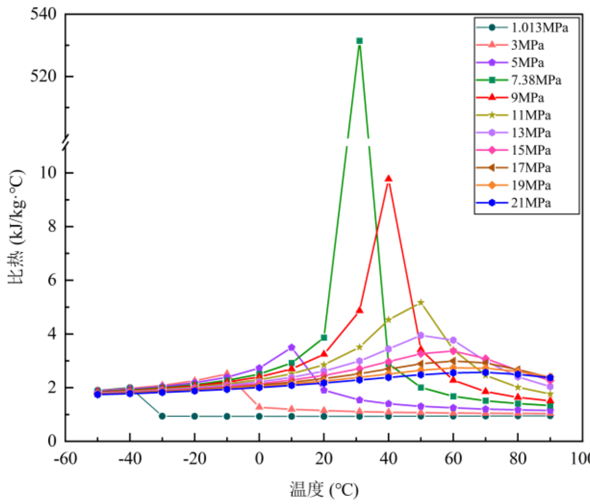

Figure 3: Heat capacity variation law of pure carbon dioxide

It can be seen from Figure 3 that near the supercritical region, the specific heat change of pure CO_2 is greatly affected by temperature and pressure, and the specific rules are as follows:

1) The specific heat under different pressures first rises to the maximum value with the increase of temperature, and then begins to fall to the minimum value and finally tends to be stable, the greater the pressure, the higher the temperature at which the specific heat reaches the maximum value;
2) When the temperature is -40 °C and -50 °C, the specific heat decreases with the increase of pressure, and when the temperature is 90 °C, the specific heat increases with the increase of pressure;
3) The specific calorific value of the critical point soars to the maximum, much higher than other areas, at this time the heat absorption and heat release capacity of CO_2 is the strongest, and the temperature change of the fluid is greatly affected during the actual transportation process, so the critical point should be avoided as much as possible when setting the temperature and pressure.

2.4 Thermal conductivity

Thermal conductivity refers to the inherent ability of a substance to transfer or conduct heat, similar to specific heat, which is a temperature-related physical property parameter. The greater the thermal conductivity, the increase in the speed of heat transfer from the entire conveying system to the outside world, and the increase in the temperature drop of the system affects the conveying efficiency, so the thermal conductivity is also one of the important factors affecting pipeline transportation. The change law of the thermal conductivity of simulated pure CO_2 is shown in Figure 4.

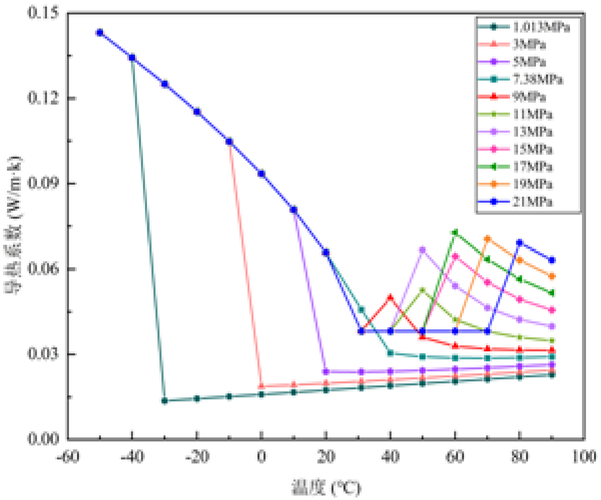

Figure 4: Thermal conductivity variation law of pure carbon dioxide the change of pure CO_2 thermal conductivity is more complex, and the specific rules are as follows:

1) When the temperature is less than -40 °C, the thermal conductivity under different pressures decreases with the increase of temperature and the value remains equal, which is not affected by pressure changes;
2) When the temperature exceeds -40 °C and the pressure does not exceed 7.38MPa, the thermal conductivity instantly decreases to the minimum value at a specific point, that is, the phase change point, and then begins to rise slowly with the increase of temperature; and when the temperature exceeds -40 °C and the pressure is greater than 7.38MPa, the thermal conductivity gradually decreases, and when it drops to a certain extent, it begins to increase again, and begins to slowly decline when it reaches the maximum value, because when the pressure is too large, the change law of thermal conductivity no longer follows the Fourier thermal conductivity expression.
3) The greater the thermal conductivity, the corresponding increase in heat transfer speed, in order to reduce the temperature drop loss and ensure the efficiency of pipeline transportation, the supercritical state is more suitable for pipeline transportation.

2.5 Compression coefficient

The compression coefficient is a physical quantity that describes the compressibility of an object, CO_2 shows different phases with temperature and pressure changes, the compression coefficient is different, and the compression coefficient is also one of the main physical properties affecting the pipeline throughput, so it is very important to analyze the change law of the compression coefficient for the reasonable allocation of pipeline throughput. The change law of the compression coefficient of pure CO_2 after simulation is shown in Figure 5.

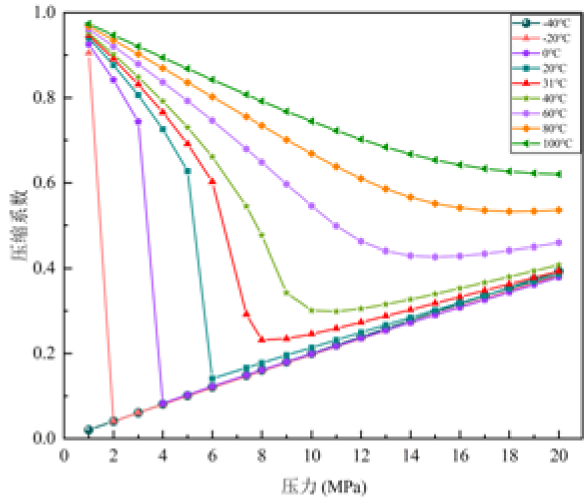

Figure 5: Compression coefficient variation law of pure carbon dioxide

It can be seen from Figure 5 that the compression coefficient varies greatly with the increase of temperature and pressure, and the specific law is as follows:
1) When the temperature is less than -40 °C, with the increase of pressure, the compression coefficient gradually increases and the value at each temperature is equal, which is not affected by temperature;
2) When the temperature rises from -20 °C to 60 °C, as the pressure increases, the compression coefficient first decreases to the minimum value and then begins to rise, but the downward trend is different at different temperatures and pressures. Below the critical point, the compression coefficient decreases instantaneously and then begins to rise slowly; Above the critical point, the downward and upward trend of the compression coefficient is relatively flat.
3) When the temperature is greater than 80 °C, as the pressure increases, the compression coefficient slowly decreases and eventually tends to be stable, without obvious upward trend.

3. Conclusions

It is believed that the physical properties of CO2 in the supercritical region are good, in which the density is close to liquid, the viscosity is close to gas, the specific heat and thermal conductivity are small, and the compression coefficient is large, and the supercritical region has a positive impact on the CO2 transport efficiency, so the supercritical state is more suitable for pipeline transportation.

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