

Temperature-Pressure and Phase Change of Impure Carbon Dioxide in Wellbore

Ling Liu^{1*}, Longxiang Lu¹, Yongqiang Ren², Chao Zhang¹, Fang Yu²

1 China University of Petroleum (East China), Qingdao 266000, China

2 Downhole service Branch of CNPC Bohai Drilling Engineering Company Limited, Renqiu 062550, China
(Corresponding Author*: liuling@upc.edu.cn)

ABSTRACT

During the process of carbon dioxide sequestration in saline aquifers, the presence of impurities in the gas source significantly impacts the temperature and pressure distribution as well as the phase state of the fluid within the wellbore, thereby influencing the injection conditions and geological storage properties. This study established a coupled temperature-pressure model to explore the phase change mechanism of non-pure carbon dioxide flowing through a wellbore. Based on field data, a numerical simulation study validated the effectiveness of the model in predicting temperature and pressure distributions of non-pure carbon dioxide along the wellbore, as well as determining its phase transition position, which could provide a crucial theoretical and decision-making support for wellhead injection technology in the sequestration of non-pure carbon dioxide in saline aquifers.

Keywords: sequestration in saline aquifers, impure carbon dioxide, temperature-pressure in wellbore, phase change of fluid

NONMENCLATURE

Symbols

ρ	Fluid density
v	Flow rate
P	Fluid pressure
θ	Shaft inclination
f	Friction coefficient of the fluid against the inner wall of the casing

T_e	Formation temperature
T	Fluid temperature in the casing
U	Total heat transfer coefficient of the wellbore
W	Mass flow rate of the fluid
C	Specific heat capacity of the fluid
η	Joule-Thomson coefficient

1. INTRODUCTION

In the field of Carbon Capture, Utilisation, and Storage (CCUS) technology, deep saline aquifer storage is considered the most promising method for carbon reduction[1-2]. As of June 2024, several large-scale saline aquifer carbon storage projects have been implemented worldwide. Notable examples include the Sleipner and Snøhvit projects in Norway, as well as the In Salah project in Algeria. These projects, characterized by their long operational periods, large scales, and significant storage capacities, are exemplary cases of successful commercial operations. In China, the development of saline aquifer carbon storage started later, with the Shenhua project in the Ordos Basin currently serving as a demonstration project[3]. From the perspective of carbon sources stored in recent CCUS projects, the vast majority consist of pure carbon dioxide with a purity of 99%, as shown in Table 1.

The high-purity carbon sources often originate from large-scale industrial emission sources, which are captured and subsequently purified and processed. The complex and high-cost purification technologies are currently an inescapable obstacle to achieving large-

scale Carbon Capture, Utilization, and Storage (CCUS). Utilizing non-pure carbon dioxide as a sequestration gas

Table. 1. CCUS projects using high-purity carbon dioxide as the storage gas source.

Project name	Industrial capture type	CO ₂ purity (%)	Cost (CNY/t)
Ordos Basin saline aquifer project	Coal-to-liquid	99.5	249
Shanbei coal chemical CO ₂ capture and demonstration	Coal-to-gas	99.8	120
Jilin Oilfield CO ₂ -EOR research and demonstration	Natural gas processing	99.9	166
Huaneng Gaobeidian power plant	Coal-fired power plant	>99.9	
Shengli Oilfield CO ₂ -EOR project	Coal-fired power plant	99.997	450
Chongqing Shuanghuai power plant carbon capture demonstration project	Coal-fired power plant	> 99.9	NA
HUST 35MW Oxy-fuel combustion demonstration	Coal-fired power plant	95	780~900
Dunhua Petroleum - Xinjiang Oilfield CO ₂ -EOR Project	Methanol plant	99.96	800
Wuhu Baimashan Cement Plant CO ₂ Capture and Purification Demonstration Project	Cement plant	99.99	NA
Haifeng Carbon Capture Testing Platform	Coal-fired power plant	99.99	500
East China Oilfield CCUS Full-Process Demonstration Project	Chemical plant	99	
Qilu Petrochemical - Shengli Oilfield CCUS Project	Chemical plant	99	/

Sources: Compiled from the China CCUS Annual Report (2021)

source will be one of the important pathways to achieve large-scale carbon reduction through CCUS in the future.

Firstly, the use of non-pure carbon dioxide can significantly reduce the costs of capture and purification. In traditional carbon capture and storage processes, carbon dioxide requires high-purity separation and purification. This process typically necessitates the use of expensive chemical absorbents or advanced membrane separation technologies, resulting in high costs. The use of non-pure carbon dioxide can reduce the consumables and processing steps in the purification process, thereby lowering the overall operating costs. For instance, if the captured carbon dioxide contains a small amount of other gases (such as nitrogen or oxygen), it can be directly injected into underground reservoirs in certain cases without the need for high-purity separation. This not only reduces the complexity of the purification steps but also lowers the costs associated with the use of chemicals and equipment.

Secondly, the use of non-pure carbon dioxide as an injection gas source can simplify the treatment technology. High-purity carbon dioxide capture and treatment technologies often involve complex processes and equipment, such as multi-stage

compressors, precise membrane separation devices, and efficient chemical absorption towers. These pieces of equipment are not only costly but also require professional maintenance and operation. The use of non-pure carbon dioxide reduces the reliance on these complex devices, thereby simplifying the treatment technology. For example, by employing direct capture technology, impure carbon dioxide gas can be directly injected into underground reservoirs without the need for complex separation and purification steps. This not only lowers the technical threshold but also reduces the difficulty of operation and maintenance.

Thirdly, the use of non-pure carbon dioxide can significantly reduce energy consumption. The high-purity carbon dioxide capture and treatment process usually requires a substantial amount of energy, especially when using chemical absorption methods, which require a large amount of thermal energy to regenerate the absorbent. Non-pure carbon dioxide does not require purification steps and high-energy-consuming separation processes. Moreover, the simplified treatment technology will also reduce the demand for electricity and thermal energy, improving the overall system's energy efficiency.

It is evident that by reducing operating costs, improving energy efficiency, and simplifying the technical process, more enterprises and projects can

become economically feasible. At the same time, policy support and market mechanisms (such as carbon trading and carbon taxes) can further promote the development of these projects, making the use of non-pure carbon dioxide an economically sustainable choice.

The phase state of fluids in wellbore mainly depends on temperature and pressure. Currently, studies on temperature and pressure modelling of wellbore fluids mainly focus on carbon dioxide oil repulsion (CCUS-EOR) and fracturing scenarios[4-5]. Zhou et al[6] established a pressure drop prediction model for CO₂-driven wells with high gas-to-liquid ratio based on the solubility of CO₂ in crude oil and the phase change of CO₂ flow along the wellbore, and Feng et al[7] established a model of cement ring seal failure under temperature change-induced stresses in response to the failure of cement ring seals due to the change of wellbore temperatures in the process of CO₂-driven oil. In fracturing, Guo et al [8] established a coupled model of wellbore pressure drop and heat transfer under CO₂ fracturing based on the interaction between wellbore temperature and pressure changes and CO₂ physical properties, while Li et al [9], Xiao [10], and Wu et al[11] established a wellbore temperature and pressure model to reveal the effects of injection temperature, construction displacement, drag reduction effect, and tubing size on temperature and pressure. Related studies on carbon sequestration in saline aquifers mainly focus on the potential, formation conditions, and technology of geological sequestration of pure CO₂ [12-15]. Lei et al [16-17] explored the mechanism and thermodynamic modelling of impure CO₂ fluids containing two components in shallow saline aquifers. In general, there are fewer studies on the temperature-pressure and phase change in the wellbore during the injection of non-pure carbon dioxide carbon fluids into deep saline aquifers.

Saline aquifer carbon sequestration typically requires that the carbon dioxide reaching the reservoir be in a supercritical state. Supercritical carbon dioxide possesses the characteristics of low gas viscosity and high liquid density, which gives it strong mass transfer capabilities and a large diffusion coefficient, thereby providing strong diffusion and dissolution abilities. It brings good stability and safety to the sequestration, aiding in achieving long-term effectiveness of the storage.

This study focuses on the temperature, pressure, and phase transition of non-pure carbon dioxide as it flows through the wellbore, revealing the flow scheme of non-pure carbon dioxide in the wellbore. The

ultimate goal of the study is to provide a theoretical basis for optimizing wellhead injection schemes, that is, under the premise of ensuring the safe and stable injection of carbon dioxide, to meet the dual objectives of injection efficiency and storage effect by adjusting the fluid injection temperature, pressure, and injection rate at the wellhead. To this end, we constructed a temperature and pressure distribution model of the fluid in the wellbore and verified the effectiveness of this model with data from the field.

2. ASSUMPTIONS

2.1 Wellbore Conditions

Drawing on the current experience of wellbore structure design for EOR and saline formation carbon sequestration[18-19], the wellbore during injection is structured by three parts, shown in Figure 1. Each part has different layers of casing and cement ring, with regular structure and good gas tightness.

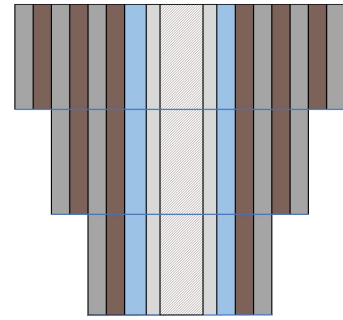


Fig. 1. Schematic diagram of wellbore structure

The basic parameters are set according to the sequence of locations from the inside to the outside in the upper wellbore is i , i is an integer between 1 and 8. The inner and outer diameters of the medium in bit i sequence are r_i and r_{i+1} , respectively. The inner surface temperature and outer surface temperature are T_i and T_{i+1} respectively. The thermal conductivity of the medium is λ_i . For the lower and middle shafts, the outer diameter of the outermost cement ring is not equal to the outer diameter r_5 , r_7 of the corresponding sequence cement ring of the upper shaft ($i=4, 6$), so they are set as r'_5 , r'_7 respectively.

Additionally, the study also provides hypothetical descriptions regarding the fluid components and their heat transfer environment in the wellbore during the initial period of injection. The state of heat transfer between the non-pure CO₂ fluid and the wellbore is assumed as steady, while that between the wellbore and the formation is unsteady.

2.2 Fluid properties

The Fluid is a mixture composed of CO₂ with a content of less than 90%, and one or more impurity gases, such as N₂, O₂, CH₄, H₂, H₂S, CO, SO₂, NO₂. The key physical property parameters of the critical point are obtained through custom operations in the REFPROP property library when the fluid mix is determined.

2.3 Boundary and Initial Conditions

The wellbore is seen as a complex system full of fluid in equilibrium, with the wellhead as input boundary and the well bottom as the output.

Only radial heat transfer is considered in wellbore, and the temperature, pressure, and physical parameters of the mixture are kept consistent in the radial direction.

The initial formation temperature varies linearly with the depth of wellbore.

3. MODELLING

Combining the mass conservation theorem of fluid and the momentum balance principle, the wellbore pressure gradient equation can be obtained.

$$\frac{dp}{dz} = \rho g \sin \theta - \frac{f \rho v^2}{4r_1} - \rho v \frac{dv}{dz} \quad (1)$$

Combining the energy conservation equation, mass conservation equation and heat transfer equation, the wellbore temperature model can be obtained as follows:

$$\frac{dT}{dz} + \frac{2\pi r_1 U}{wc} T = \frac{2\pi r_1 U}{wc} T_e + \eta \frac{dp}{dz} + \frac{dp}{c_p dz} + \frac{fv^2}{2dc} \quad (2)$$

The heat transfer coefficients of the upper, middle and lower parts of the shaft are also different due to the number of solid wall layers, which can be expressed as:

$$U_u = \frac{1}{r_1} \left[\frac{f(t)}{\lambda_e} + \sum_{i=1}^8 \left(\frac{\ln \frac{r_{i+1}}{r_i}}{\lambda_i} \right) + \frac{1}{r_1 h_f} \right]^{-1} \quad (3)$$

$$U_m = \frac{1}{r_1} \left[\frac{f(t)}{\lambda_e} + \frac{\ln \frac{r_7}{r_6}}{\lambda_6} + \sum_{i=1}^5 \left(\frac{\ln \frac{r_{i+1}}{r_i}}{\lambda_i} \right) + \frac{1}{r_1 h_f} \right]^{-1} \quad (4)$$

$$U_l = \frac{1}{r_1} \left[\frac{f(t)}{\lambda_e} + \frac{\ln \frac{r_5}{r_4}}{\lambda_4} + \sum_{i=1}^3 \left(\frac{\ln \frac{r_{i+1}}{r_i}}{\lambda_i} \right) + \frac{1}{r_1 h_f} \right]^{-1} \quad (5)$$

4. SIMULATION

Since the phase state of the fluid at any depth after injection into the wellbore depends on the difference between the temperature and pressure of the wellbore and the critical temperature and pressure at which the fluid undergoes a phase transition. To predict the location of the phase transition of the non-pure CO₂ fluid in the wellbore, the temperature-pressure

distribution in the wellbore first needs to be solved using the temperature-pressure model constructed in this paper.

In this paper, the numerical method is used to solve the wellbore by dividing it longitudinally into units of equal length

4.1 Data source and processing

Assuming the injected fluid is a mixture of liquid carbon dioxide (90%) and nitrogen (10%). Other basic data are shown in Table 2.

Table 2 Basic data and value for simulation

Subscripts	Unit	Value
Injection temperature	°C	20
Injection speed	t/a	40000
Surface temperature	°C	15
The depth of the drilling I	m	480
The depth of the drilling III	m	2547
Radius of the drilling II	mm	173
Injection casing inner radius	mm	50.17
Production casing inner radius	mm	79.71
Technical casing inner radius	mm	125.095
Surface casing inner radius	mm	192.07
Inject casing wall roughness	mm	0.0152
Production casing thermal conductivity	W/(m·°C)	43.27
Surface casing thermal conductivity	W/(m·°C)	43.27
Annular fluids thermal conductivity	W/(m·°C)	0.6
Formation diffusion coefficient	m ² /s	0.0036
Injection pressure	MPa	27()
Injection time	day	200
Geothermal gradient	°C/hm	3.06
The depth of the drilling II	m	1000
Radius of the drilling I	mm	254
Radius of the drilling III	mm	120.65
Injection casing outer radius	mm	57.15
Production casing outer radius	mm	88.9
Technical casing outer radius	mm	136.525
Surface casing outer radius	mm	203.2
Injection casing thermal conductivity	W/(m·°C)	43.27
Technical casing thermal conductivity	W/(m·°C)	43.27
Cement ring thermal conductivity	W/(m·°C)	0.52
Formation thermal conductivity	W/(m·°C)	2.09
Well inclination angle	°	90

4.2 Data source and processing

Using the aforementioned solution approach and data, the temperature and pressure distribution of impure carbon dioxide fluid in the wellbore as a function of depth were obtained. These results were compared with two sets of field measurements, with temperature and pressure errors both being less than 1%, as shown in Figure 2.

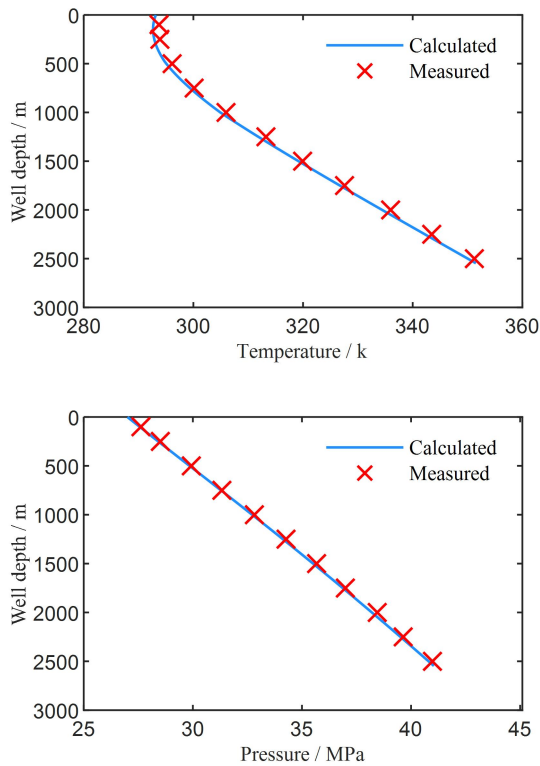


Fig.2. Temperature and pressure of the wellbore

This indicates that the model is effective and can be used to predict the effects of fluid composition and other factors on temperature and pressure distribution, as well as phase state.

For the binary system which contains only one impurity, nitrogen, and the mole fraction content of CO₂ changes from 100% to 80%, that is, N₂ from 0 to 20%, the temperature along wellbore is always lower than the initial formation temperature and the position of phase transition moves upwards.

For the ternary system such as a mixture of carbon dioxide (80%) and nitrogen (10%) and methane (10%), the temperature along wellbore is always lower the initial formation temperature, same with the binary system above, but the position of phase transition moves downwards comparing to the binary system.

5. CONCLUSION

This study has showed the specific injection mechanism of impure CO₂ systems in wellbore. As injected in liquid state, the mixture will affect the temperature-pressure distribution of the fluid along the wellbore, and further affect the phase transition position of the fluid. Simulation results show that by predicting the fluid temperature-pressure distribution and phase transition position along the well, it can provide decision support for optimizing the injection scheme to achieve energy conservation, safe, and stable injection. Some areas for improvement include limited experiments, scattered results, thus insufficient universality.

ACKNOWLEDGEMENT

This work is supported by the Foundation of CNPC Bohai Drilling Group's major science and technology project(2023ZD17Y) and the National Natural Science Foundation of China under the Youth Science Foundation Program (52204068).

DECLARATION OF INTEREST STATEMENT

THE AUTHORS DECLARE THAT THEY HAVE NO KNOWN COMPETING FINANCIAL INTERESTS OR PERSONAL RELATIONSHIPS THAT COULD HAVE APPEARED TO INFLUENCE THE WORK REPORTED IN THIS PAPER. ALL AUTHORS READ AND APPROVED THE FINAL MANUSCRIPT.

REFERENCE

- [1] Global CCS Institute,2023[R].Global Status of CCS:Australia,2023.
- [2] X.Zhang, X.Yang et al. China Carbon Dioxide Capture, Utilization and Storage (CCUS) Annual Report (2023)[R]. China Agenda 21 Management Center, Global Carbon Capture and Storage Research Institute, Tsinghua University, 2023.
- [3] GCCSI. Global Status of CCS 2022 Report[R].Global CCS Institute, 2022.
- [4] Y. Chen, L. Zhang, et al. Comparison of crude oil properties in CO₂-driven and H₂O-driven recovered fluids[J]. Journal of petroleum (petroleum processing),2013,29(03):508-512.
- [5] M. Zhang, H. Mei, et al. Gas-liquid-solid three-phase simulation of oil and gas systems[J]. Journal of petroleum processing,2002(05):80-85.
- [6] Y. Zhou, R. Pan,et al. Predictive modeling of wellbore pressure drop in CO₂ driven high gas-to-liquid ratio oil wells in Jilin Oilfield[J]. Oil Field Equipment,2023,52(06):9-16.

- [7] Y. Feng, Y. Wang, et al. Effect of wellbore temperature variation on cemented cement ring seal integrity in CO₂-EOR wells[J]. Scientific and Technological Innovation,2022,(31):5-8.
- [8] X. Guo, X.Sun, et al. Heat transfer law of wellbore for supercritical CO₂ fracturing[J]. Drilling Fluid and Completion Fluid,2021,38(06):782-789.
- [9] X. Li, G. Li, et al. A wellbore flow modeling and coupled solution for supercritical CO₂ fracturing[J]. Journal of China University of Petroleum(Edition of Natural Science),2018,42(02):87-94.
- [10] B. Xiao. Coupled temperature-pressure field calculation method for supercritical carbon dioxide dry fracturing[J]. China Sciencepaper,2020,15(01):119-124.
- [11] L. Wu, Z. Luo, et al. Research on temperature and pressure and phase control of wellbore for supercritical carbon dioxide fracturing[J]. Journal of Southwest Petroleum University(Science & Technology Edition),2023,45(02):117-125.
- [12] Y. Wang, X. Peng, et al. Mechanisms of CO₂ transport in a stratified brackish water layer under the synergistic effect of buoyancy and capillary forces[J]. Journal of China University of Petroleum(Edition of Natural Science),2023,47(03):96-106.
- [13] Z. Li, Q. Zhang, et al. Determination of CO₂ dissolved burial potential in saline aquifers[J]. Petroleum Geology and Recovery Efficiency,2023,30(02):174-180.
- [14] Y. Bai. Research on the mechanism of freezing and plugging in the wellbore of supercritical CO₂ and water alternating injection wells[D].Northeast Petroleum University,2021.
- [15] Y. Lin, Y. Deng, et al. Carbon dioxide solubility determination in formation water and predictive modeling[J]. Journal of China University of Petroleum(Edition of Natural Science),2021,45(01):117-126.
- [16] H. Lei, J. Li, et al. An improved TOUGH2 module for simulating non-isothermal multiphase and multicomponent flow in CO₂-H₂S-CH₄-brine systems with high pressure, temperature and salinity[J]. Computers & Geosciences,2016,94:150-161.
- [17] H. Lei, J. Li, et al. Numerical modeling of co-injection of N₂ and O₂ with CO₂ into aquifers at the Tongliao CCS site[J]. International Journal of Greenhouse Gas Control,2016,54:228-241.
- [18] L. Dou, G. Li, et al. Wellbore pressure and temperature prediction model and its affecting factors for CO₂ injection wells. Petroleum Drilling Techniques 41.1 (2013): 76-81.
- [19] R. Zhang, J. Li, et al. Analysis of coupled wellbore temperature and pressure calculation model and influence factors under multi-pressure system in deep-water drilling. Energies 12.18 (2019): 3533.