

“Developing Transient Model and Simulating the Effects of Soil Properties on a Small Hole Leakage and Diffusion Characteristics in the Buried CO₂ Pipelines.”

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Highlights:

- An innovative transient model is developed for the small-hole leakage in the buried CO₂ pipelines.
- Leakage and seepage diffusion characteristics of the buried CO₂ pipelines are systematically investigated.
- Temperature-based leak detection exhibits a significant delay compared to the concentration-based methods.
- The effect of soil properties on the CO₂ seepage diffusion is systematically examined and tested.
- The variations of soil temperature around the CO₂ pipes are simulated and validated against the experimental results.

Abstract:

The Carbon dioxide (CO₂) pipelines are subject to the significant risk factors of leakage,

primarily due to the mechanical damages, corrosion, and third-party interference. The CO₂ pipe leakage, which involves the intricate phase of the transition processes, and it is characterized by the pronounced fluctuations in the pressure and temperature, creates considerable challenges to the pipeline reliability and environmental safety. Therefore, a comprehensive analysis on the leakage and seepage diffusion in the buried CO₂ pipelines is essential for the accurate risk assessment and decreasing the response time associated with the leak detection. This study develops a transient model to examine the small hole leakages' behavior in the buried CO₂ pipelines. By integrating discharge model and seepage diffusion model coupling with the thermo-fluid-solid and multi-physical fields, the research study focuses on the dynamic variations in pressure, velocity, temperature, and concentration of the soil during the leakage. Additionally, this research examines the effects of the soil properties, including porosity, permeability, and types with the CO₂ leakage and seepage diffusion behavior. The key indicators such as Warning Alert Time (WAT), Temperature Detection Time (TDT), and Pipeline Brittle Range (PBR) are introduced to define the hazardous boundaries, providing a systematic framework for the risk assessment. The findings demonstrate that the physical properties of the soil play a crucial role in determining the leakage behavior and hazardous range of the seepage diffusion in the buried CO₂ pipelines. The developed transient numerical model helps to predicts the dynamic characteristics of the leakage and seepage diffusion within the soil more effectively, offering a robust theoretical foundation and technical support for the assessing the consequences of the CO₂ leakage.

Keywords: Carbon dioxide; Buried pipelines; seepage diffusion characteristics; Soil properties; Numerical simulation

1. Introduction

In recent years, the extreme climate events such as heavy rains, droughts, hurricanes, and floods have occurred frequently around the world.^{1,2} The impact of ever-increasing greenhouse is harshly affecting the human survival and societal development.³ The

Carbon Capture, Utilization, and Storage (CCUS) technologies provide a promising pathway for reducing CO₂ emissions and addressing impact from the climate change.⁴ In the CCUS technology chain, pipelines are widely recognized as the most cost-effective and efficient method for transporting CO₂.^{5,6} However, pipeline leaks inevitably occur due to several factors such as corrosion, external interference, and construction defects.^{7,8} This is particularly true for the buried pipelines.⁹ The leakage incidents can be classified based on the size of the leak: small holes (where the ratio of the leak size to the pipeline diameter is $d/D < 0.2$), large holes ($0.2 \leq d/D < 0.6$), and the full pipeline ruptures ($d/D \geq 0.6$).¹⁰ The small hole leaks compare to others are mostly concerning due to their multiple leakage points, strong concealment, difficulty in detection, and high potential danger.¹¹ However, the current detection technology for CO₂ in the buried pipelines is not yet advanced enough to promptly identify these leaks, which can result in missing the optimal rescue time.¹²

Over the past decade, researchers have achieved notable advancements in the study of CO₂ leakage and dispersion.^{13–15} Guo et al.^{16,17} categorized the leakage into three phases: 1) rapid expansion, 2) metastable, and 3) slow decay. These are based on their observed positions of the Mach disk and the patterns of the visible gas cloud. They found that increasing the size of the leakage holes or the leakage volume expands both within a low-temperature region and around the diffusion radius. Teng et al.¹⁸ conducted experiments utilizing high-pressure cylinders and nozzles and revealed that a maximum fluid velocity of 250 m/s near the leakage hole is increasing first and then decreasing with the CO₂ concentration along the leakage axis. Moreover, the larger leakage sizes correlated with the lower temperatures near-field. Hu et al.¹⁹ discovered that the dry ice particles formed during the leakage process, but did not accumulate on the ground. As the leaks size increased, the jet intensity and the rate of visible gas cloud decay both intensified. They identified a danger zone extending 80 meters from the axis of the leakage hole and 8 meters along the length of the pipeline.

Currently, the research on the above-ground CO₂ pipeline leaks is relatively well-

developed, with a wealth of technical methods that facilitate observation and simulation of the leakage process.^{20–22} In contrast, the research on the underground CO₂ pipeline leaks is less common due to the stringent design requirements for the underground leakage experiments, involving high construction costs and difficulties in data collection. Furthermore, underground pipeline leakage involves multiple interacting factors and assist in increasing the complexity of the leakage process. As early as 2016, the team led by Yu at Dalian University of Technology initiated experimental research on the buried CO₂ pipeline leaks and found that the substantial amounts of dry ice formed after the CO₂ leakage, causing a significant decrease in the soil temperature.²³ The team further discovered that the formation of dry ice and permafrost do not only reduced the soil temperatures but also increase additional compressive stress on the pipeline, causing it to displace from its original installation path.²⁴ This displacement heightened the risk of brittle fracture, particularly in low-temperature and stress-concentrated areas. Compared to above-ground pipelines, the underground pipelines leaks pose a greater threat to the structural integrity. Subsequent research analyzed the changes in the volume and shape of dry ice spheres during the CO₂ leakage process. It revealed that the upward leakage produced at the largest dry ice spheres provides the same size of leakage hole, followed by the horizontal leakage but the downward leakage formed is the smallest. Additionally, the CO₂ in the soil spread toward areas of lower resistance, with the flow direction determining the shape of the dry ice spheres rather than the leakage direction.²⁵ Liu et al.²⁶ measured the changes in the temperature field using thermocouples placed in the soil pits. Their study revealed that the temperature distribution in the soil formed a funnel shape and at the same horizontal elevation, temperatures were lowest in the direction of the leakage. The isotherms expanded outward in a nearly circular pattern due to the uniformity of the soil medium.

This study on the buried CO₂ pipeline leakage primarily focuses on the experimental methods with the limited attention to the theoretical studies. While experimental work has made progress in revealing changes in the soil temperature field, these methods often face the constraints related to the equipment complexity, high costs, and the

limitations in data collection, making it challenging to comprehensively reflect complex conditions.²⁷ This paper establishes a small-hole leak model for the buried CO₂ pipelines through the scientific study of the leakage and seepage diffusion characteristics of the buried CO₂ pipelines. The developed model helps to integrate the discharge and seepage diffusion processes, coupling the thermal, fluid, and solid multi-physical fields. To ensure the accuracy and reliability of the research findings, a three-dimensional model was employed to replicate the real scenarios, and the numerical model was validated against the experimental data for the computational precision. This paper also examines the changes in the pressure field, velocity field, streamlines, concentration field, and temperature field following the leaks in the buried CO₂ pipelines. Furthermore, the study expands the definition of the Warning Alert Time (WAT), the Pipeline Brittle Range (PBR), and the Temperature Detection Time (TDT). By analyzing different scenarios, the paper discusses the impact of soil porosity, soil permeability and soil types on the leakage and seepage diffusion characteristics, as well as on the hazard boundaries. This study provides a crucial theoretical support for a deeper understanding of the leakage mechanisms and improving safety assessments of the buried CO₂ pipelines.

2. Development of the mathematical model

2.1 Basic assumptions

To facilitate the calculation, several necessary assumptions were made as below:

- 1) Dry ice and liquid CO₂ are considered condensed phases, simplifying the leakage process to a two-phase flow.
- 2) The CO₂ inside the pipe leaks into the soil through the leak hole. Due to the minimal friction and heat transfer at the leakage point, this process can be considered an isentropic expansion process.
- 3) Due to the brief duration (milliseconds) of the study, the heat transfer between the fluid and pipe walls is disregarded.

- 4) The soil is assumed to be an isotropic porous medium that remains unchanged during the leakage process.

2.2 Fluid properties calculation model

Under the high-pressure conditions, CO₂ exhibits significant physical properties. In the event of a leak, the CO₂ undergoes rapid phase transitions, shifting from a liquid or supercritical state to a gaseous or gas-liquid mixed state, which quickly mixes with the surrounding air. This complex transition phase profoundly affects not only the initial jet characteristics of the leak but also the seepage diffusion behavior. Therefore, accurately describing the changes in the physical properties of CO₂ is a critical first step in predicting the consequences of leaks. To address this issue, it is essential to select an appropriate fluid property calculation method. Zhao et al.²⁸ conducted a comparison of various equations of state, concluding that the Peng - Robinson (PR) equation is the most suitable for calculating the vapor-liquid equilibrium and physical properties of polar substances like the CO₂. In relevant standards, such as the Recommended Practice DNVGL-RP-F104-2021 'Design and Operation of Carbon Dioxide Pipelines' and SH/T 3202-2018 'Specifications for Engineering of Carbon Dioxide Pipeline Transportation,' the PR equation is also recommended for calculating the thermodynamic properties of CO₂.²⁹⁻³¹ Despite the simplicity of the cubic equations of state, they are widely recognized for their accuracy in modeling the vapor-liquid behavior of CO₂ while providing high computational efficiency.^{32,33}

In this model, the PR EOS is used to calculate the density of CO₂. The PR equation is expressed as follows:

$$P = RT/(V - b) - a(T)/(V^2 + 2bV - b^2) \quad (1)$$

Where T denotes the temperature. V represents specific volume. R refers to the universal gas constant. The empirical parameters $a(T)$ and b account for molecular interactions and the finite volume occupied by molecules, respectively.

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

$$b = 0.07780 \frac{RT_c}{P_c} \quad (3)$$

Where T_c and P_c represent the critical temperature and pressure, respectively. $\alpha(T)$ is a temperature-dependent function.

$$\alpha(T) = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{T_r})]^2 \quad (4)$$

When using the PR equation of state, the speed of sound can be approximately calculated through Equation (5).

$$c = \sqrt{\kappa \frac{RT}{M}} \quad (5)$$

Where κ is the isentropic exponent, $\kappa = C_p/C_v$. M represents the molar fraction of the gas.

Enthalpy can be obtained by integrating the heat capacity, as shown in Equation (6).

$$H = H_{ideal}(T) + \int_{v_{ideal}}^v \left[T \left(\frac{\partial P}{\partial T} \right)_v - P \right] dv \quad (6)$$

Where H_{ideal} represents the enthalpy of an ideal gas.

The entropy value of a real fluid can be calculated using Equation (7).

$$S = S_{ideal}(T) - R \ln \left(\frac{v-b}{v} \right) + \int_{v_{ideal}}^v \frac{T \left(\frac{\partial P}{\partial T} \right)_v}{T} dv \quad (7)$$

Where S_{ideal} represents the entropy of an ideal gas.

2.3 Orifice flow state and discharge models

The orifice flow state and discharge models include the gas dynamics models, isentropic processes, reverse hysteresis processes, and vena contracta effects. As the fluid transitions start from a high-pressure region to a low-pressure region, it undergoes acceleration. According to the principles of gas dynamics, when the initial pressure within the pipeline exceeds the critical pressure for the choked flow, the discharge velocity of the CO₂ approaches to the local speed of sound. In this scenario, the leak flow rate matches the local speed of sound of CO₂, and the mass flow rate reaches its

maximum.³⁴ This phenomenon is referred to as choked flow. The critical pressure for choked flow is calculated using Equation (8).

$$\frac{P_c}{P_e} = \left(\frac{\gamma + 1}{2} \right)^{\gamma/(\gamma-1)} \quad (8)$$

Where P_c is the critical pressure for choked flow, MPa. P_e is the ambient pressure, MPa. γ is the adiabatic index, dimensionless, with a value of $\gamma=1.29$ for CO₂.

The critical pressure P_c for CO₂ choked the flow and it is calculated to be approximately 0.185 MPa. This shows that the pressure in the CO₂ transport pipelines is much higher than the calculated value. Therefore, any leak in the CO₂ pipelines can be considered the choked flow at the leak point. Under these conditions, the leakage flow rate matches the speed of sound for the fluid. However, the speed of sound is not constant; it is influenced by the equation of state, as well as temperature and pressure conditions. In this model, the acoustic velocity of CO₂ can be calculated using the PR EOS.

Due to minimal friction and heat transfer at the leakage point, the leakage of CO₂ through the small hole can be regarded as an isentropic expansion process. In this context, when the fluid slows to zero velocity, the process is called stagnation, and the zero-velocity state is defined as the stagnation state. Because the flow velocity within the pipeline is two orders of magnitude lower than the jet velocity at the leakage point, the CO₂ inside the pipeline can be assumed in a stagnation state. The CO₂ flow from the pipeline to the leakage point can be viewed as the reverse of the stagnation process, known as the "reverse stagnation process." The relationship between any state within the stagnation process and the stagnation state is described by Equation (9).

$$h_0 = h + \frac{u_1^2}{2g} \quad (9)$$

Where h_0 is the enthalpy in the stagnation state, J/kg. h is the enthalpy in any arbitrary state, J/kg. u_1 is the flow velocity, m/s. g is gravitational acceleration, m/s².

Here, enthalpy, a function of temperature and pressure, is calculated using the PR EOS. Subsequently, the flow velocity can be determined by iteratively solving for the speed

of the sound closest to the flow velocity. The fluid's temperature and pressure at the leakage point can be inferred. The flow contracts at leaks, forming a flow path smaller than the cross-sectional area. This phenomenon is known as the vena contracta effect, as shown in the Figure 1. Therefore, the influence of the vena contracta coefficient must be considered when calculating the leakage rate.

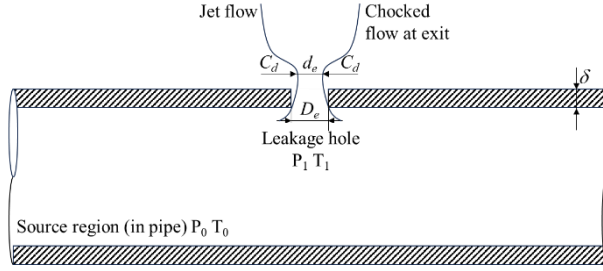


Figure 1. Schematic diagram of the vena contracta effect

In summary, based on the isentropic expansion process, the synergistic variation between temperature and pressure during leakage can be determined, which in turn allows for the calculation of the speed of sound. Through the reverse stagnation process, the change in fluid velocity can be derived. By coupling the flow velocity with the speed of sound, the fluid state at the leakage points can be deduced. Finally, the discharge model is established, as shown in Equation (10).

$$Q_1 = \rho_1 u_{a,1} C_d A \quad (10)$$

$$C_d = \frac{P_0}{2P_0 - P_1} \quad (11)$$

Where ρ_1 represents the density at the leakage point in kg/m^3 , which can be calculated based on the corresponding temperature and pressure. $u_{a,1}$ is the acoustic velocity of the fluid at the leakage point in m/s . C_d is the vena contracta coefficient. A is the leakage area in m^2 .

2.4 Leakage and seepage diffusion models

The leakage of a buried CO_2 pipeline involves the seepage diffusion of compressible gas in porous media. We employed a multiphase Eulerian mixture model to analyze the external flow field around the pipeline. The mathematical model for the leakage and

seepage diffusion process of CO₂ in the soil encompasses mass conservation, momentum conservation, energy conservation, equation of species transport, non-equilibrium phase transition models and turbulence models.

2.4.1 Conservation equation of mass

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \bar{u}_m) = 0 \quad (12)$$

Where the subscript m denotes the properties of the mixture. ρ_m and $\bar{u}_m$ represent the mixture's density and mass-averaged velocity, respectively.

2.4.2 Conservation equation of momentum

$$\begin{aligned} \frac{\partial(\rho_m \bar{u}_m)}{\partial t} + \nabla \cdot (\rho_m \bar{u}_m \bar{u}_m) = & -\nabla p_m + \nabla \cdot [\mu_m (\nabla \bar{u}_m + \nabla \bar{u}_m^T)] + \rho_m \bar{g} + S_i + \\ & \nabla \cdot \left(\sum_{k=1}^2 \alpha_k \rho_k (\bar{u}_k - \bar{u}_m)(\bar{u}_k - \bar{u}_m) \right) \end{aligned} \quad (13)$$

Where the subscript k represents a specific phase. ∇p_m represents the mixture pressure. $\rho_m \bar{g}$ represents the gravitational body force. μ_m represents mixture viscosity. As shown in Equation (14), S_i is the momentum source in term of porous media, composed of two parts. The first term on the right side of the equation is Darcy's viscous resistance loss, while the second term accounts for the inertial resistance loss.

$$S_i = -\left(\frac{\phi^2 \mu}{\alpha} v_i + \frac{\phi^3 C_2}{2} \rho v^2 \right) \quad (14)$$

The viscous resistance coefficient and inertial resistance coefficient of the soil can be determined using the Equations (15) and (16).

$$\frac{1}{\alpha} = \frac{150\mu}{D_p^2} \cdot \frac{(1-\phi)^2}{\phi^3} \quad (15)$$

$$C_2 = \frac{3.5}{D_p} \cdot \frac{(1-\phi)}{\phi^3} \quad (16)$$

2.4.3 Conservation equation of energy

$$\frac{\partial}{\partial t}(\phi \rho_f E_f + (1-\phi) \rho_s E_s) + \nabla \cdot (\bar{u}_f (\rho_f E_f + p)) = \nabla \cdot \left(k_{eff} \nabla T - \sum_{j=1}^2 h_j \bar{J}_j + (\bar{\tau}_{eff} \cdot \bar{u}) \right) + S_f^h \quad (17)$$

Where the subscript f represents fluid, while s denotes the soil medium. The subscript j denotes specific species within the vapor phase (CO₂ or air). k_{eff} represents the effective conductivity that encompassing both the standard and turbulent thermal conductivities. The term ϕ represents porosity of the solid. E_f represents the total fluid energy. E_s represents the total soil energy. S_f^h represents the heat source associated with the energy involved in the phase transition process. $\bar{\tau}_{eff} \cdot \bar{u}$ refer to the viscous dissipation.

2.4.4 Equation of species transport

This paper proposes a multiphases and multicomponent groups of the transport model for the minor CO₂ leaks. Since no chemical reactions occur during the seepage diffusion process, the rate of mass change for the CO₂ is controlled solely by the net diffusion rate, as shown in Equation (18).

$$\frac{\partial}{\partial t}(\rho_v \alpha_v Y_j) + \nabla \cdot (\rho_v \alpha_v \bar{u}_{vj} Y_j) = -\nabla \cdot \alpha_v \bar{J}_j \quad (18)$$

Where Y_j denotes the local mass fraction of each species. $\bar{u}_{vj}$ represents diffusion velocity vector. $\bar{J}_j$ represents diffusion flux.

2.4.5 Non equilibrium phase transition models

This model employs pressure dynamics to explore the non-equilibrium phase behavior of CO₂. It integrates mass and energy source terms to accurately simulate phase transitions. When P_l falls below P_{sat} , the liquid phase transforms into the gas phase. Conversely, when P_v exceeds P_{sat} , the gas phase condenses back to the liquid phase. The processes of evaporation and condensation are represented by Equations (19) and

(20)³⁵

$$P_l < P_{sat}, \quad \dot{m}_{lv} = C_{ev} \alpha_l \rho_l \frac{P_{sat} - P_l}{P_{sat}} \quad (19)$$

$$P_l > P_{sat}, \quad \dot{m}_{vl} = C_{con} \alpha_v \rho_v \frac{P_v - P_{sat}}{P_{sat}} \quad (20)$$

Where C_{ev} and C_{con} represent the evaporation and condensation coefficients, respectively.

In this study, both the dry ice and liquid-phase CO₂ are treated as condensate phases. To enhance the model's physical fidelity, an energy source term, S_f^h , is introduced to account for energy exchanges during the phase transitions (Equation 21). Heat transfer between the liquid and gas phases is characterized as the latent heat of vaporization, whereas the solid and gas phases is defined as the latent heat of sublimation. The latent heat associated with these transitions is temperature-dependent and is computed using a piecewise polynomial formulation (Equation 22).³⁶

$$S_f^h = \Delta h_{lv} \cdot \dot{m}_{lv} \quad (21)$$

$$\Delta h_{lv} = h_{vsat} - h_{lsat} = \begin{cases} -1307.5T + 633590 & (173.15 \leq T < 216.59) \\ -0.45T^3 + 325.82T^2 - 80101T + 7000000 & (216.59 \leq T < 304.15) \end{cases} \quad (22)$$

Where, h denotes enthalpy in J/kg. The temperature of 216.59 K corresponds to the triple point of CO₂, while 304.15 K represents its critical temperature.

2.4.6 Turbulence models

The standard k - ε turbulence model was applied, incorporating a compression function into the equation for calculating the dissipation rate to address compressive effects. The transport equations that govern the turbulence kinetic energy (k) and its rate of dissipation (ε) are as follows:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (23)$$

and

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\varepsilon u_i) = \frac{\partial}{\partial x_j}[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial\varepsilon}{\partial x_j}] + G_{1\varepsilon}\frac{\varepsilon}{k}(G_k + C_{3\varepsilon}G_b) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon \quad (24)$$

Turbulence kinetic energy generated by mean velocity gradients is represented by G_k , while G_b denotes the production of turbulence kinetic energy due to buoyancy effects. The term Y_M accounts for the influence of fluctuating dilatation in compressible turbulence on the total dissipation rate. The constants $C_{1\varepsilon}$, $C_{2\varepsilon}$, and $C_{3\varepsilon}$ are included, along with the turbulent Prandtl numbers σ_k and σ_ε for k and ε , respectively. Additionally, S_k and S_ε represent user-specified source terms.

The model constants are assigned the default values listed in Table 1.

Table 1. The default values of the model constants.

Constants	$C_{1\varepsilon}$	$C_{2\varepsilon}$	$C_{3\varepsilon}$	σ_k	σ_ε
Default values	1.44	1.92	0.09	1.00	1.30

3. Algorithm design for the Physical Model

3.1 Physical model

In this study, a three-dimensional physical model was developed to simulate the leakage and seepage diffusion behavior of the high-pressure CO₂ leakage from a buried pipeline through a small orifice, as shown in Figure 2. The model employed a 3D Cartesian coordinate system, with the origin O located at the center of the leakage hole. The simulation domain is a 4 m × 4 m × 2.5 m porous medium region representing the soil environment. The 250 mm diameter pipeline is buried at a depth of 1.5 m, with the leakage hole located at its geometric center. This model considered the influence of soil resistance in three dimensions, overcoming the limitations of one- and two-dimensional models, which often neglect the soil resistance and pipeline length. This study investigates the small-hole leakage in the buried pipelines, focusing on a 6 mm circular orifice for the experiment and data analysis.

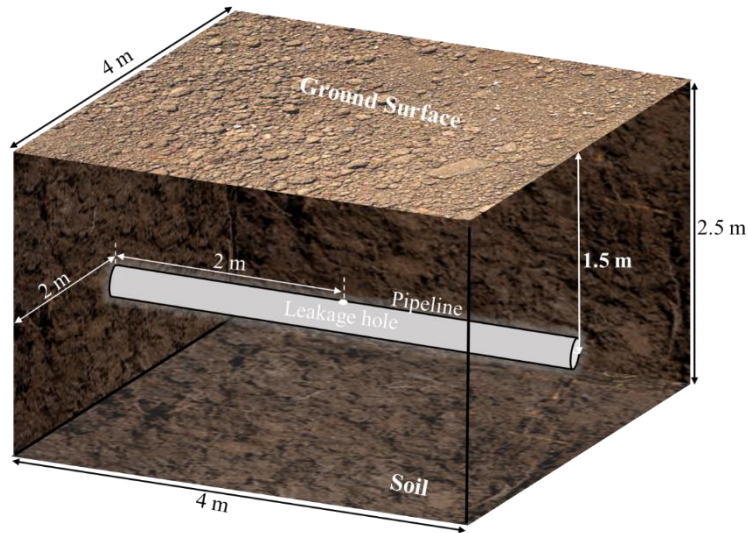


Figure 2. Schematic diagram of the physical model.

3.2 Computation algorithm

In this study, the numerical method for modeling the buried CO₂ pipeline leakage is divided into three stages: the initialization, the orifice jet, and the seepage dispersion, as shown in Figure 4. At first stage, the initial conditions are obtained. The physical properties of CO₂ are calculated based on the fluid state. Next stage, the reverse choked flow model is used to determine the pressure, temperature, and flow rate at the leakage hole. Final stage, the seepage diffusion process of CO₂ through a small hole in the buried pipeline is simulated using ANSYS FLUENT 2022 R1. Given the transient nature of the process, the PISO algorithm is employed to address the coupling of velocity and pressure. To account for the sudden changes in pressure gradient inside and outside the pipeline, a least-squares cell-based method is used to compute the gradient, and the PRESTO scheme is applied for pressure interpolation. Other terms are discretized using second-order upwind schemes for the improved accuracy. The time step is set to 0.01 seconds. The maximum number of iterations is limited to 50 steps. The time step is chosen based on the leakage duration, with a total leakage time of 100 seconds corresponding to 10,000 steps.

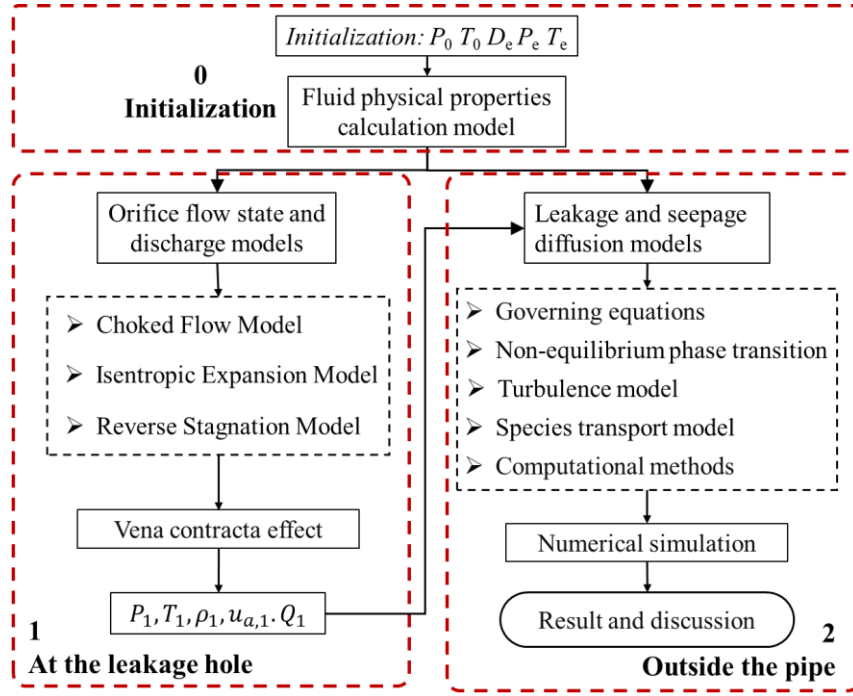


Figure 3. Flowchart for solving the leakage and seepage diffusion process of a buried pipeline.

3.3 Soil property

Soil is considered a typical porous medium, with a porous media model constructed by incorporating a momentum source term into the momentum equation. This approach translates the fluid resistance within the porous zone into a distributed resistance throughout the fluid, enabling the simulation of fluid seepage diffusion through the soil. The calculation methods for inertia resistance factor and viscous resistance factor are provided in Equations (15) and (16). This study focuses on three primary soil types, with their respective characteristics presented in Table 2.³⁷

Table 2. Characteristics of the soils.

Soil types	Particle diameter D_p (mm)	Porosity ϕ	Viscous resistance $1/\alpha$ (1/m ²)	Inertial resistance C_2 (1/m)
Sandy	0.50	0.50	2.16e+10	3.36e+05
Loam	0.05	0.43	2.45e+11	5.02e+05
Clay	0.01	0.30	2.73e+12	9.07e+05

3.4 Boundary condition

During an instantaneous leak from a buried CO₂ pipeline, the CO₂ rapidly ejects as a

high-speed jet. Some researchers argue that when the leak size is much smaller than the pipeline's diameter, the pressure at the leak hole can be approximated as equal to the pipeline's operating pressure.^{38,39} However, this assumption neglects the actual fluid dynamics during transient processes, particularly under high-pressure conditions, making it unsuitable for such scenarios. In this study, the throttling effect of small hole leaks are accounted in the experiment. Based on the orifice flow state and discharge models, The temperature, pressure, and leak rate at the leak hole are calculated by treating these factors as boundary conditions at the orifice. Detailed settings for other boundary types are shown in Table 3.

Table 3. Type of the boundary conditions.

Boundary location	Boundary type	Parameter setting
Leakage hole	Pressure inlet	Gauge pressure, turbulence, phase, temperature.
Ground surface	Pressure outlet	Gauge pressure, species, temperature.
Surface of pipeline	wall	No-slip, roughness
Surrounding surface of soil domain	Symmetry	Keep the default
Bottom surface of soil domain	Wall	No slip, adiabatic boundaries with zero mass flow.

3.5 Simulation scenarios

This research employed the control variable method to examine the impact of the key soil parameters on the leakage and seepage diffusion characteristics in the buried CO₂ pipelines. As shown in Table 4, a comparative analysis was conducted across 5 simulation scenarios. Based on Case 1, the transient behavior during the leakage and seepage diffusion process of the buried CO₂ pipelines was further explored in detail.

Table 4. Basic parameters of work scenarios.

Case	Initial pressure MPa	Leakage size mm	Leakage direction	Soil type	Porosity	Permeability
Case 1	9	6	Upward	Loam	0.43	4.14d
Case 2	9	6	Upward	Sandy	0.25	46.91d
Case 3	9	6	Upward	Sandy	0.50	46.91d
Case 4	9	6	Upward	Loam	0.43	24.14d
Case 5	9	6	Upward	Clay	0.30	0.37d

Currently, the consequences of CO₂ leakage are primarily assessed by evaluating the concentration range of CO₂ in the leak environment. According to relevant standards, a CO₂ concentration of 5000 ppm is considered the safe exposure limit for an 8-hour work environment, while a concentration of 50,000 ppm poses a severe threat to life.⁴⁰ When a buried pipeline leaks, CO₂ diffuses through soil pores, eventually reaching the surface and entering the atmosphere. Therefore, this study defines the Warning Alert Time (WAT) as the time required for the surface CO₂ concentration to reach 50,000 ppm (corresponding to a mass fraction of 7.4%) after a leak. This time serves as a metric to evaluate the potential danger to personnel on the ground. Additionally, CO₂ leakage can lead to low-temperature hazards. During leakage, the rapid expansion of CO₂ causes a sharp temperature dropping in the surrounding environment, resulting in dry ice formation. The presence of dry ice reduces the toughness of the pipeline material, increasing the risk of brittle fracture. Consequently, the Pipeline Brittle Range (PBR) is defined as the area around the pipeline where the risk of brittle fracture increases due to the low-temperature effect. To further assess the impact of the low-temperature effect, multiple temperature monitoring points are established along the leakage direction to record the Temperature Detection Time (TDT) at each point. The TDT criterion is set as a 5 K drop in soil temperature, indicating that the low-temperature effect induced by the leakage has reached that monitoring point. This criterion includes a margin to exclude noise interference. The spatial positions of the monitoring points and lines are illustrated in Figure 4, with specific coordinates listed in Table 5. Monitoring Point P7 is designated to observe the WAT across various conditions. Monitoring Line A tracks the PBR range for each scenario, and Monitoring Points PT0-PT4 monitor the TDT under each condition.

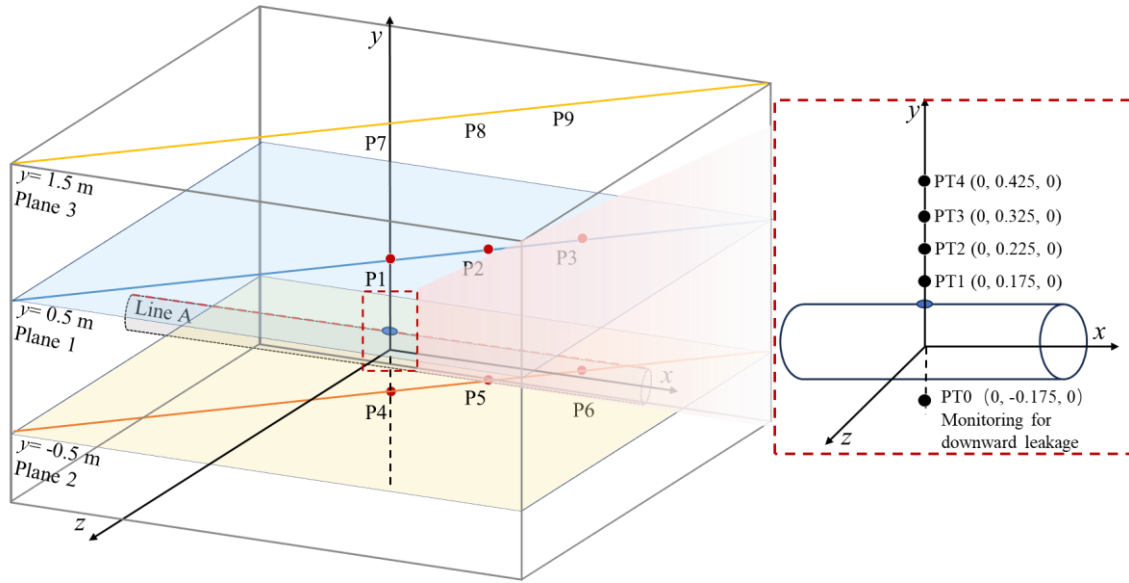


Figure 4. Spatial locations of monitoring points and lines.

Table 5. Location of monitoring points.

No.	Type	Location	No.	Type	Location
P1	Concentration	(0, 0.5, 0)	P8	Concentration	(0.5, 1.5, -0.5)
P2	Concentration	(0.5, 0.5, -0.5)	P9	Concentration	(1, 1.5, -1)
P3	Concentration	(1, 0.5, -1)	PT0	Temperature	(0, -0.175, 0)
P4	Concentration	(0, -0.5, 0)	PT1	Temperature	(0, 0.175, 0)
P5	Concentration	(0.5, -0.5, -0.5)	PT2	Temperature	(0, 0.225, 0)
P6	Concentration	(1, -0.5, -1)	PT3	Temperature	(0, 0.325, 0)
P7	Concentration	(0, 1.5, 0)	PT4	Temperature	(0, 0.425, 0)

4. Validation of the developed models

4.1 Validation of grid independence

This study employs Fluent meshing to create the meshes for the leakage domain, utilizing the Poly-Hexcore volume mesh generation method, which is based on the "mosaic" technology. This approach allows for co-node connectivity between hexahedral and polyhedral meshes without the need for interface surfaces, but combining the advantages of both mesh types more effectively. It not only provides the efficient computational capabilities but also handles complex boundaries more effectively.⁴¹ Figure 5 illustrates the computational domain and meshes formation.

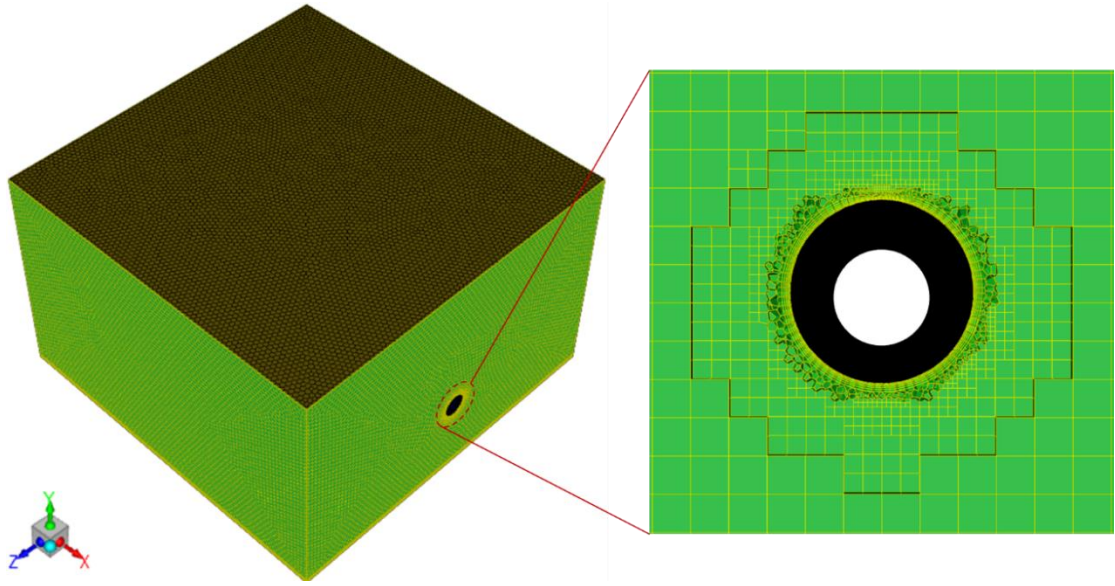


Figure 5. Computational domain and mesh for CO₂ dispersion from the buried pipelines with high pressure.

The quality of the mesh plays a critical role in determining computational speed and accuracy. To ensure that the results remain unaffected by the mesh quantity while maintaining computational efficiency. This study performed a mesh sensitivity analysis based on the Scenario 1 as shown in Table 4. Four mesh levels were tested with the Grid numbers of 640,253, 777,773, 801,781, and 921,256, respectively. The variations in CO₂ concentration over time were monitored at measurement points (P1, P4, P7) along the leakage hole axis. As shown in Figure 6, the calculated results of CO₂ concentration stabilizes when the grid number exceeds 777,773. To balance the computational accuracy and efficiency, the mesh scheme with 777,773 grids was selected for the subsequent numerical simulations.

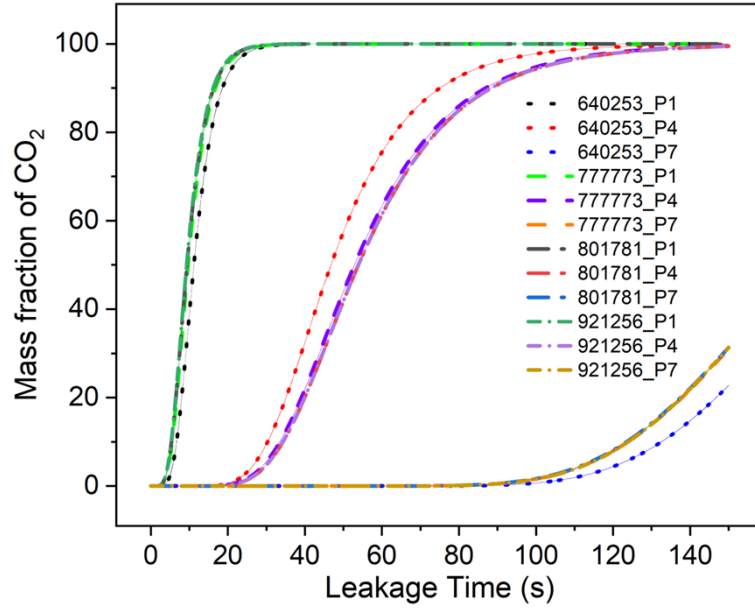


Figure 6. Grid independence verification of CO₂ concentration over time at measurement points P1, P4, and P7.

4.2 Validation of numerical model

The accuracy of the numerical model was validated against experimental results from leakage tests on a buried CO₂ pipeline conducted by Yu et al.²⁵ As shown in Table 5, the relevant experimental parameters were listed. The numerical model was constructed based on these conditions, including boundary conditions, soil type, and monitoring point locations.

Table 6. Parameters related to experimental conditions

Experimental parameters	Values	Experimental parameters	Values
Pipeline Diameter	100 mm	Leak size	3 mm
Pipeline Burial Depth	1.5 m	Leak direction	Horizontal
Operating pressure	8.8 MPa	Soil type	Sandy
Operating temperature	33.4 °C	Monitoring Type	Temperature

Figures 7a and 7b show the sandbox structure used to simulate the buried CO₂ pipeline leaks. The thermocouples distribution is shown in Figure 7c and 7d, with thermocouples 0-d, 0-e, and 0-f placed along the horizontal leakage jet axis at distances of 300 mm, 400 mm, and 500 mm from the leakage point. In experiment 5, the temporal variations in temperature at different monitoring points were presented in Figure 8. At monitoring

points 0-d, which is located closer to the leakage site, displayed the experimental data a relatively smooth downward trend, whereas the simulation results shown a more rapid temperature decrease. This discrepancy was likely attributed to the longer response time of the thermocouples. Notably, after the temperature had reached its lowest point, the simulation results gradually converged with the experimental data. In contrast, at monitoring point 0-f, which is positioned 1100 mm from the leakage site, the rapid cooling effect of the leaking gas was less noticeable, resulting in a higher degree of agreement between the simulation predictions and the experimental observations. Overall, the simulation demonstrated the strong performance in predicting the steady-state temperature distribution, despite deviations during the rapid cooling phase. Significantly, the average deviation between simulation and the experimental data remained below than 10%. Therefore, the proposed numerical and physical model in this study proved that this would be highly reliable and safe for analyzing the leakage and seepage diffusion characteristics of the buried CO₂ pipelines.

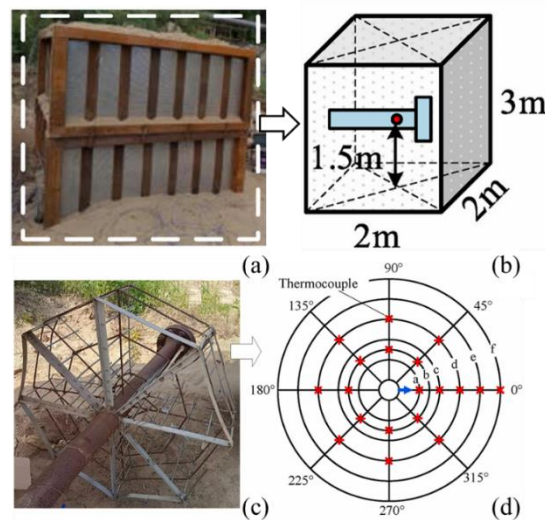


Figure 7. Leakage experiment scenario. (a) Photograph of sandbox. (b) Schematic diagram of sandbox. (c) Photograph of the steel bracket. (d) Schematic diagram of thermocouple distribution for horizontal. ²⁵ Reproduced with permission from Ref. ²⁵ Copyright 2024 ELSEVIER.

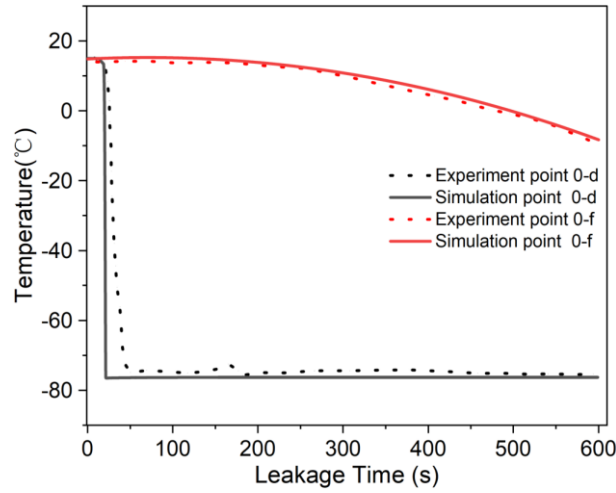


Figure 8. Experimental verification of the numerical model.

5. Results and discussions

In this section, the leakage and seepage diffusion characteristics of the buried CO₂ pipelines are scrutinized and discussed. The influence of the soil properties is discussed in detail from three perspectives: 1) soil porosity, 2) soil permeability, and 3) soil types.

5.1 Leakage and seepage diffusion characteristics

5.1.1 Pressure, velocity and streamline distributions

When a minor leak occurs in a buried CO₂ pipeline, high-pressure CO₂ rapidly escapes through the leak points and infiltrate the surrounding soil. This process creates a localized high-pressure zone near the leak hole (indicated in red), where the pressure gradually decreases outward, forming a typical concentric pressure gradient, as shown in Figure 9a. Over time, as the leak continues, the diffusion range of CO₂ in the soil expands, leading to a more uniform gas pressure distribution, while the overall pressure remains higher than the undisturbed soil. Due to the proximity to the atmosphere above the pipeline, CO₂ can escape through the soil, releasing pressure in that area. In contrast, the CO₂ accumulation persists due to the limited diffusion pathways below the pipeline, resulting in longer gas retention and a broader low-pressure zone, which is illustrated in Figure 9b.

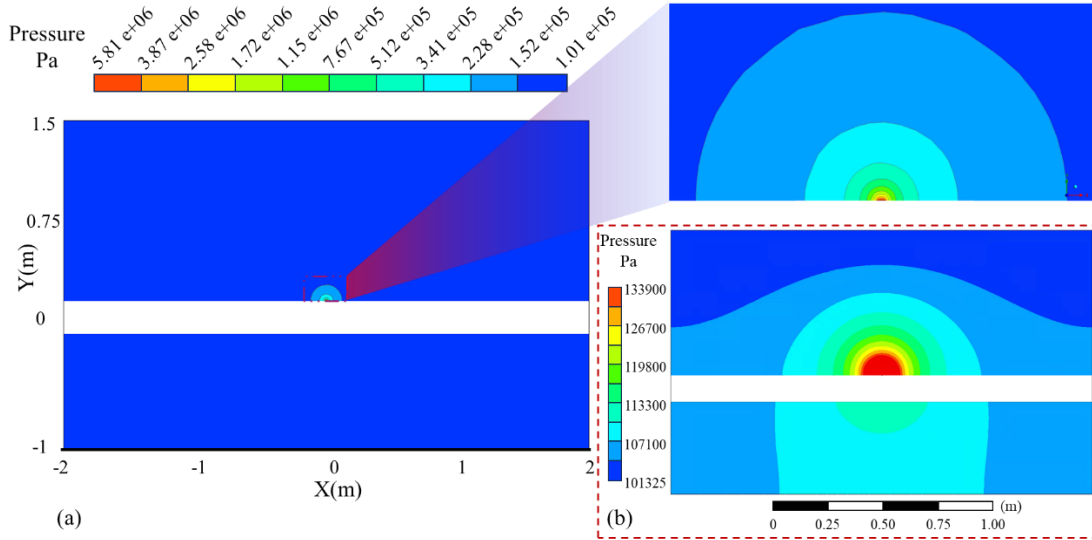


Figure 9. Pressure contour plot of the CO₂ leakage domain (a) Full Range (b) Low-Pressure Zone Detail.

Figure 10 illustrates the variation in velocity within the leak domain. Notably, the fluid velocity in this scenario differs from that observed in overhead pipeline leaks. In the case 1, the maximum velocity at the leak point reaches 33.4 m/s, whereas in overhead pipeline leaks, the velocities can attain supersonic levels.⁴² This discrepancy is primarily due to soil resistance. The slower diffusion rate of CO₂ in soil results in leaks from buried pipelines, which is being more discreet and harder to detect.³⁹ As the distance from the leak increases, the diffusion mechanism transitions to molecular diffusion driven by concentration gradients, significantly reducing the diffusion rate. For example, at 0.7 meters from the leak point, the velocity falls below 0.01 m/s.

Figure 10b illustrates the diffusion streamlines of CO₂ in the soil following a leak. Upon leakage, CO₂ diffuses in all directions within the soil. Influenced by the pipeline structure, some gas is deflected downward and creating a backflow that eventually rises to the surface due to the buoyant force in the soil.⁴³ The porosity and permeability of the soil significantly affect the migration path and diffusion rate of the gas.

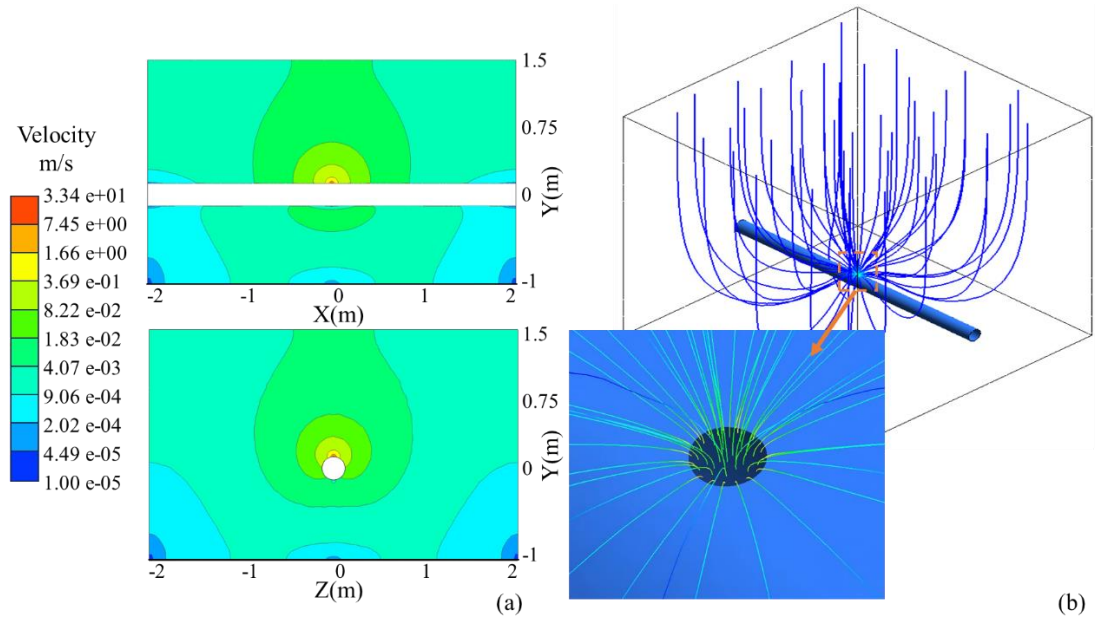


Figure 10. (a) Gas velocity contour plots around the leakage point in the soil. (b) The gas streamlines distribution in the soil.

5.1.2 Concentration distributions

Figure 11 illustrates the distribution of CO₂ concentration in the soil at different time intervals (50s, 200s, and 1000s). Assuming the soil is an isotropic porous medium, the concentration above the leak hole forms an approximately hemispherical shape. Within the first 50 seconds of the leak, the CO₂ diffuses rapidly and spreads outward. It is found that some of the CO₂ has already reached the surface by 150 second. As time progresses, the diffusion range continues to expand. As shown in Figure 12, the distribution of CO₂ concentration along the pipeline direction is notably symmetric and follows a Gaussian distribution.

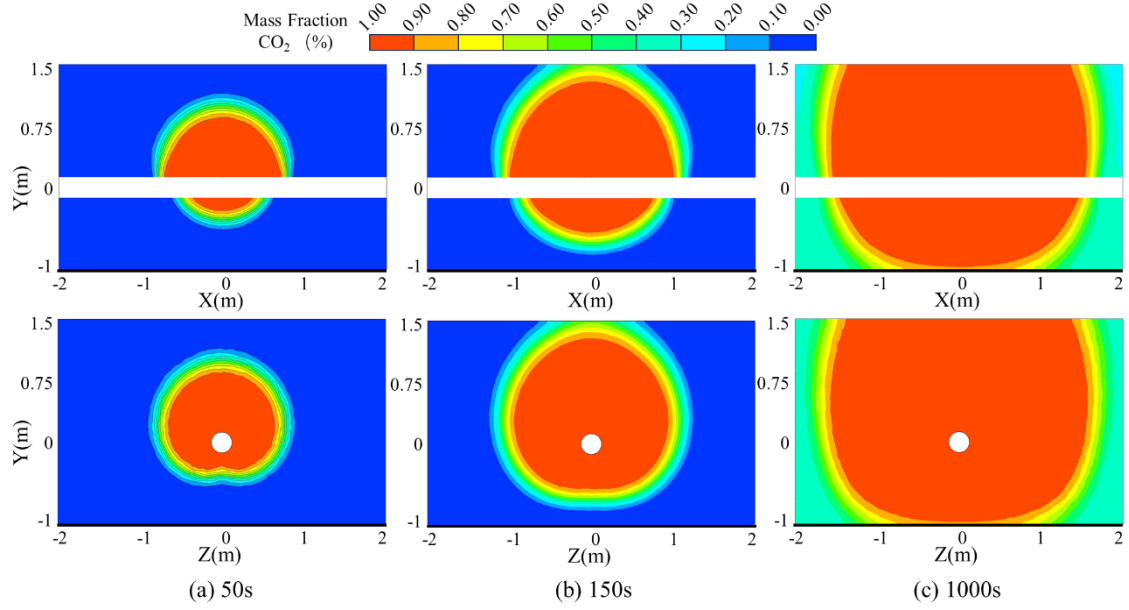


Figure 11. Contour plot of CO₂ concentration at different leak times. (a) 50s. (b) 150s. (c) 1000s.

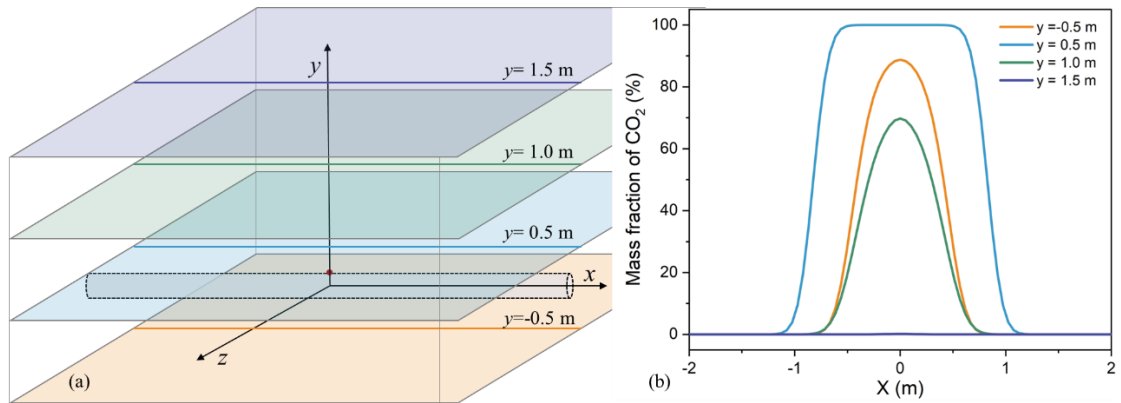


Figure 12. (a) Spatial locations of monitoring lines. The distribution of CO₂ concentration on different monitoring lines at 80s.

As shown in Figure 13, the monitoring points of the CO₂ concentration along the vertical axis of the leak hole (P1, P4, and P7) exhibit a faster growth rate compared to other points on the same plane. After 13 seconds of leakage, the mass fraction of the CO₂ at P1 approaches 100%. This rapid increase in concentration is attributed to the pipeline pressure, which drives gas diffusion around the leak. As the diffusion distance increases, the leak pressure gradually decays (see Figure 9) and this help to reducing the driving force of CO₂ seepage. Additionally, the soil resistance further slowdown the gas diffusion rate. Consequently, the concentration growth rate at P3 is significantly

lower than at P1 and P2, which are closer to the leak.

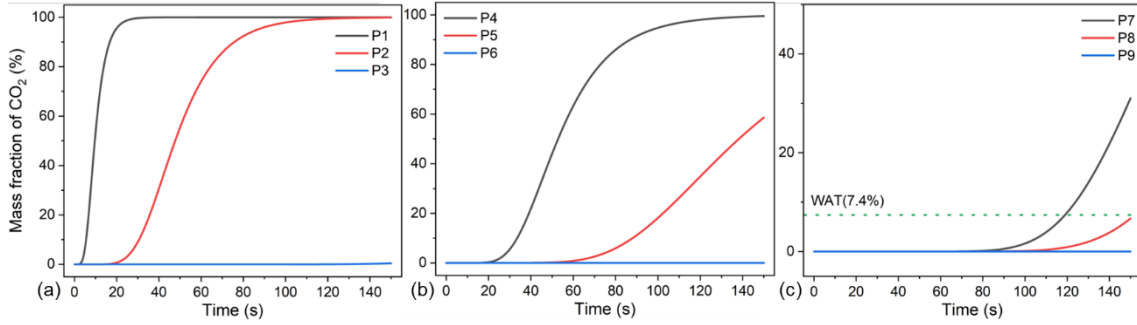


Figure 13. Variation of CO₂ mass fraction over time at different measurement points.

(a) Plane 1 (b) Plane 2 (c) Plane 3

5.1.3 Temperature distributions

Due to the unique physical and phase-change properties of the CO₂, the throttling cooling effect during its leakage is particularly pronounced. When CO₂ escapes through the leak hole, the sudden pressure drop causes rapid expansion of the gas, absorbing a significant amount of heat. Some of the gas undergoes phase change to dry ice and adheres to the pipeline walls. This results in a sharp drop in wall temperature, which transfers cold to the surrounding soil, forming permafrost. As leakage continues, the dry ice spheres grow larger, and the permafrost layer expands outward, encasing the dry ice. Figure 14 illustrates the temperature variation in the soil domain 150 seconds after the leak. The continuous leakage causes the low-temperature region to expand outward, creating a distinct temperature gradient within the soil.

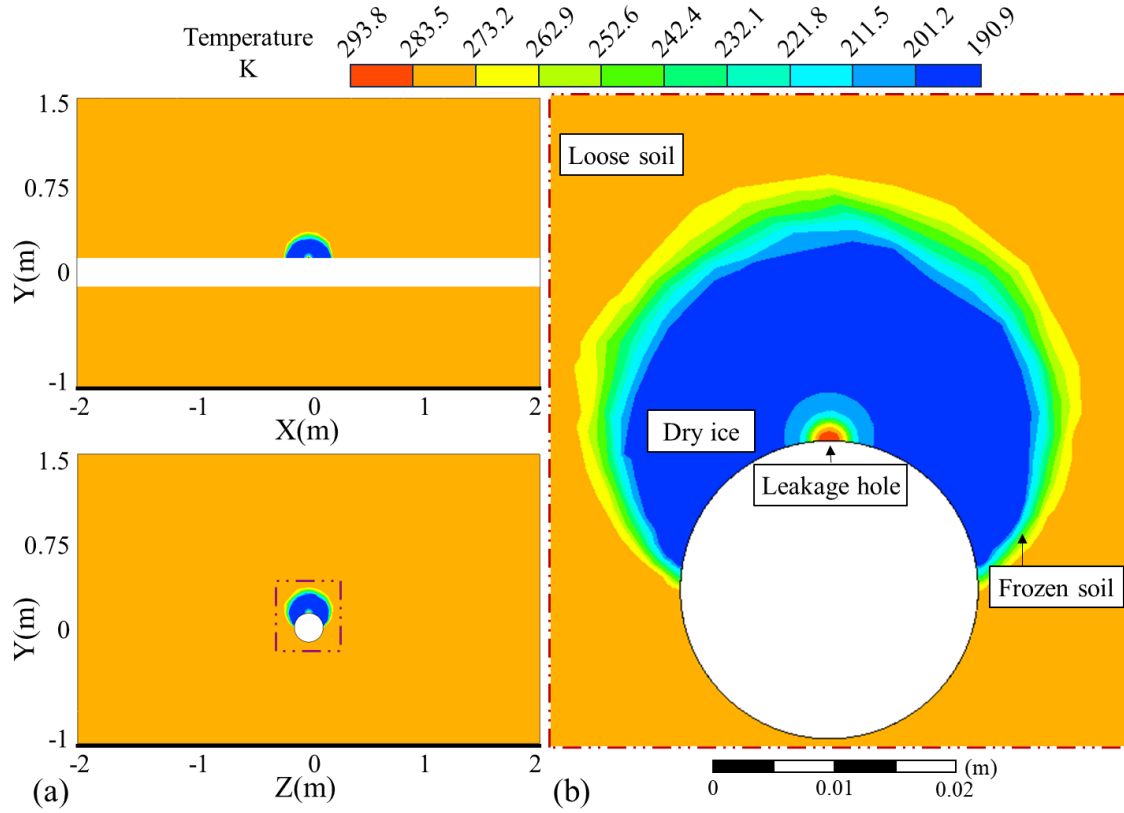


Figure 14. Temperature contour plot of the CO₂ leakage domain (a) Full Range (b) Low-Temperature Zone Detail.

According to safety requirements for oil and gas pipelines, the detection cable should be installed at least 300 mm from the pipe wall.^{44,45} In case 1, the TDT at point PT1, located 50 mm from the leak hole, is 1.25 seconds, while at point PT4, positioned 300 mm from the leak hole, it is 467 seconds (See Table 7). This indicates that as the distance from the leak increases, the rate of temperature decreases significantly. In compared to the WAT alarm time (98.71 seconds), temperature monitoring exhibits a delay, particularly in the areas farther from the leak, where the response time to temperature changes is longer. Therefore, relying solely on temperature detection for leak monitoring has limitations. To enhance the timeliness and accuracy of the leak detection, temperature monitoring should be combined with other methods, ensuring more effective risk control and emergency response.

Table 7. WAT and TDT response times under multiple scenarios. Unit: s

Alarm Time \ No.	Case 1	Case 2	Case 3	Case 4	Case 5
	Case 1	Case 2	Case 3	Case 4	Case 5
WAT	118.94	106.93	4.7	102.13	224.49
PT1_50 mm	1.25	1.07	1.00	0.63	3.17
PT2_100 mm	8.91	8.47	9.13	5.95	30.07
PT3_200 mm	97.94	86.39	71.23	62.20	236.55
PT4_300 mm	467.59	329.80	389.10	242.03	954.09

5.2 Effect of soil porosity

Porosity represents the volume of voids within the soil that can accommodate fluids. Initially, the gas fills the pores near the leak hole and then diffuses outward. As porosity increases, the gas diffusion rate gradually decreases, and the WAT increases. When the porosity is 0.25 (Case 2), the maximum flow rate at the leak hole reaches 80.23 m/s, whereas at a porosity of 0.5 (Case 3), the maximum flow rate drops to 42.74 m/s, as shown in Figure 15. Moreover, the diffusion rate is higher along the leak direction, whereas the diffusion rate contour lines display a “flame-like” distribution pattern. The combined effect of cooling and the increased storage capacity expands the low-temperature region, thus enabling the monitoring points PT1-PT4 to detect temperature changes more quickly (see Table 7).

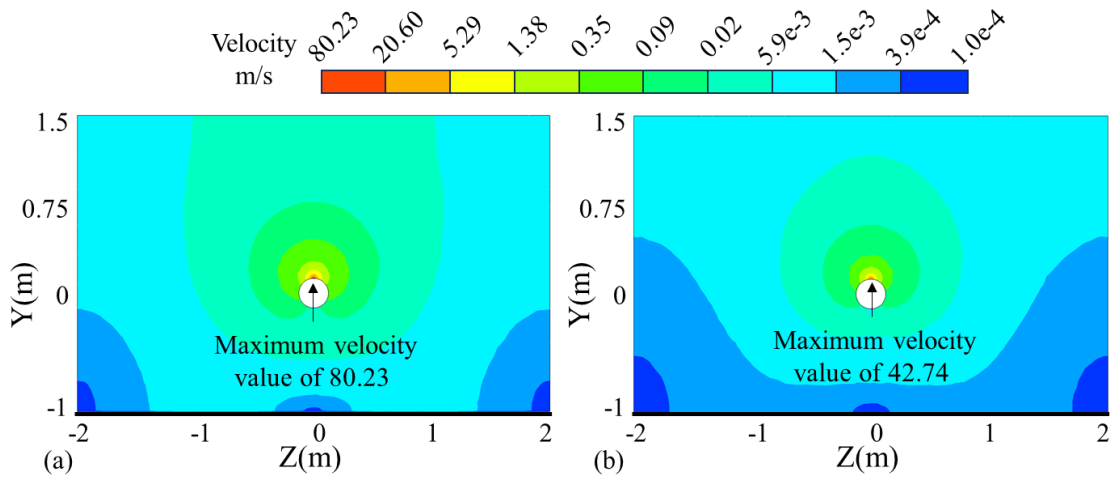


Figure 15. Velocity contour plots in the soil. (a) Sandy soil with a porosity of 0.25. (b) Sandy soil with a porosity of 0.5.

The expansion of fluid storage capacity, combined with the cooling effect of the CO₂,

significantly expands the coverage of low-temperature regions. As illustrated in Figure 16, increasing soil porosity allows temperature monitoring points PT1 to PT4 to detect temperature changes more rapidly. Meanwhile, the PBR expands significantly within the same time.

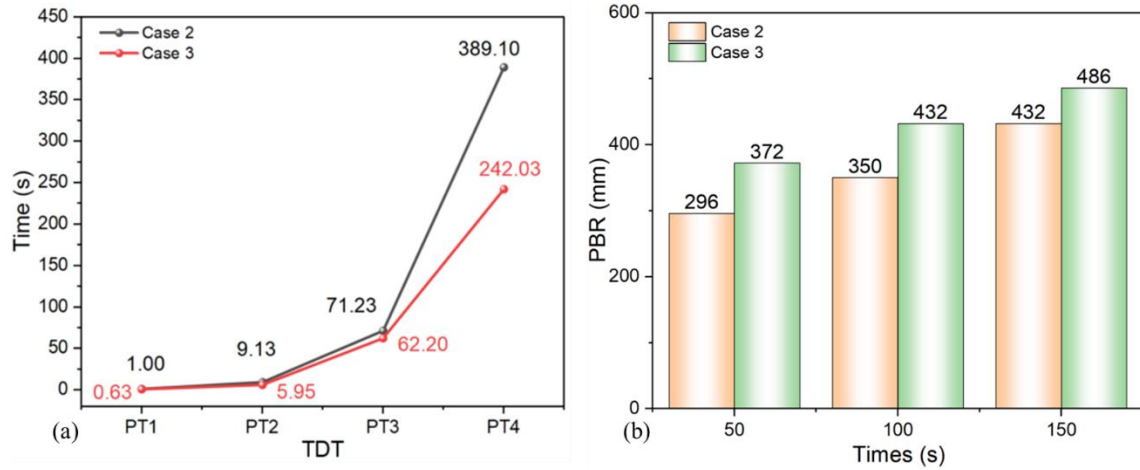


Figure 16. Seepage diffusion characteristics of different soil porosity. In Case 2, porosity is 0.25. In Case 3, porosity is 0.5. (a) TDT. (b) PBR.

5.3 Effect of soil permeability

Soil permeability reflects how easily CO₂ seeps through the soil. According to Darcy's law, the permeability of loam in case 1 is 4.1 d, while in Case 4, it is 24.1 d. The results (see Table 7) show that the WAT response time for case 1 is 118.94 seconds, whereas for Case 4, it is 102.13 seconds. This suggests that the higher permeability enables CO₂ to reach the surface more quickly, thus significantly reducing the WAT and increasing potential risks to the surface personnel.

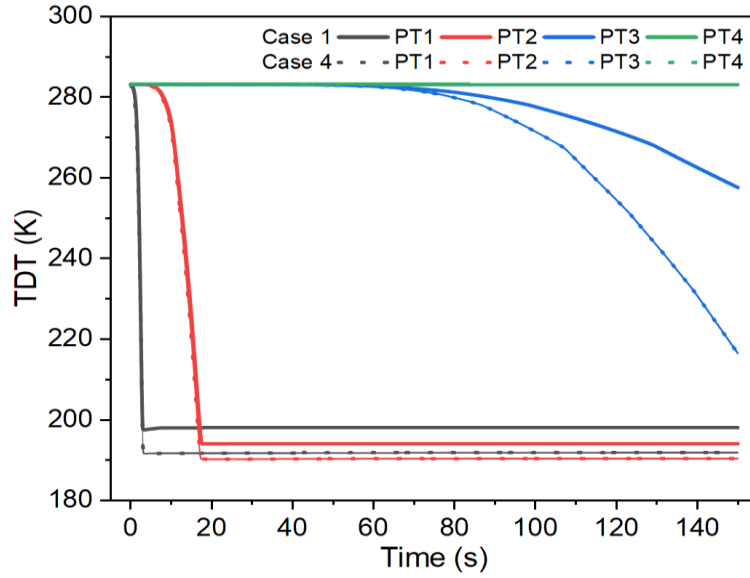


Figure 17. Temperature variation over time at each point in Case 1 and Case 4.

The increase in permeability also intensifies the cooling effect. As the gas seeps more rapidly through the soil, it removes more heat. In Case 8, the TDT at various monitoring points is shorter than in Case 1 (see Table 7). Additionally, the minimum temperatures recorded at each monitoring point in Case 4 are lower than those in Case 1, as shown in Figure 17. This demonstrates that under high-permeability conditions, the cooling effect is more pronounced, posing a greater threat to the safety of buried pipelines.

5.4 Effect of soil type

After clarifying the impact of key soil properties (porosity and permeability) on the seepage diffusion, this study comprehensively compares the effects of three typical soil types: loam, sandy soil, and clay. As shown in Figure 18a, the mass flow rate is the highest under sandy conditions, followed by loam, but the lowest flow rate under clay. In sandy soil, the mass flow rate is 2.6 times that of the clay. This is due to the smaller particle size and lower permeability of the clay, which significantly restrict the diffusion rate of CO₂. This result is also supported by the time characteristics of seepage diffusion under different soil environments. In clay, the WAT is 224.49 seconds, and the TDT at PT4 is 954.09 seconds; whereas in sandy soil, the WAT is reduced to 102.13 seconds, and the TDT at PT4 is 242.03 seconds. Figure 17b illustrates the PBR under different soil types. Due to the higher permeability and lower viscosity of the sandy soil, the CO₂

diffuses the fastest rate in sandy. As a result, under the same conditions, the PBR in the sandy soil is larger than in the loam and clay (Figure 18b).

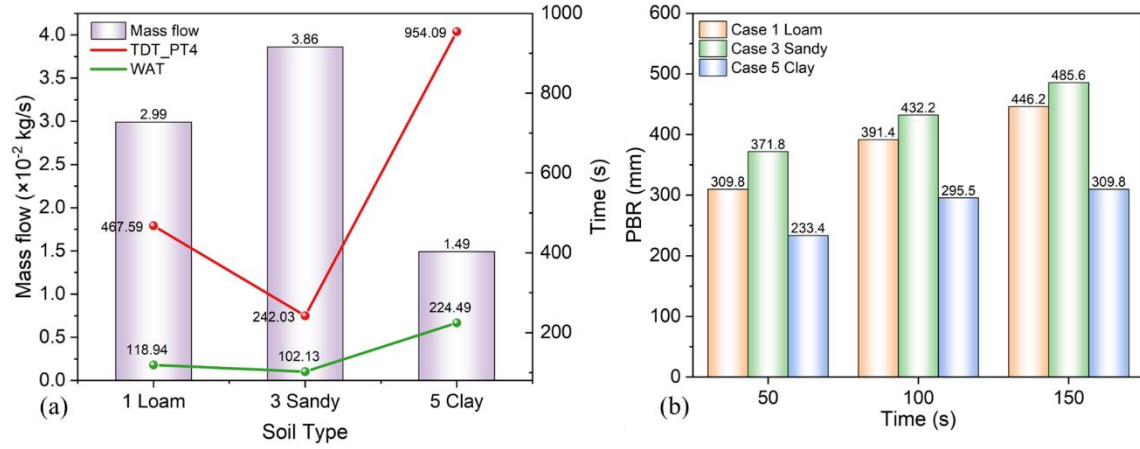


Figure 18. Seepage diffusion characteristics in different soil types (a) Mass flow rate, TDT, and WAT (b) PBR.

6. Conclusions

This study presents a transient model for the small hole leakage in the buried CO₂ pipelines by integrating the thermal, fluid and solid multi-physical fields. The leakage and seepage diffusion behavior are systematically analyzed, with particular attention to the influence of the soil properties, including porosity, permeability, and types, during the seepage diffusion. The key findings of this research are summarized as follows:

1. The leaked CO₂ initially exhibits a very high instantaneous flow velocity due to the high operating pressure of the pipeline, However, once it escapes at the leakage point, the gas velocity decreases sharply due to the soil resistance, creating by a pronounced velocity gradient around the site of leakage. Under the influence of the pipe wall, a portion of the CO₂ deflects downward and generates backflow, while the remaining gas diffuses upward and toward the surface, driven by buoyancy forces.
2. The CO₂ diffuses outward from the leakage points with the diffusion velocity being significantly higher in the leakage direction compared to other directions. It is found that the velocity contours deliver a distinct "flame-shaped" pattern. The CO₂ concentration distribution exhibits notably symmetric and horizontally, while along the

pipeline direction, the concentration follows a Gaussian distribution. Over time, the diffusion radius expands gradually, although the diffusion rate decreases progressively. Within a 1-meter radius of the leakage point, the diffusion velocity declines sharply from 10 m/s to less than 0.01 m/s.

3. The low thermal conductivity of soil results in relatively slow heat transfer. At a monitoring point, which is 300 mm from the leakage site, it is found that the TDT is 467 seconds, whereas the WAT is 118.94 seconds. This discrepancy indicates a lag in temperature-based leak detection. Therefore, integrating temperature monitoring technology with other detection methods in pipeline safety management can improve response speed and accuracy in the leak detection, thereby enhancing overall pipeline operational safety.

4. As soil porosity increases, the diffusion rate of the CO₂ decreases, leading to an extended WAT response. Furthermore, the higher porosity allows the soil to retain greater amounts of low-temperature CO₂, thereby expanding the low-temperature region and enabling temperature sensors to detect leaks more rapidly. These findings highlight that soil porosity influences do not impact only the diffusion dynamics of CO₂ but also the timeliness and effectiveness of the leak detection.

5. High soil permeability allows CO₂ to reach the soil surface more rapidly, significantly reducing the WAT and increasing the safety risks for personnel on the surface. Additionally, the elevated permeability amplifies the cooling effect, thus intensifying low-temperature hazards and posing greater threats to the structural integrity and operational safety of the buried CO₂ pipelines.

6. Soil type plays a critical role in determining the hazardous boundaries of the leakage and seepage diffusion in the buried CO₂ pipelines. The simulation results indicate that transitioning from the sandy soil to clay results in a 2.6-fold decrease in CO₂ mass flow rate, a 2.2-fold increase in the WAT, and a nearly fourfold increase in the TDT. These findings suggest that the clay soil significantly reduces the effectiveness of the leak detection, making it more challenging to identify and respond to the CO₂ leaks. Finally, it concludes that this study has developed a more precise mathematical and physical model that helps for predicting the hazardous radius while defusing CO₂ and offering

a scientific guidance for the risk assessment and emergency response planning in the buried CO₂ pipeline.

7. Future research study

Future research will focus on the multi-condition simulations that will incorporate a wider range of different types of variables, such as pipeline transport conditions, leak size, leak type, and soil temperature. This will further be expanded and diversified in the simulation dataset.

Acknowledgements

This work was supported by Xinjiang Uygur Region "One Case, One Policy" Strategic Talent Introduction Project (No. XQZX20240054), Autonomous Region Tianshan Innovation Team for Research and Application of High-Efficiency Oil and Gas Pipeline Technology (No. 2022TSYCTD0002) and Innovation Environment Building Program (Innovative Talents) Project of Karamay (No. 20232023hjcxrc0004).

CRedit authorship contribution statement

Yan Shang: Conceptualization, Methodology, Writing – original draft, Formal analysis.

Xiaokai Xing: Supervision, Funding acquisition. Xiaoling Chen: Writing - Review & Editing, Funding acquisition. Ming Yang: Software, Data curation, Validation.

Raj Shah: Comprehensive Review of the full paper

Xinyu Pang:

Declaration of competing interest

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.

Nomenclature

Nomenclature		γ	Adiabatic index
A	Leakage area, m ²	ε	Turbulence rate of dissipation
C_2	Inertial resistance coefficient	κ	Isentropic exponent
C_d	Vena contracta coefficient	μ	Viscosity, kg/m s
E	Total energy, J	ρ	density, kg/m ³
g	Gravitational acceleration, 9.81 m/s ²	σ	Turbulent Prandtl number
H	Enthalpy, J/kg	Γ	Effective diffusivity, m ² /s
k	turbulence kinetic energy	φ	Porosity of the soil
M	molar fraction of the gas	Subscript	
P	Pressure, MPa	0	Stagnation/initial state
Q	Mass flow rate, kg/s	1	Fluid state at the leakage point
R	Universal gas constant, 8.134 J/kg K	2	Fluid state outside the pipe
S	Entropy, J/K	c	Critical value
S_i	Momentum source term of soil	e	Ambient value
S_f^h	Heat source associated with the energy	f	fluid
T	Temperature, K	k	Specific phase
u	Flow velocity, m/s	j	Specific species within the vapor phase
u_a	Speed of sound, m/s	l	Liquid phase
V	Specific volume, m ³ /kg	m	Properties of the mixture
Y	local mass fraction	sat	Saturated state
Greek letters		s	Soil medium
$1/\alpha$	Viscous resistance coefficient	v	Vapor phase

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