

DISSERTATION

NUMERICAL AND EXPERIMENTAL STUDIES OF MULTIPHASE, MULTICOMPONENT
TRANSPORT FOR SUBSURFACE GAS MIGRATION AND REMOVAL IN THE VADOSE
ZONE USING SOIL AERATION

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ABSTRACT

NUMERICAL AND EXPERIMENTAL STUDIES OF MULTIPHASE, MULTICOMPONENT TRANSPORT FOR SUBSURFACE GAS MIGRATION AND REMOVAL IN THE VADOSE ZONE USING SOIL AERATION

Subsurface methane (CH_4) released from natural gas (NG) pipeline leaks can migrate through the vadose zone, accumulate in confined subsurface infrastructure, and pose flammability hazards. Isolating or repairing a leak source does not necessarily eliminate the subsurface hazard immediately. Residual CH_4 can remain stored in the vadose zone, continue to migrate, and, in some cases, rebound after active mitigation stops. This creates a practical need for post-repair remediation of accumulated subsurface CH_4 . However, predicting plume evolution and mitigation of residual subsurface CH_4 after leak isolation or repair requires a mechanistic understanding of coupled multiphase (gas and water) flow and multicomponent transport in variably saturated porous media under both variable atmospheric conditions and induced pressure gradients. Despite decades of vadose-zone research, predicting gas transport in variably saturated porous media remains limited by two unresolved challenges. First, transient leak behavior remains difficult to infer reliably from sparse near-surface CH_4 observations because the measured signals are influenced by transport in the vadose zone and the changes in soil and atmospheric conditions. Second, predictive understanding of soil aeration for remediation remains limited because the coupled effects of soil properties and design parameters on induced airflow pathways and diffusion-limited mass transfer during soil aeration are not quantitatively resolved.

Therefore, this dissertation integrated field-scale experiments with numerical modeling to advance understanding of subsurface gas (i.e., CH₄) migration and removal under both natural and induced pressure gradients and translate that understanding into a validated, field-relevant decision-making tool. The first contribution is to demonstrate that estimating transient subsurface gas migration and leak behavior requires integrating near-surface observations with subsurface transport properties. Controlled experiments demonstrate that belowground near-surface (BNS) measurements respond earlier and persist longer than surface measurements. Within a 4 m monitoring radius, BNS CH₄ concentrations are on average 20 to 486% higher than surface concentrations. Incorporating these observations into an inverse gas-migration model enables estimation of transient leak behavior with strong agreement with measurements (slope $m = 0.99$; $R^2 = 0.77$). These results support that transient source characterization benefits from a monitoring strategy aligned with vadose-zone transport physics rather than from short-duration surface observations alone.

The second contribution is to use a modified multiphase multicomponent transport model to investigate the dominant mechanisms governing subsurface gas removal and to quantify how soil properties, water saturation, vacuum pressure, and bar-hole configuration interact to control removal performance. Integrating six controlled field-scale soil-aeration experiments with a transport model and 108 scenario simulations shows that subsurface gas removal follows a two-stage process. This process first includes rapid depletion dominated by advection during aeration, followed by diffusion-limited release from weakly aerated regions and less-connected pore space. Moderate vacuum pressure strengthens advective capture and accelerates cleanup, whereas increasing vacuum beyond this range can reduce efficiency by enhancing preferential airflow bypass and competition for removal. Low-permeability conditions are more effectively addressed

by increasing bar-hole density and improving plume alignment than by increasing vacuum alone. Across tested conditions, optimized bar-hole number and layout achieve 80 to 98% subsurface CH₄ removal, while improper spacing reduces removal efficiency by 20 to 30%. Overall, these results provide a mechanistic basis for predicting subsurface CH₄ removal under the tested soil, moisture, and operating conditions, enabling the selection of bar-hole layouts and vacuum levels that maximize capture while minimizing bypass and diffusion-limited persistence.

The third contribution is a reduced-order, physics-based decision-making framework that predicts subsurface CH₄ removal efficiency and aeration duration from measurable site conditions (soil type, moisture, and plume geometry) and controllable design parameters (vacuum level, aeration duration, and bar-hole layout). The framework shows good agreement with controlled experiments ($R^2 = 0.74$) and enables rapid screening of configurations that improve capture and reduce bypass under site-specific constraints. Therefore, this dissertation advances understanding of subsurface gas transport in the vadose zone and provides a field-validated pathway from detection and transient source estimation to mechanistically informed CH₄ mitigation design.

Overall, this dissertation provides a foundation for a more practical approach to subsurface gas-leak response by integrating near-real-time detection, leak behavior quantification, and subsurface CH₄ removal. The broader implication is that subsurface explosion hazards associated with CH₄ accumulation in the vadose zone can be more effectively evaluated and mitigated when monitoring data, transport physics, and mitigation design are integrated within a unified framework. Future research should extend and evaluate this framework under more complex site conditions, including layered and heterogeneous soils, surface sealing and subsurface infrastructure, and variable atmospheric conditions, while incorporating uncertainty quantification and real-time decision support. These next steps would not only improve scientific understanding

of subsurface gas transport and removal but also optimize the design and operation of field subsurface gas-leak response strategies.

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Chapter 1. Introduction

1.1 Background and Motivation

Natural gas (NG) is a major component of energy systems, supporting residential, commercial, and industrial energy demand. In the United States, NG is delivered through an extensive buried pipeline system. Pipeline and Hazardous Materials Safety Administration (PHMSA) annual report data for 2025 indicate 2,395,772 miles of gas distribution mains and estimated service lines, 300,017 miles of natural gas transmission pipelines, and 113,005 miles of gathering pipelines (Pipeline and Hazardous Materials Safety Administration, 2025). Despite advances in pipeline integrity management, underground NG leaks still occur due to corrosion, aging infrastructure, material defects, excavation damage, and operational errors (Murvay & Silea, 2012). Pipeline and Hazardous Materials Safety Administration (2023) reported that, between 2003 and 2022, excavation damage was the leading cause of serious gas distribution incidents (28%), followed by other outside force damage (23%) and incorrect operation (14%). Its current performance measures continue to identify excavation damage as a leading cause of life-threatening gas pipeline incidents, indicating that these risks remain relevant in 2025.

Leaks from low-pressure distribution systems are of particular concern because they can persist undetected for extended periods and allow methane (CH_4), the primary component of NG, to migrate through the vadose zone and accumulate in confined or partially confined structures such as basements, crawlspaces, utility vaults, and other subsurface utilities. Weller et al. (2020) estimated approximately 659,000 leaks in the U.S. local distribution system, with an average of about 0.51 leaks per main mile. These leaks lead to methane (CH_4) emissions of about $0.69 \text{ Tg CH}_4 \text{ yr}^{-1}$. The widespread occurrence of these leaks across diverse subsurface conditions indicates

the need for an understanding of subsurface CH₄ transport behavior and effective remediation across variable site conditions.

Accumulation of CH₄ can elevate concentrations to explosive levels, approximately 5 to 15 percent by volume in air, increasing explosion risk and enabling vapor intrusion driven by pressure gradients between the subsurface and indoor environments (Truex et al., 2013; U.S. Environmental Protection Agency, 2018). Based on PHMSA gas pipeline incident-report data for reporting years 2002–2024, NG pipeline incidents resulted in 1,139 injuries in the United States, with most injuries occurring in distribution systems (974) compared to transmission systems, including gathering (165) (Pipeline and Hazardous Materials Safety Administration, 2026). Although these totals are not limited to subsurface leak scenarios, they indicate that distribution pipeline failures remain a critical safety concern. Subsurface NG migration can therefore threaten building occupants, utility workers, and emergency responders when CH₄ accumulates in confined or poorly ventilated spaces before the hazard is recognized.

In addition to explosion risk, subsurface CH₄ migration also raises public-health exposure concerns because hazardous atmospheres may develop in enclosed or poorly ventilated spaces before elevated concentrations are recognized. This is particularly relevant for residents occupying overlying buildings, utility workers entering vaults, manholes, or other confined subsurface spaces, and emergency responders tasked with assessing whether an atmosphere is hazardous during leak response (GPTC, 2023; Pipeline and Hazardous Materials Safety Administration, 2020). Therefore, subsurface CH₄ migration can create hazards beyond explosion risk at near-LEL concentrations, including CH₄ accumulation in enclosed or poorly ventilated spaces that may not be detected immediately during occupancy or emergency response.

Elevated CH₄ in the vadose zone is also a climate concern because subsurface CH₄ can ultimately be emitted to the atmosphere, contributing to greenhouse gas emissions, if not effectively removed (Cho et al., 2020; U.S. Environmental Protection Agency, 2025, 2026). Therefore, subsurface NG leak response should not be limited to leak identification but requires integrated detection and monitoring to support appropriate grading and quantification of subsurface gas leak behavior. In practice, operators grade leaks to determine risk to public safety and the environment and to prioritize repair actions (GPTC, 2023; Pipeline and Hazardous Materials Safety Administration, 2023). However, the grading and quantification depend on measurements collected under complicated environmental conditions, strongly impacting the gas migration from subsurface to atmosphere (Cho et al., 2020; Jayarathne, Kolodziej, et al., 2022a; Lo et al., 2024; Riddick et al., 2021; Smith et al., 2003; Ulrich et al., 2019; van de Griend & Owe, 1994). These factors motivate mechanistic and quantitative frameworks that remain defensible under variable field conditions and that can support the detection and quantification in the field.

Leak repair or source isolation does not necessarily mean that the subsurface hazard has been eliminated. After leak identification and repair, the residual CH₄ in the vadose zone can still slowly migrate to the confined subsurface spaces (e.g., basement), gradually increasing CH₄ concentration in confined spaces and leading to explosions (Cho et al., 2020; Jayarathne et al., 2024; Pipeline and Hazardous Materials Safety Administration, 2017). If post-repair monitoring does not adequately capture this residual subsurface gas, a site may appear repaired while hazardous gas remains stored belowground. Therefore, active subsurface CH₄ removal may be required to reduce subsurface CH₄ concentrations below safety thresholds and limit the potential for continued accumulation in confined subsurface regions. When post-repair monitoring indicates that residual subsurface gas remains or that hazardous concentrations may persist near structures or other

confined subsurface pathways, active venting or NG soil aeration may be used to remove gas from the vadose zone and reduce subsurface CH₄ concentrations (Jayarathne et al., 2024; National Transportation Safety Board, 2025, 2026; Pipeline and Hazardous Materials Safety Administration, 2017; U.S. Environmental Protection Agency, 2018). NG soil aeration is typically implemented by drilling boreholes, commonly referred to as bar holes, near confirmed or suspected leak locations. The airflow is then induced to migrate from the surrounding vadose zone toward these bar holes through passive venting or active vacuum assisted aeration. Aeration is generally performed iteratively, with additional bar holes installed and operations repeated until an approved clearance criterion is met, such as 0.1% LEL or 50 ppmv (Jayarathne et al., 2024), with follow-up monitoring after shutdown to evaluate rebound.

In field practice, soil aeration is commonly conducted intermittently from hours to several days. However, the removal performance of NG soil aeration is highly variable across sites and over time because gas removal depends strongly on site-specific transport controls, including intrinsic permeability, heterogeneity, and water content (Minnesota Pollution Control Agency, 2025; Sarabia, 2019; Spectrum News, 2019). This challenge motivates the need for mechanistic understanding and quantitative guidance that link subsurface CH₄ transport behavior to aeration design and operation. However, existing practice and much of the published literature provide limited mechanistic and field-validated guidance for predicting aeration performance across variable site conditions, highlighting the need for a unified framework that integrates controlled field operation with physics-based modeling to support decision-making.

This problem is not limited to detection or mitigation alone. Subsurface NG leak response remains constrained by uncertainty in detecting and quantifying transient belowground gas behavior and by the lack of field guidance for post-repair mitigation. Because site conditions

strongly influence gas migration, residual hazard persistence, and soil aeration performance, effective response requires more than isolated measurements or decisions based on experience. A field-relevant framework is needed to connect subsurface monitoring, transient leak quantification, and post-repair gas removal, enabling belowground hazards to be evaluated and mitigated more defensibly under variable site conditions.

1.2 Literature Review

1.2.1 Multiphase and Multicomponent Transport in the Vadose Zone

Multiphase (gas and water) transport in the vadose zone occurs in variably saturated soils where air and water occupy the pore space simultaneously. The system is commonly characterized by porosity ϕ , water (S_w) and gas (S_g) saturations ($S_w + S_g = 1$), and phase pressures P_w and P_g , which represent the pore-water pressure and pore-gas pressure. Their difference defines capillary pressure. Phase coupling is described by capillary pressure ($P_c = P_g - P_w$) and the soil water characteristic curve. Saturation-dependent relative permeabilities then define how changes in S_w modify air and water mobility (Brooks & Corey, 1964; Mualem, 1986; van Genuchten, 1980). These relationships explain why variations of water saturation strongly alter air-phase connectivity and transport pathways in the vadose zone.

Previous studies and technical guidance for soil vapor extraction (SVE) and soil venting commonly describe pressure-driven gas flow in the vadose zone using Darcy's law (Bear, 1972; Johnson et al., 1990; Stewart, 2022; U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1991, 2018). In SVE, vacuum extraction creates a negative pressure gradient that induces vapor movement through the air-filled pore space toward extraction wells. Therefore, vapor flow is controlled by soil properties, such as porosity and air permeability, gas properties

including viscosity and density, and the applied pressure gradient (Johnson et al., 1990; Suthersan et al., 1999; U.S. Environmental Protection Agency, 1991). Johnson et al. (1990) used Darcy's law and continuity equation to estimate the radial vapor flow toward an extraction well by assuming laminar, steady-state vapor flow, isothermal conditions, negligible gravitational effects, and no significant changes in porous medium structure due to the change in pressure. Therefore, Darcy's law provides a practical framework for describing field-scale gas migration toward extraction wells in the vadose zone.

Pressure gradients drive water and gas flow through the pore space in the vadose zone. Darcy's law is used to describe water and gas flow:

$$\mathbf{u}_i = -\frac{k k_{ri}}{\mu_i} (\nabla P_i - \rho_i \mathbf{g}) \quad (\text{Eq. 1. 1})$$

where $\mathbf{u}_i$ [LT^{-1}] is the Darcy velocity of phase i , k [L^2] is intrinsic permeability, k_{ri} [-] is the relative permeability of phase i , μ_i [$ML^{-1}T^{-1}$] is the dynamic viscosity of phase i , ρ_i [ML^{-3}] is the density of phase i , P_i [$ML^{-1}T^{-2}$] is the pressure of phase i , and $\mathbf{g}$ [LT^{-2}] is gravitational acceleration. The key feature is that k_{rg} decreases as S_w increases, which decreases air-filled porosity and suppress pressure-driven gas flow under wet conditions.

The gas phase in this study includes CH_4 and air. The CH_4 transport in the vadose zone is described by advection and diffusion in the gas-filled pore network:

$$\frac{\partial(\phi S_g C_{CH_4,g})}{\partial t} + \nabla \cdot (\mathbf{u}_g C_{CH_4,g}) - \nabla \cdot (\phi S_g D_{\text{eff}} \nabla C_{CH_4,g}) - q_{CH_4} = 0 \quad (\text{Eq. 1. 2})$$

where ϕ [-] is porosity, S_g [-] is the gas saturation, $C_{CH_4,g}$ [ML^{-3}] is the gas-phase CH_4 concentration, D_{eff} [L^2T^{-1}] is the effective diffusion coefficient in porous media, and q_{CH_4} [$ML^{-3}T^{-1}$] represents sources or sinks.

Diffusion in porous media is strongly impacted by air-filled porosity and tortuosity. The model is a first-order estimation of the effective diffusion coefficient, which relates gas diffusion to air-filled porosity (Davarzani et al., 2014; Gao et al., 2021; Moldrup et al., 2000). The effective diffusion coefficient in this dissertation can be estimated using Millington and Quirk's (1961) model:

$$D_{eff} = D_0 \frac{(\phi S_g)^{10/3}}{\phi^2} \quad (\text{Eq. 1. 3})$$

where $D_0 [L^2 T^{-1}]$ is the diffusivity in free air (Millington, 1959; Moldrup et al., 2000).

The relative importance of advection and diffusion depends on permeability structure, saturation, and boundary conditions (Fig. 1. 1). Under an induced pressure gradient, advective airflow preferentially follows connected, higher-permeability pathways in sand, which is used to represent coarse-grained soil condition. In contrast, CH_4 stored in silt loam, which is used to represent lower-permeability fine-grained soil condition, or in wetter regions with limited air connectivity, is released into the pore network increasingly by diffusion.

Fig. 1. 1 illustrates gas transport in a layered vadose zone using conceptual sand and silt loam cases to represent higher- and lower-permeability conditions. In this dissertation, the silt loam is used as a representative lower-permeability soil to study restricted airflow behavior during soil aeration. Although sorption of gas-phase contaminants may occur in the fine-grained mineral soils (Ertefai et al., 2010; J. Li et al., 2016; Wang et al., 2020; Ziemiański et al., 2020), previous SVE studies suggest that the effect of sorption on removal is more commonly associated with long-term remediation behavior, such as late-time tailing and rebound during SVE (Carroll et al., 2012; Kaleris, 2002; U.S. Army Corps of Engineers, 2002; Yoon et al., 2008). Therefore, relative to the shorter aeration duration considered in this dissertation, CH_4 sorption capacity is not treated in this dissertation as a first-order control on subsurface CH_4 removal. Furthermore, non-Darcy or

nonlinear gas flow behavior may also occur in the clay-rich soils (H. H. Liu & Birkholzer, 2012; V. Nguyen et al., 2021; Schjønning et al., 2013; Teng et al., 2024). However, these mechanisms are not explicitly represented in the present transport model. The silt loam is used to study restricted airflow behavior under the assumptions of the present model, rather than as a general clay-rich soil behavior. Under these conditions, subsurface CH_4 behavior in this dissertation is expected to be governed primarily by gas-phase advection, restricted air-phase connectivity, and diffusion-limited release from regions with limited gas connectivity.

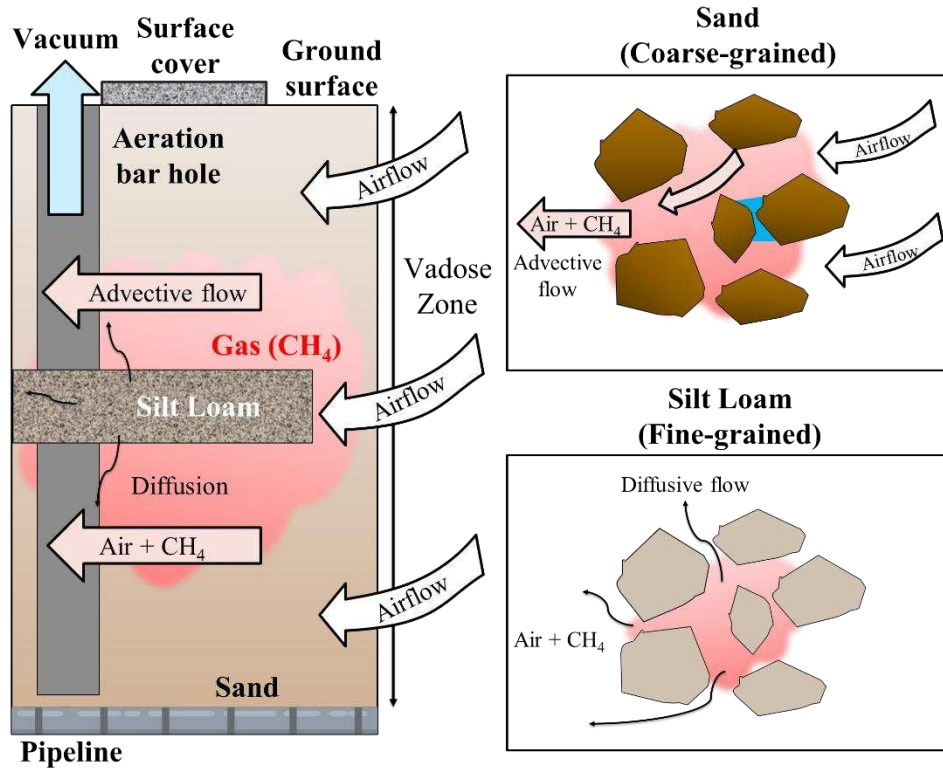


Fig. 1. 1. Conceptual scheme of advective and diffusive gas transport in a layered vadose zone with induced airflow. Advective airflow preferentially follows connected, higher-permeability pathways in sand, rapidly transporting subsurface gas toward an aeration bar hole. In contrast, CH_4 stored in silt loam is transported to the pore network primarily by diffusion. Surface cover and subsurface heterogeneity modify airflow pathways and can promote lateral spreading and bypass. The contrasting soils describe conceptual soil conditions under the present transport model assumptions.

Several environmental factors control gas transport behavior. Soil structure, permeability, and air-filled porosity primarily impact advection and diffusion. Sand often presents broader airflow distribution, while silt loam restricts advective airflow and increases the importance of diffusion-dominated storage and release. Soil water saturation is a dominant control because high water saturation can reduce air permeability and advective transport. Transient wetting can therefore shift pathways and increase subsurface gas accumulation. Field-scale observations show that rainfall increases soil moisture, increasing and expanding lateral gas migration while reducing gas loss to the atmosphere (Deepagoda et al., 2016; Jayarathne, Kolodziej, et al., 2022a; Smith et al., 2003; van de Griend & Owe, 1994). Heterogeneity and preferential pathways, including layering, macropores, fractures, utilities, and backfill, can promote bypass and short-circuiting (Fig. 1. 2) and create spatially variable advection and diffusion regimes at short length scales. Surface cover and sealing alter the effective top boundary condition, which can suppress upward exchange and promote lateral spreading. Atmospheric forcing can further control near-surface pressure gradients, contributing to time-varying exchange and surface observation (Levintal et al., 2019; Nachshon et al., 2012; Poulsen et al., 2018).

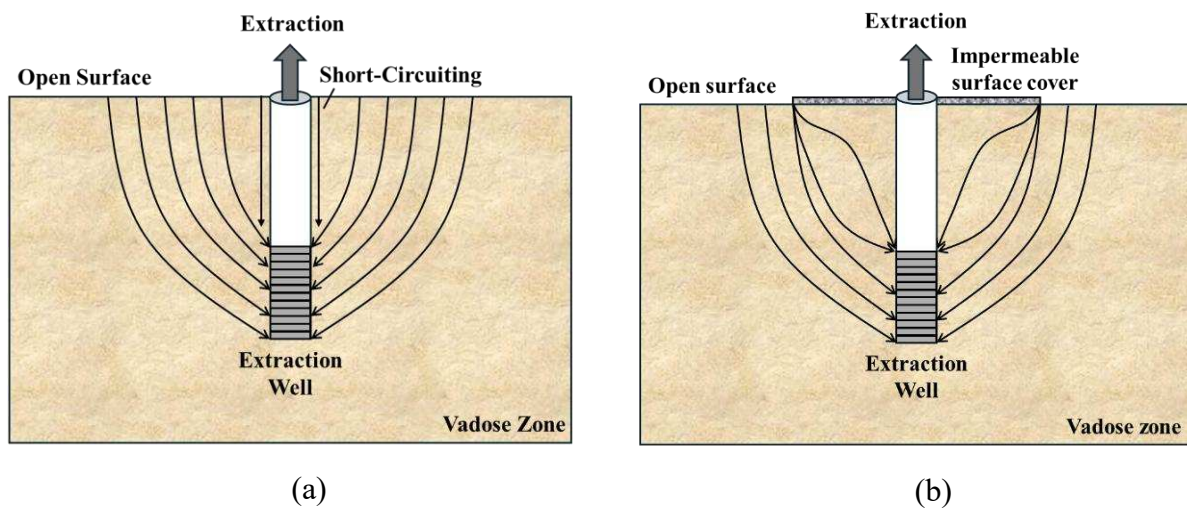


Fig. 1. 2. Conceptual scheme of impermeable surface cover effects on induced airflow pathways during soil vapor extraction. (a) With an open surface, air can enter near the extraction point,

promoting near-well “short-circuiting” and reducing capture from the subsurface. (b) With an impermeable surface seal, near-surface air entry is suppressed, forcing airflow to be drawn from greater distances and increasing the effective capture zone. This figure was designed based on figures Johnson et al (1990) and U.S. Army Corps of Engineers (2002)

Gas composition and chemical properties impact gas transport in the vadose zone by affecting gas density, viscosity, and molecular diffusivity, as well as potential partitioning into pore water and biotic sinks (Suthersan et al., 1999; U.S. Army Corps of Engineers, 2002). For multicomponent gas mixtures, gas density and viscosity influence pressure-driven advection, while molecular diffusivity governs diffusion and the effective diffusivity. For volatile contaminants that exist as nonaqueous or liquid-phase sources, the maximum gas-phase concentration can be approximated by equilibrium relationships and the ideal gas law using vapor pressure and molecular weight. However, for gas migration in the vadose zone, where contamination does not typically involve a liquid-phase source, vapor pressure is not a meaningful predictor of transport or removal behavior. Instead, the relevant coupling is between gas-phase transport and the soil water saturation that controls gas connectivity and diffusion.

Partitioning between the gas phase and pore water is commonly described using Henry’s law, which links dissolved concentration to gas-phase partial pressure and provides a framework for evaluating how much of a compound may dissolve into pore water as saturation increases (Suthersan et al., 1999). In soil venting, vapor pressure and Henry’s law constant are often used as screening indicators for feasibility and expected performance. For gas, dissolution into pore water is typically limited by low aqueous solubility. For example, CH₄ solubility in water is approximately 0.022 mg/mL (Lide, 1995), suggesting that gas-phase transport generally dominates CH₄ migration under most vadose-zone conditions.

Sorption can affect contaminant transport in the vadose zone by partitioning mass from the gas phase into the solid phase or pore water. This behavior reduces gas-phase concentrations, retards transport, and may contribute to delayed release or rebound after active vapor extraction or removal slows or stops. These processes are important for many volatile organic compounds (VOC) considered in soil vapor extraction (SVE) (Kaleris, 2002; Rivett et al., 2011; Roy & Griffin, 1991; Switzer & Kosson, 2007; Unger et al., 1996). However, relative to many VOCs, CH₄ has low aqueous solubility (Böttger et al., 2016; Kim et al., 2016; Serra et al., 2006).

In addition, CH₄ adsorption on mineral surfaces is somewhat greater on clay-rich minerals than on silica-rich soils and reduced in the presence of adsorbed water. In sand, adsorption is expected to be of secondary importance relative to gas-phase storage and transport. In silt loam, greater surface area and more tortuous pore structure may increase CH₄ retention. However, pipeline backfill is typically specified as clean, granular, mineral soil that is free of organic material or excessive organic matter (Howard, 1996; Pacific Gas and Electric Company, 2020; Truckee Meadows Water Authority, 2011). Therefore, CH₄ is not expected to be strongly affected by sorption under the low-organic-matter mineral soil conditions considered in this dissertation. Furthermore, the overall operation time of aeration is from minutes to hours. Compared to slower sorption-related effects, which are typically more important during long-term tailing and rebound in SVE systems (Carroll et al., 2012; Kaleris, 2002; Switzer & Kosson, 2007), sorption is less likely to dominate removal during soil aeration. Therefore, the main influences on CH₄ migration and removal are reduced air-filled porosity, permeability, and effective diffusivity rather than adsorption and aqueous partitioning of CH₄ (Deepagoda et al., 2011; Jayarathne et al., 2023; Ji et al., 2012; D. Liu et al., 2013; Moldrup et al., 2000; Onawole et al., 2021).

Biodegradation can also act as a sink for gaseous components in soil venting. In bioventing, induced airflow supplies oxygen that supports aerobic biodegradation by microorganisms, and biodegradation rates depend on factors such as pH, water content, oxygen availability, and temperature (Baker, 2015; Briassoulis & Mistrionis, 2018). Low soil moisture can reduce biodegradation rates, whereas higher moisture can increase microbial uptake by enhancing dissolved availability for some compounds (Zwick et al., 1995). For CH₄, low aqueous solubility can limit microbial availability and make biodegradation less effective when gas residence times are short, although oxidation may become more relevant under conditions that promote longer contact times and sustained oxygen supply (Vergara-Fernández et al., 2019).

These multiphase and multicomponent processes provide a mechanistic basis for detection, quantification, and mitigation of subsurface CH₄, but they also expose three unresolved challenges that limit current field practice. First, detection based on surface or near-surface concentrations remains unreliable for characterizing subsurface leak behavior because surface expression is displaced and intermittent, modulated by soil water saturation changes, surface cover, and atmospheric forcing (Deepagoda et al., 2016; Gao et al., 2021; Gundapuneni et al., 2026; Riddick et al., 2021; Tian et al., 2022a; Ulrich et al., 2019). Existing approaches do not systematically integrate belowground observations with the transport properties that govern how gas migrates from source to sensor. Second, quantification of transient NG leak rates from sparse near-surface measurements remains poorly constrained because available models either assume steady-state conditions or rely on surface signals alone, without accounting for the time-varying coupling among soil moisture, surface boundary conditions, and subsurface transport pathways that control what fraction of subsurface CH₄ reaches the measurement domain (Cheptonui et al., 2023; Deepagoda et al., 2016; Lo et al., 2024; Tian et al., 2022a). Third, mitigation through soil aeration

lacks a predictive framework that connects measurable site conditions (e.g., soil type, water saturation, and plume geometry) to the design parameters that govern removal performance, such as bar-hole configuration, applied vacuum, and aeration duration. In particular, the transition from advective or pressure-driven early-time removal to diffusion-limited late-time tailing and rebound is well established conceptually in subsurface gas transport and vapor remediation (Brooks & Corey, 1964; Carroll et al., 2012; Deepagoda et al., 2016; Yoon et al., 2008; Zhao & Zytner, 2008). However, it has not been quantitatively resolved across representative soil conditions in a way that supports field decision-making. These unresolved issues highlight the need for further research on transient leak quantification, mechanistic controls on soil-aeration performance, and field-relevant design approaches.

1.2.2 Subsurface Natural Gas Leak Detection

A key challenge for subsurface NG leakage is that the leak source is difficult to identify and locate. Heterogeneous soil properties and variable saturation strongly control gas and water transport mechanisms in the vadose zone. At the same time, the surface expression of CH₄ is highly sensitive to atmospheric forcing and surface cover (Cho et al., 2020; Deepagoda et al., 2016; Jayarathne, Kolodziej, et al., 2022a; Levintal et al., 2019; Lo et al., 2024; Nachshon et al., 2012; Poulsen et al., 2018; Riddick et al., 2021; Smith et al., 2003; Ulrich et al., 2019). As a result, the same leak can produce surface and subsurface CH₄ behaviors that vary substantially in space and time even when the leak rate is unchanged. These complicated conditions impact both detection and quantification, especially when decisions must be made from field measurements collected over limited time windows.

These characteristics directly relate to the operational requirements. During leak response, operators must assess if leak conditions are evolving over time and gauge the severity of the release.

Once a leak is detected, operators typically grade the leak to determine risk to public safety and the environment and to prioritize repair actions (GPTC, 2023; Pipeline and Hazardous Materials Safety Administration, 2023). Standard grading approaches aim to distinguish immediate hazards requiring urgent repair from conditions suitable for scheduled repair or longer-term monitoring. However, grading reliability depends on measurements collected under conditions that may not represent the subsurface hazard. Multiple studies show that atmospheric conditions, surface cover, subsurface structures, and soil properties can substantially impact measured concentrations and migration behavior (Cho et al., 2020; Deepagoda et al., 2016; Ulrich et al., 2019).

For detection, surface or near-surface concentrations are usually used to identify the subsurface leak level. While these indicators are effective for screening, atmospheric conditions and surface coverage influence the observation of surface gas migration. Wind-driven pressure variability can couple to soil-gas flow through permeable surfaces and impact subsurface migration pathways and surface expression (Levintal et al., 2019; Nachshon et al., 2012; Poulsen et al., 2018). Short-term and long-term barometric pressure variations can also induce pressure gradients that drive advective flow and influence subsurface migration. Surface conditions further affect detection results. Pavements and surface sealing can impede upward migration and promote lateral redistribution and underground accumulation. This can extend surface expression from the leak source and increase the potential for gas entry into subsurface structures (Jayarathne, Kolodziej, et al., 2022a; Ulrich et al., 2019). In urban environments, heterogeneous surface and subsurface conditions and obstructions such as buildings, basements, and vegetation can bias transport from subsurface to surface and distort the spatial pattern of measured CH₄. Practical constraints, including private property boundaries, can also limit spatial coverage and repeatability of field measurements, adding uncertainty to detection interpretation. Overall, these effects show that

surface and near-surface concentrations are effective for screening but can be biased by forcing and surface conditions. Therefore, robust detection benefits from integrating subsurface information and monitoring over time rather than relying on single-pass surface surveys.

1.2.3 Subsurface Natural Gas Leak Quantification

A wide variety of approaches have been used to quantify underground NG leak conditions and to estimate surface emission rates. Real-time transient modeling approaches use variations in temperature, pressure, and concentration to evaluate leak occurrence and magnitude. However, they often require dense instrumentation, specialized equipment, and substantial operator training. These requirements constrain deployment across large networks. Statistical approaches use pressure and flow observations along pipelines to identify leak locations and leak rates. Nevertheless, they often provide area-scale estimates and may not resolve site-scale temporal variability in leak behavior (Murvay & Silea, 2012). Downwind approaches estimate emission rates using dispersion modeling, including Lagrangian frameworks that relate measured enhancements to source strengths under specified meteorological conditions (Denmead, 2008; Flesch et al., 1995; Riddick et al., 2017, 2019, 2021; Tian et al., 2022a). While these approaches can be effective for estimating emission rates, they typically require sufficient monitoring duration and stable measurement conditions. They also do not directly quantify gas accumulation and migration in the vadose zone that drive near-field hazard and persistence. For example, Tian et al. (2022a) reported that multi-hour measurement periods were needed to support flux estimation in their deployment design. Unmanned aerial vehicle (UAV) approaches and other mobile detection technologies show promise for rapid detection and localization, particularly for screening and mapping. However, they have limited applicability for defensible emission estimation and long-term monitoring at specific sites under variable atmospheric and surface conditions (Iwaszenko et

al., 2021; Lu & He, 2017). Therefore, constraints related to cost, data availability, deployment feasibility, and environmental heterogeneity motivate the development of low-cost monitoring networks capable of continuous operation, resolving environmental variability, and enabling inference of non-stationary leak dynamics beyond short-duration measurement campaigns (Lo et al., 2024).

Previous studies have advanced models that use measured CH₄ concentrations and key environmental parameters to interpret surface expression. Cho et al. (2020) developed an analytical approach to estimate emissions using surface concentration data and soil conditions. However, inferred migration distance and emissions can depend on the assumed threshold above background and on soil saturation conditions (Cho et al., 2020). The Estimating Surface Concentration Above Pipeline Emission (ESCAPE) model estimates surface CH₄ enhancements using resistance concepts with meteorological observations and known underground leak information under steady leak conditions (Riddick et al., 2021). These approaches provide links between observations and estimated subsurface leak behavior. However, a key limitation is that these methods cannot adequately represent time-varying coupling among soil, surface, and atmospheric conditions, particularly when subsurface migration pathways vary with changes in soil moisture, surface sealing, or rapidly varying atmospheric forcing. Field-scale experiments further indicate that incorporating subsurface observations is crucial for describing belowground leak behavior. Lo et al. (2024) reported that elevated belowground-near-surface concentrations persisted prior to elevated surface concentrations. The difference between surface and belowground near-surface concentrations varied widely under fluctuating atmospheric conditions. These observations motivate integrated approaches in which time-varying aboveground and belowground conditions are incorporated into quantification models to better infer potential variations in leak rate and to

more accurately represent gas transport behavior in the vadose zone. Consequently, these studies indicate that robust quantification requires more than short-duration surface-based estimation. It benefits from continuous monitoring and an integrated surface-subsurface modeling framework that explicitly represents how surface and subsurface conditions control gas migration from subsurface to atmosphere.

1.2.4 Subsurface Natural Gas Leak Mitigation

Following leak identification and quantification, repair is the primary action. However, repair does not necessarily eliminate subsurface CH₄ immediately. Residual CH₄ can remain stored in the vadose zone and continue migrating after the leak is isolated. Subsurface CH₄ concentrations can remain elevated under diffusion-dominated conditions with weak advection, higher water saturation that reduces gas-phase permeability, and surface covers that suppress upward venting and promote lateral spreading. Residual CH₄ may also accumulate in critical zones within the built environment, including poorly ventilated dead zones near basement floors, increasing the potential for gas entry into structures (Truex et al., 2013; U.S. Environmental Protection Agency, 2018). These safety concerns motivate mitigation as part of pipeline safety management, particularly where asphalt, snow, or other covers impede vertical transport and extend the footprint of residual subsurface plumes (Jayarathne, Kolodziej, et al., 2022a; E. Six, 2014). The practical mitigation challenge is not only reducing concentration at a monitoring point. It is also reducing total subsurface CH₄ mass to levels that minimize rebound after the mitigation process stops (Carroll et al., 2012; Høier et al., 2009).

Soil aeration is widely used to remove residual NG from the vadose zone after a leak has been identified and repaired. In field practice, one or more boreholes (“bar holes”) are drilled at or near

confirmed or suspected leak locations. Gas removal occurs by passive venting or active aeration induced by vacuum, which establishes a pressure gradient that drives soil gas migration toward the bar holes. Aerated gas may be collected for treatment or released to air, depending on site constraints and operating practice (U.S. Environmental Protection Agency, 2017). Aeration is typically continued or periodically repeated until subsurface CH₄ concentrations meet an approved criterion (e.g., 0.1% LEL or 50 ppmv) with follow-up monitoring after shutdown to evaluate concentration rebound. Soil aeration applies vacuum at bar holes to create pressure gradients that drive advective airflow in the vadose zone. CH₄ trapped in low-mobility soils reaches these flow pathways mainly by diffusion. This mechanism induces two-stage removal behavior. Early-time removal is rapid where airflow accesses connected pore space. Late-time behavior is diffusion-limited and can rebound after shutdown. Removal performance is governed by the extent of the advective capture zone and back-diffusion from low-mobility soils or poorly aerated zones.

In practice, the design of NG soil aeration is commonly guided by operational constraints and rapid field interpretation rather than a detailed analysis of the site-specific transport in the vadose zone. Bar-hole depth is selected to target the zone of elevated subsurface CH₄ while avoiding buried utilities and the pipeline. Bar-hole diameter is chosen to allow rapid installation and sufficient removal without extensive well construction. In general, bar-hole diameter is from 3 cm to 6 cm. The number, spacing, and layout of bar holes are often determined from the observed concentration pattern and accessible locations, with bar holes placed near the highest CH₄ concentration and then expanded outward if concentrations remain elevated. The applied vacuum level is primarily constrained by field equipment, including air-compressor capacity and the bar-hole purger design. Within these constraints, operators adjust the operating point to achieve concentration reductions while maintaining stable aeration, although higher vacuum, which

induces the pressure drawdown related to the atmosphere pressure, does not always yield proportional improvements when airflow preferentially follows high-permeability pathways. The operation period is typically selected to meet clearance criteria (e.g., 50 ppmv) at designated monitoring locations, and operations may be repeated if concentrations rebound after shutdown.

In current field practice, site-specific NG soil aeration design and operation are often guided by operator experience and generalized rules developed under practical constraints. Deployment typically occurs under limited time windows, restricted access, and incomplete subsurface information. As a result, key soil factors that control advective and diffusive transport in the vadose zone, including soil types, permeability, and water saturation, are not consistently incorporated into decisions on bar-hole layout, applied vacuum, operation time, or shutdown criteria. This contributes to large variability in performance across sites and can lead to insufficient removal, prolonged operations, and rebound after initial concentration reductions. Post-incident analyses attributed the prolonged cleanup to low intrinsic permeability and elevated water content that restricted gas transport (E. Six, 2014; Spectrum News, 2019; U.S. Environmental Protection Agency, 2019). These limitations and challenges highlight the need to consider soil characteristics in the design and operation of NG soil aeration to improve subsurface CH₄ removal. Similar limitations have also been reported for soil vapor extraction (SVE). Federal Remediation Technologies Roundtable (2003) mentioned that six soil vapor extraction case studies at drycleaner sites, two systems failed under high-soil-moisture conditions, and another site showed rebound after initial operation, with removal rates dropping sharply over time.

Soil vapor extraction (SVE), a well-established remediation technology for volatile contaminants in the vadose zone, provides established design concepts and practical guidance that link pressure response and site properties to system configuration and performance expectations

(Carroll et al., 2012; Hutzler & Murphy, 1988; Kuo, 2014; Sun et al., 2023; Suthersan et al., 1999; U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1995). SVE uses vacuum extraction wells to generate advective airflow through contaminated soil, and removal is governed by advection, diffusion, phase partitioning, and mass-transfer limitations (Hers et al., 2003; Johnson et al., 1990; U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1993, 1996). Pressure drawdown testing is used to assess how applied vacuum propagates and to infer effective air permeability at the scale relevant to operation (U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1991). Radius of influence (R_I) is commonly defined using a threshold drawdown criterion relative to applied vacuum and is used to approximate an effective capture or aeration area (Johnson et al., 1990; Kuo, 2014; Sun et al., 2023; Suthersan et al., 1999; U.S. Army Corps of Engineers, 2002). Practical design often applies R_I -based coverage logic to select well numbers and locations, commonly visualized by overlapping circles on site maps to ensure that the targeted zone is covered (Fig. 1. 3). Previous SVE studies also emphasize airflow bypass and short-circuiting under surface sealing, preferential pathways, and heterogeneity, as well as diminishing returns when increasing vacuum does not expand the effective capture zone.

SVE also offers a long history of laboratory tests, pilot studies, and field case reports that clarify when venting succeeds or stalls. Field evidence repeatedly indicates that high-permeability soils such as sand and gravel induce more successful extraction, whereas low-permeability and layered soils tend to prolong tailing and residual mass persistence (D. H. Bass et al., 2000; Marley & Bruell, 1995; Suthersan et al., 1999; U.S. Environmental Protection Agency, 1995). Quantitative case studies in SVE further illustrate the range of outcomes and the importance of site-specific transport limitations. For example, one field SVE application reported the removal of

approximately 95700 kg of total petroleum hydrocarbons (TPH) by SVE-based soil venting operations (Khan et al., 2004; Khan & Husain, 2003; Kirtland & Aelion, 2000; U.S. Environmental Protection Agency, 1995). However, even after substantial removal using SVE, a small residual mass in fine-grained layers can persist and require additional venting phases. For example, SVE was conducted at a highly heterogeneous site, where more than 726 lb of extracted contaminant was reported removed, while a residual mass on the order of 6 lb remained in a clayey silt layer and required further soil venting (U.S. Environmental Protection Agency, 2018). Therefore, these cases indicate that limited airflow access and diffusion-limited mass transfer often control cleanup time and rebound. This directly affects when systems can be shut down with confidence.

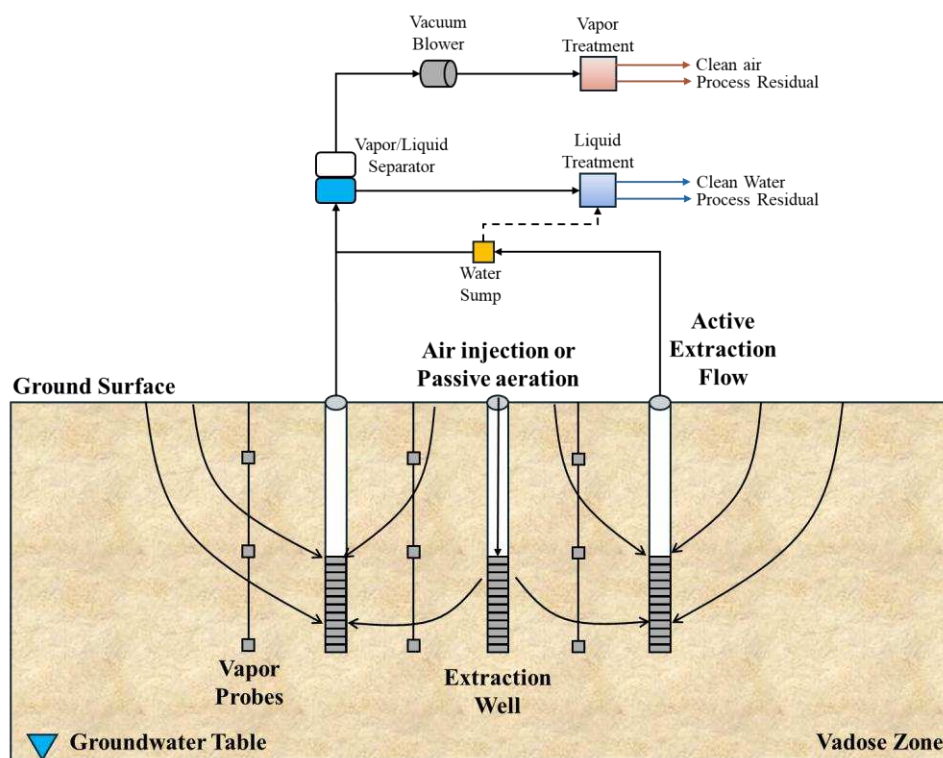


Fig. 1. 3. Schematic of a soil vapor extraction (SVE) system. The system includes extraction wells, active extraction, and monitoring points (vapor probes). The advective airflow is drawn toward the wells under an induced negative-pressure gradient and conveyed through a vapor/liquid separator and vacuum blower to vapor or liquid treatment units, producing clean air and clean water with process residuals. Arrows indicate representative subsurface vapor flow paths above the water

table. The gray squares indicate the well screens. This figure was designed based on figures in Stewart et al (2018).

In parallel, numerical models have been used to represent coupled flow and transport processes and to identify the parameters most relevant to soil remediation technology (e.g., SVE). AIR3D was developed to estimate unsaturated-zone permeability from SVE tests and to simulate three-dimensional airflow in heterogeneous, anisotropic settings (Joss & Baehr, 1995). MISER integrated multiphase flow, multicomponent compositional transport with non-equilibrium interphase mass transfer, and aerobic biodegradation, and highlighted that SVE efficiency depends strongly on airflow access to contaminated zones and on mass-transfer limitations (Rathfelder et al., 2000). Additional tools such as VENT3D and SVE-3D were developed to simulate three-dimensional gas transport and support well number and spacing decisions and cleanup-time estimation (Benson, 2011; Scientific Software Group, 2011), while later developments incorporated non-equilibrium transient mass transfer in multiphase, multicomponent settings (V. T. Nguyen et al., 2013). Consequently, these field and modeling studies provide a rich reference for the processes and measurements relevant to SVE or subsurface gas removal, including pressure response interpretation, capture-zone coverage, bypass behavior, and diffusion-limited mass transfer that drives tailing and rebound.

Despite the conceptual overlap between SVE and NG soil aeration, SVE guidance is not directly sufficient for NG soil aeration because objectives, time scales, and field constraints differ. SVE commonly targets sustained remediation over months to years and across treatment footprints that can be large. In contrast, NG soil aeration is often implemented as an interim mitigation measure over hours to days within a constrained radius around a leak location (Pipeline and Hazardous Materials Safety Administration, 2017; U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1998). The endpoint is typically defined by a clearance criterion.

The objective is rapid concentration reduction and post-shutdown verification rather than long-term mass removal.

Operational details also differ in ways that affect induced airflow for subsurface removal. In SVE, extraction wells commonly include casing, screened intervals, filter packs, and seals that shape near-well flow and minimize solids entrainment. Engineered surface covers may also be used to reduce short-circuiting and infiltration (ASTM International, 2021, 2025; Barnes, 2003; Suthersan et al., 1999; Zhan & Park, 2002). In contrast, the bar holes in NG soil aeration are typically drilled with a small diameter and rapidly installed. They often operate with an open interface and limited construction. These features can increase sensitivity to local heterogeneity and to surface and subsurface conduits such as utilities and backfill. They can also increase the likelihood of bypass and short-circuiting under certain site configurations.

NG soil aeration is further influenced by transient boundary conditions that are common in leak response settings. Wetting events, surface sealing, and environmental constraints can modify airflow paths in the vadose zone, impact residual gas distribution, and affect monitoring (Jayarathne et al., 2024; Lo et al., 2024; U.S. Army Corps of Engineers, 2002). Under these conditions, concentration reductions at a few monitoring points may not reflect total residual mass, especially when diffusion-limited mass transfer controls late-time migration behavior. These differences imply that bypass, back-diffusion, and rebound dynamics may depart from simplified assumptions often adopted in conventional SVE practice. Therefore, SVE provides a useful reference framework rather than a direct design template. NG soil aeration design and operation should link measurable site conditions, including soil properties, water saturation, and surface and subsurface conditions, to bar-hole configuration and operation decisions. This linkage is critical

for defensible field decisions on system setup, operation, and shutdown. It also motivates adapting reduced-order, field-applicable decision tools from the SVE studies to the NG soil aeration context.

Johnson et al. (1990) provided a practical approach to the design, operation, and monitoring of in-situ soil venting. A crucial contribution of this approach is that it translates limited field measurements into actionable decisions and highlights where performance is constrained by transport and mass-transfer limitations. Within SVE practice, these simplified tools are often paired with performance indicators, including radius of influence, extracted concentration, achievable flow rate, and removal efficiency. They are also used alongside operational criteria for cleanup time and rebound evaluation, which help interpret tailing behavior and residual mass persistence in the vadose zone (Brusseau et al., 2010, 2015; U.S. Army Corps of Engineers, 2002). Analytical and numerical studies have also focused on estimating cleanup time and tailing under heterogeneity and alternative operating strategies, such as intermittent (on–off) extraction (Armstrong et al., 1994; Jury et al., 1991; Kaleris & Croisé, 1997; Kuo, 2014; Yoon et al., 2008). These concepts provide a practical template for defining performance indicators and supporting design and operational decisions for NG soil aeration under field constraints.

However, few studies and few multiphase, multicomponent modeling frameworks have been tailored to the short-duration soil aeration relevant to pipeline safety, where objectives, operating constraints, and transient boundary conditions differ from conventional SVE remediation. In current practice, NG soil aeration monitoring often focuses on concentration changes at aeration locations, while environmental conditions such as soil moisture are rarely integrated systematically into operational interpretation. A quantitative approach that links measurable site conditions to bar-hole configuration, removal efficiency, and shutdown decisions remains limited. This gap motivates the need for a reduced-order, physics-informed, site-specific tool for NG soil aeration

that connects measurable field parameters to time-resolved subsurface CH₄ removal performance while minimizing rebound risk.

1.3 Objectives and Hypotheses

The overarching objective of this dissertation is to address unresolved challenges in estimating transient subsurface gas leak behavior, understanding the mechanisms controlling subsurface gas removal during soil aeration, and developing a practical framework for field-scale design and operation. To address these challenges, the following objectives and associated hypotheses are proposed.

Objective 1: Estimate subsurface gas leak rate by incorporating surface and belowground near-surface (BNS) gas concentration measurements, soil properties, and atmospheric conditions

Hypotheses (Obj. 1):

- **H1.1:** Variation of BNS gas concentration responds more consistently to changes in subsurface gas leak behavior than that of surface gas concentration.
- **H1.2:** Integrating surface and BNS gas concentration measurements with soil properties and atmospheric conditions improves the quantification of transient subsurface gas leak rates compared with using only surface gas concentration measurements and atmospheric conditions

Test of Hypotheses (Obj. 1):

- **H1.1:** Comparing variations in surface and BNS gas plumes and concentrations to changes in the controlled gas leak rate during the field-scale controlled experiments.

- **H1.2:** Comparing estimated subsurface gas leak rates from an inverse gas migration model using (1) only surface gas concentration measurements and atmospheric conditions, and (2) surface and BNS gas concentration measurements, soil properties, and atmospheric conditions. Modeled performance was evaluated against known subsurface gas leak rates in controlled experiments using R^2 with a value greater than 0.7.

Objective 2: Estimate subsurface gas migration and removal during soil aeration across different soil characteristics and soil aeration designs using a multiphase multicomponent transport model and field-scale controlled experiments

Hypotheses (Obj. 2):

- **H2.1:** Subsurface gas removal during soil aeration is a time-varying process that transitions from an advection-dominated stage to a diffusion-limited stage.
- **H2.2:** Aeration designs selected based on soil characteristics govern subsurface gas advection and diffusion during soil aeration, controlling subsurface gas removal.

Test of Hypotheses (Obj. 2):

- **H2.1:** Analyzing the changes in subsurface gas concentration, removal efficiency, and residual gas concentration during field-scale soil aeration experiments and numerical simulations to determine if subsurface gas removal transitions from an advection-dominated stage to a diffusion-limited stage.
- **H2.2:** Comparing subsurface gas transport and removal under different soil characteristics and aeration designs using field-scale experiments and numerical simulations. Modeled

performance was evaluated against removal efficiency in controlled experiments using R^2 with a value greater than 0.7.

Objective 3: Develop a reduced-order, physics-based model to predict subsurface gas removal efficiency, estimate aeration duration, and determine bar-hole configuration for soil aeration using site-measurable parameters

Hypotheses (Obj. 3):

- **H3.1:** A reduced-order, physics-based model using site-measurable parameters, including soil properties, vacuum pressure, subsurface gas plume geometry, can predict subsurface gas removal efficiency under representative conditions.

Test of Hypotheses (Obj. 3):

- **H3.1:** The predictions from a reduced-order, physics-based model are compared with results from controlled experiments across representative soil properties, plume geometry, and operating conditions. Modeled performance was evaluated against removal efficiency in controlled experiments using R^2 with a value greater than 0.7.

1.4 Dissertation Outline

This dissertation consists of 5 chapters and 6 appendices. Chapter 2 investigates the responses of surface and belowground near-surface gas concentration observations to subsurface gas leak behavior and quantifies transient subsurface gas leak rates by integrating surface and belowground near-surface gas concentration measurements, soil properties, and atmospheric conditions with an inverse gas migration model. Because this chapter is reprinted from Lo et al. (2024), the

introductory statistics and cited literature reflect the state of the literature and publicly available data at the time the manuscript was prepared. More recent PHMSA incident-report data are synthesized in Chapter 1 to frame the dissertation as a whole. Chapter 3 investigates the impacts of soil properties and aeration designs on subsurface gas migration and removal during soil aeration, using field-scale controlled soil aeration experiments and multiphase (gas and water) transport simulations. Based on the insights from Chapter 3, Chapter 4 introduces a reduced-order, physics-based framework to predict subsurface gas removal efficiency, required aeration duration, and optimal bar-hole number and layout. Finally, Chapter 5 summarizes the main contributions of this dissertation, discusses their broader implications for subsurface gas monitoring, quantification, and mitigation, and provides directions for future research. Appendix A summarizes instrumentation, calibration, and data acquisition procedures. Appendix B provides additional details of the controlled experiments at METEC. Appendix C presents experimental data processing procedures. Appendix D includes numerical model setup and supplementary transport results. Appendix E provides supplementary derivations and framework calculations. Appendix F lists supplemental electronic files.

Chapter 2. Quantifying Non-steady State Natural Gas Leakage from the Pipelines Using an Innovative Sensor Network and Model for Subsurface Emissions¹

Abstract

Detecting and quantifying subsurface leaks remains a challenge due to the complex nature and extent of belowground leak scenarios. To address these scenarios, monitoring and evaluating changes in gas leakage behavior over space and time is crucial for ensuring safe and efficient responses to known or potential gas leaks. This study demonstrates the capability of linking environmental and gas concentration data obtained using a low-cost, near real-time methane (CH₄) detector network and an inverse gas migration model to capture and quantify non-steady state belowground natural gas (NG) leaks. The Estimating Surface Concentration Above Pipeline Emission (ESCAPE) model was modified to incorporate the impact of soil properties on gas migration. Field-scale controlled NG experiments with leakage rates ranging from 37 to 121 g/h indicate that elevated belowground near-surface (BNS) gas concentrations persist long before elevated surface concentrations are observed. On average, BNS CH₄ concentrations were 20% to 486% higher than surface CH₄ concentrations within the monitoring radius of 4 meters from the leak location. An increase in the BNS CH₄ concentration was observed within 3 hours as the leak rate increased from 37 to 89 g/h. However, due to the atmospheric fluctuations, any changes in surface CH₄ concentrations could not be confirmed within this period. The plume area of the BNS CH₄ extended approximately two times farther than that of the surface CH₄ as the gas leak rate

¹ Reprinted with permission, *Environmental Pollution*, 2024, 341. This chapter is a reproduction of the paper entitled “Quantifying non-steady state natural gas leakage from the pipelines using an innovative sensor network and model for subsurface emissions-InSENSE.” by Lo, J. H., Smits, K. M., Cho, Y., Duggan, G. P., & Riddick, S. N., which was published in *Environmental Pollution*, 341, 122810 (2024). doi: <https://doi.org/10.1016/j.envpol.2023.122810>

increased from 37 to 121 g/h. The estimated NG leak rates by the modified ESCAPE model agree well with the experimental NG leak rates ($m=0.99$ and $R^2=0.77$), demonstrating that including soil characteristics and BNS CH₄ measurements can advance estimations of non-steady NG leak rates in low and moderate NG leak rate scenarios. The CH₄ detector network and model show potential as an innovative tool to improve operators' risk assessment and NG leakage response.

2.1 Introduction

Natural gas (NG) is an important energy source, supporting 21% of the world's energy demand with 3.4 billion cubic meters of gas produced each year. In the United States, NG is transported using three million miles of distribution pipelines (U.S. Energy Information Administration, 2021). However, gas pipelines may leak due to corrosion, aging infrastructure, and human error. The leaks from low-pressure pipelines could migrate unnoticed for long periods and accumulate in confined areas of buildings (e.g., basement). The Pipeline and Hazardous Materials Safety Administration (PHMSA) reported that pipeline leakage resulted in 1,030 injuries between 2002 and 2021, with 6 from gathering lines, 157 from transmission lines, and 867 from distribution lines (Pipeline and Hazardous Materials Safety Administration, 2022).

To improve NG pipeline safety, operators grade the leak to determine the risk to public safety and the environment once the leak is detected (GPTC, 2023; Pipeline and Hazardous Materials Safety Administration, 2023). In general, Grade 1 leaks present an immediate hazard to people and are immediately repaired; Grade 2 are non-hazardous leaks but prioritized for repair; Grade 3 leaks are considered non-hazardous and repaired based on a longer time scale, varying based on the local level regulations, typically within 6 to 12 months of grading. Nevertheless, changes in surface cover or ongoing construction may alter the grading of an existing gas leak (Jayarathne, Kolodziej,

et al., 2022a, 2022b; Jayarathne, Smits, et al., 2022). Therefore, continuous monitoring of the leak is necessary to evaluate potential changes in the leak rate and the belowground gas behavior.

A wide variety of approaches are used to detect underground NG leaks. For example, real-time transient modeling uses variations in temperature, pressure, and concentrations to determine the occurrence of a gas leak. However, the disadvantage of this approach is the requirement for substantial instrumentation and equipment along with operator training. The statistical analysis utilizes targeted pressure and flow rates at potential gas leak areas along the pipeline to determine the gas leak rates and locations. Nevertheless, this approach provides area estimates of emissions rather than an understanding of changes in leak behavior over time (Murvay & Silea, 2012). Downwind methods use Lagrangian dispersion models to quantify emission rates (Denmead, 2008; Flesch et al., 1995; Riddick et al., 2017, 2019, 2021; Tian et al., 2022a). Nevertheless, Tian et al. (2022a) indicated that a minimum of 3 hours of data was required for reasonable estimations. In addition, topography and surface obstructions (e.g., trees and buildings) highly influence results due to the difficulty of monitoring the change in leakage over time with reasonable accuracy. The unmanned aerial vehicle (UAV) methods show promise in leak detection (Iwaszenko et al., 2021; Lu & He, 2017) but have limited applicability to emission estimation and monitoring over time. In addition, previous studies indicate that changes in environmental conditions including ambient temperature, wind velocity, and soil conditions affect the measurement of NG concentrations (Cho et al., 2020; Deepagoda et al., 2016; Ulrich et al., 2019). Jayarathne, Kolodziej, et al. (2022a) showed that heavy rain events can quadruple the lateral underground distribution of CH₄ within 6 hours. Thus, current approaches of detection may not be suitable to effectively monitor underground gas leaks under transient conditions due to cost, data accessibility, deployment approach, and varied environmental conditions.

The low-cost gas sensor networks capable of detecting underground gas leaks are a potential development. Metal oxide semiconductor (MOS) sensors have been evaluated in multiple studies and demonstrated promising performance (Cho et al., 2022; Eugster & Kling, 2012; Honeycutt et al., 2021). Cho et al. (2022) developed the low-cost CH₄ detector using a MOS sensor (Figaro Engineering Inc., n.d.) and environmental sensors to study the influence of temperature and relative humidity on the change in CH₄ concentrations. The evaluation of a low-cost CH₄ detector with a portable cavity ring-down spectroscopy (CRDS) analyzer indicated that the low-cost CH₄ detector could detect CH₄ concentrations as low as 100 parts per million volumes (ppmv). Therefore, a low-cost CH₄ sensor network could be used to monitor changes in gas leak behavior and leak rate over time.

Cho et al. (2020) developed an analytical tool to study subsurface gas migration by utilizing surface concentration data and key environmental parameters. However, the migration distance of CH₄ in their approach is influenced by the threshold level above background levels and soil saturation. The Estimating the Surface Concentration Above Pipeline Emission (ESCAPE) model (Riddick et al., 2021) utilizes above-ground meteorological measurements and known underground leak information under steady conditions to estimate surface CH₄ enhancements over time. In the ESCAPE model, CH₄ emissions were calculated from the surface and background CH₄ concentrations and estimates of atmospheric resistance. However, a limitation of the ESCAPE model is the assumption that micrometeorological and surface conditions are the sole factors affecting the development of surface CH₄ emissions. Emissions resulting from underground leaks are highly influenced by dynamic interaction among soil, surface, and atmospheric conditions. Hence, the considerations of both time-varying above and below-ground conditions could enhance our understanding of potential variations in leak rate and gas transport behavior.

The present study introduces an innovative approach to quantify underground natural gas (NG) leak rates under non-steady conditions using an inverse gas migration model and surface near-real-time low-cost CH₄ detector network. The inverse gas migration model is developed based on the ESCAPE model to incorporate soil properties and the belowground near-surface (BNS) CH₄ concentration variations to estimate non-steady underground NG leak rates. To evaluate the performance of the model, field-scale controlled gas release experiments were conducted at Colorado State University's Methane Emission Technology Evaluation Center (METEC) under varying leak and environmental conditions. The key hypothesis is that the non-steady gas migration from the leak point to the surface is described by the interaction between surface and BNS characteristics. This study can also be used for various applications such as monitoring high-risk or highly visible pipeline locations during underground construction operations or monitoring problematic pipeline locations awaiting repair or replacement.

2.2 Materials and Methods

2.2.1 Model for Estimating Non-steady State Natural Gas (NG) Leak Rates

The model was modified based on the ESCAPE model (Riddick et al., 2021) to incorporate above-ground atmospheric measurements, soil properties, and known underground NG leak conditions to quantify underground NG leak rates. In the modified ESCAPE model, the gas flow (CH_4 and air) in the unsaturated soil was assumed to be transported under isothermal conditions. The dissolution of CH_4 in soil water was ignored due to its low solubility in water (0.022 mg/mL) and typically low water saturation in the below-ground near-surface (BNS). The modified ESCAPE model did not incorporate the scenario of heterogeneous surface covers, particularly the impermeable surface cover (e.g., asphalt) that may significantly impede the diffusion of gas, resulting in extensive migration over long distances before reaching an active atmospheric interface.

The modified ESCAPE model required time-varying measurements of surface and BNS CH_4 concentrations, wind speed, solar radiation, soil moisture, soil temperatures, the deployment of CH_4 detectors, and the depth of the leak point. Wind speed and solar radiation were used to estimate the atmospheric resistance, while soil moisture and temperature were utilized to calculate the soil resistance and diffusion coefficient of CH_4 in the soil. The atmospheric resistance described the influence of atmospheric conditions on CH_4 transportation from the surface to the atmosphere. High wind speed could create surface turbulence and lower the barrier to vertical gas transportation, resulting in a decrease in atmospheric resistance (Nemitz et al., 2001; Riddick et al., 2021). The soil resistance illustrated the effects of soil moisture on the gas migration through the soil. Elevated soil moisture could decrease soil resistance to CH_4 transportation, reducing the barrier for CH_4 to migrate through the soil (van de Griend & Owe, 1994). The wind speed profile

and soil moisture were assumed to be a homogeneous distribution with depth within the measured locations.

In the modified ESCAPE model, the non-steady NG leak rate is described by Eq. 2.1.

$$Q_L(t) = \overline{Q_L} + Q_{LT}(t) \quad \text{Eq. 2.1}$$

where Q_L (g/h) is the non-steady NG leak rate from the underground pipeline, $\overline{Q_L}$ (g/h) is the average steady-state NG leak rate estimated by the original ESCAPE model, and Q_{LT} (g/h) is the transient change in the NG leak rate.

Based on Ohm's Law analogy, the surface CH₄ flux (F_s , g/m²/h) from the surface to the air could be described by the ratio of the difference of gas concentration between the surface and air to the atmospheric resistance (Eq. 2.2) (Nemitz et al., 2001; Riddick et al., 2021).

$$F_s(t) = \frac{C_s(x, t) - C_a}{R_{at}(t)} \quad \text{Eq. 2.2}$$

where x (m) is the distance from the surface leak point to a measured location, C_s (g/m³) is the maximum surface CH₄ concentration at the measured distance x , C_a (g/m³) is the background atmospheric CH₄ concentration, which is 1.88 ppm at the experimental site, and R_{at} (s/m) is the atmospheric resistance, which is the summation of the aerodynamic resistance (R_a , s/m) and the boundary layer resistance (R_b , s/m). Details of estimation of R_{at} and R_b could be found in supplementary material (Appendix C.1).

The contribution of steady-state underground NG leak rate to surface CH₄ flux is assumed to be proportional to the travel distance in gas migration (Riddick et al., 2021). Therefore, the NG leak rates under steady-state conditions can be inversely estimated by Eq. 2.3.

$$\overline{Q_L} = A_e(x) \frac{\sum_{i=1}^{\infty} \frac{1}{\sqrt{x_i^2 + d^2}}}{\frac{1}{\sqrt{x_i^2 + d^2}}} F_s(t) \quad \text{Eq. 2.3}$$

where the subscript i represents the location of surface measurements, d (m) is the depth of the leak point (d , m), and A_e (m²) is the equivalent area of CH₄ flux. The equivalent area of CH₄ flux (A_e) can be described based on the location of measurements by Eq. 2.4.

$$A_e(x) = \pi \left[\left(\frac{x_{i+1} - x_i}{2} \right)^2 - \left(\frac{x_i - x_{i-1}}{2} \right)^2 \right] \quad \text{Eq. 2.4}$$

The variation of NG leak rates under transient conditions (Q_{LT}) could be described by the summation of the contribution of underground NG leaks to surface CH₄ emission rate (Q_s) at each measured location (Eq. 2.5 and Eq. 2.6).

$$Q_{LT}(t) = \sum_{i=1}^{\infty} \frac{Q_s(x_i, t) w_i}{\sum_{i=1}^{\infty} w_i} \quad \text{Eq. 2.5}$$

$$w_i = \frac{\frac{1}{x_i}}{\sum_{i=1}^{\infty} \frac{1}{x_i}} \quad \text{Eq. 2.6}$$

where Q_s (g/h) is surface CH₄ emission rate at the measured location (x_i) and w_i is a coefficient to describe the contribution of underground NG leak rate to the surface CH₄ emission rate. The surface CH₄ emission rate is described by the difference between the surface and BNS CH₄ fluxes on an equivalent area of CH₄ flux (Eq. 2.7).

$$Q_s(t) = A_e(F_{ns}(t) - F_s(t)) \quad \text{Eq. 2.7}$$

where F_{ns} (g/m²/h) is BNS CH₄ flux. The BNS CH₄ flux is dominated by the advection and diffusion fluxes in porous media (Eq. 2.8), which are significantly impacted by soil properties (e.g., soil moisture and permeability). The influence of atmospheric properties is less than that of the soil properties on the BNS CH₄ migration (Deepagoda et al., 2016; Cho et al., 2020; Mitton, 2018).

$$F_{ns}(t) = F_{ns_adv} + F_{ns_dif} \quad \text{Eq. 2.8}$$

where F_{ns_adv} (g/m²/h) is the advective BNS CH₄ flux and F_{ns_dif} (g/m²/h) is the diffusive BNS CH₄ flux. Based on Ohm's Law analogy, the advective BNS CH₄ flux (F_{ns_adv}) is described by Eq. 2.9.

$$F_{ns_adv}(t) = \frac{C_{ns}(x, t) - C_s(x, t)}{R_s(t)} \quad \text{Eq. 2.9}$$

where C_{ns} (g/m³) is the maximum CH₄ concentration in the BNS at measured distance x and R_s (s/m) is the soil resistance. The soil resistance varied with the change in soil moisture over time. Previous studies indicated that soil resistance is strongly related to soil moisture (P. J. Camillo & Gurney, 1986; Z. Li & Smits, 2020; van de Griend & Owe, 1994). Bittelli et al. (2008) indicated that the model proposed by van de Griend & Owe (1994) showed the best estimation of soil resistance in fine sandy loam. Thus, the van de Griend & Owe (1994) model is used to estimate soil resistance (R_s) (Eq. 2.10).

$$R_s(t) = R_{sl} e^{0.3563(\theta_{min} - \theta_{top})} \quad \text{Eq. 2.10}$$

where R_{sl} (s/m) the resistance to gas molecular diffusion across the water surface, which was given 10 (s/m), θ_{min} (m³/m³) is the empirical minimum soil moisture, which was given 0.18 in this study, and θ_{top} is the soil moisture content in the topsoil.

The diffusive BNS CH₄ flux (F_{ns_dif}) through porous media can be described based on Fick's law (Eq. 2.11).

$$F_{ns_dif} = D(\theta) \frac{C_{ns}(x, t) - C_s(x, t)}{\Delta d_m} \quad \text{Eq. 2.11}$$

where Δd_m is the depth of BNS CH₄ concentration measurement (m), θ is the soil volumetric water content (m³/m³), and D is the diffusion coefficient of CH₄ in the soil (m²/h). Previous studies developed several models to describe the soil-gas diffusivity, which is used to describe the relationship between the diffusion of gas in the air and the soil (Millington, 1959; Moldrup et al., 2000). The WLR-Marshall model (Moldrup et al., 2000) was used to calculate the diffusion coefficient of CH₄ in the soil, as is shown in Eq. 2.12.

$$D(\theta) = D_a(T) \frac{(n - \theta)^{1.5}}{n} \quad \text{Eq. 2.12}$$

where D_a is the diffusion coefficient of CH₄ in the air (m²/h), T is the soil temperature (K), and n is the soil porosity, which was given as 0.45.

2.2.2 Scenario Analysis in the Modified ESCAPE Model

Scenario analysis is a process of generating and analyzing different hypothetical scenarios based on varying input parameters in the numerical model. The maximum surface and BNS CH₄ concentrations and the equivalent area (A_e) are related to the number of measured locations. Therefore, we selected different combinations of measured locations to determine the influence of the deployment of sensors on the estimation of non-steady NG leak rates in the modified ESCAPE model. The locations at the leak point and the boundary of the detection area are two required measured locations. The normalized root mean squared error ($NRMSE$) (Eq. 2.13), is used to evaluate the results of the scenario analysis.

$$NRMSE = \frac{RMSE}{mean(y)} \quad \text{Eq. 2.13}$$

where y indicates the true NG leak rates.

2.2.3 Field Experiments at Methane Emission Technology Evaluation Center (METEC)

A 5-day field-scale experiment with controlled NG emission rates was conducted at METEC. The atmospheric conditions, such as precipitation, temperature, wind speed, and solar radiation were measured using a weather sensor (ATMOS 41, METER Group, Inc.). The testbed was designed to simulate the transportation of natural gas from the pipeline in undisturbed soil and grass areas without an impermeable surface cover to the surface (Ulrich et al., 2019).

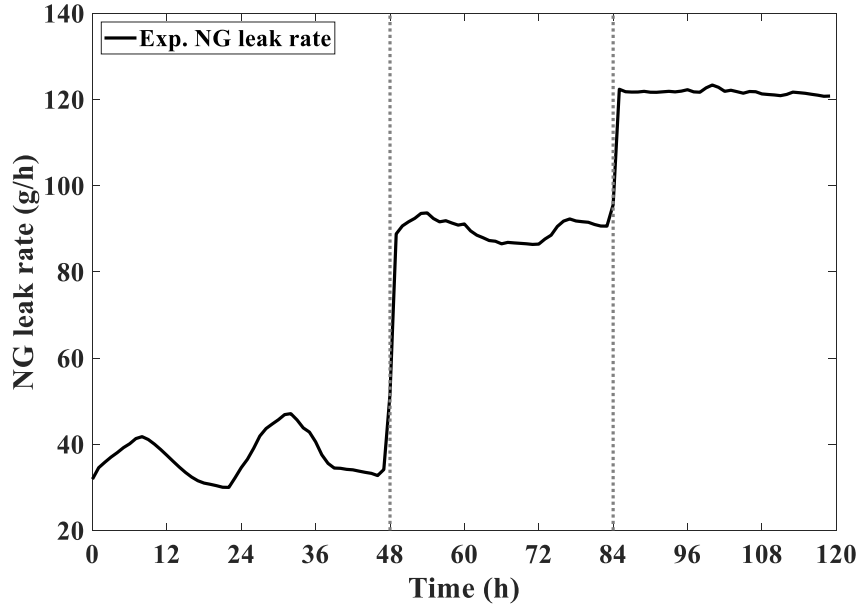
Polyvinyl chloride (PVC) pipe at a depth of 0.91 m below the ground surface (BGS), simulated a leaking pipeline at a depth consistent with the natural soil cover requirements for buried pipelines. The size and depth of the buried pipelines were selected to represent those of typical NG distribution mains. Compressed natural gas, consisting of 86% vol CH_4 , was delivered through stainless-steel tubing from 145-L cylinders, with emission rates averaging 37 ± 5 g/h for 48 hours (Level 1), 89 ± 7 g/h for 36 hours (Level 2), and 121 ± 4 g/h for 36 hours (Level 3) (Fig. 2. 1a). Each level of emission rate was initiated by regulating the gas pressure and opening the solenoid valve to achieve the intended leak rate.

Nineteen low-cost CH_4 detectors, which were modified based on CH_4 sensors in Cho et al. (2022), were deployed on the surface to measure surface and below-ground near-surface CH_4 concentrations every 5 seconds. Each CH_4 detector consists of two metal oxide semiconductors (TGS 2611-E, Figaro Engineering Inc.). The optimal detection concentration of the TGS 2611-E could be from 100 ppmv to 10000 ppmv (Cho et al., 2022). Prior to conducting experiments, the

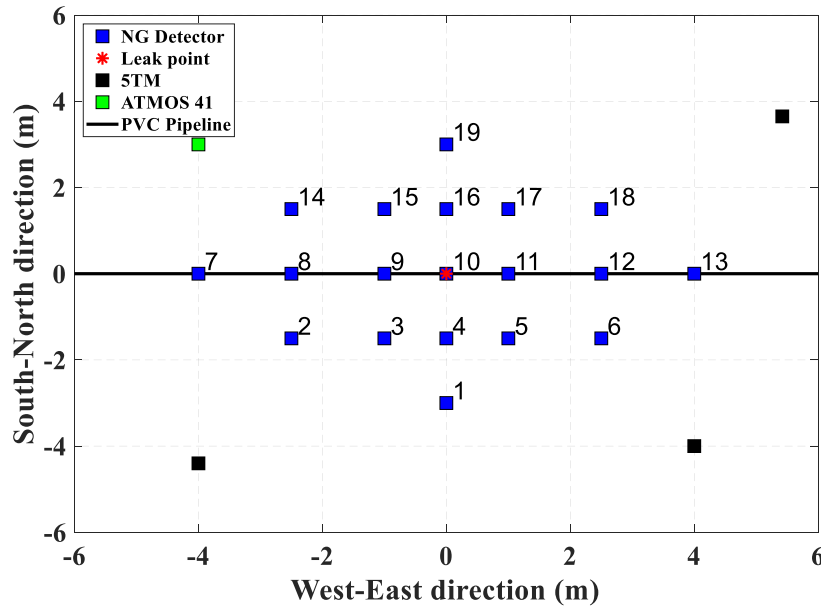
detectors were calibrated in the lab by comparing the trace gas detector analyzer (Picarro G4302). An approach suggested by Cho et al. (2022), which incorporates signals from metal oxide semiconductors, ambient temperature, and relative humidity, was applied to estimate the CH₄ concentrations. The details of the analysis and calibrations of the methane detectors can be found in Cho et al. (2022) and supplementary material (Appendix A.2) for details. The variation was correlated at an averaged R^2 value of 0.72 at the gas concentration between 500 to 1500 ppmv for various sensors. The average depth of the BNS CH₄ concentration measurement was 0.05 m (BGS). Additionally, each CH₄ detector also measured relative humidity (RH) and atmospheric temperature by an environmental condition sensor (BME280, Bosch Sensortec Inc.). The BME280 is accurate to $\pm 3\%$ RH and with a temperature range from -40 to 85 °C.

The CH₄ detectors were deployed on the soil surface in a rhombus configuration around the known subsurface emission point (Fig. 2. 1b). All low-cost CH₄ detectors were pre-heated for 24 hours before the experiment to stabilize the detector. A weather sensor (ATMOS 41, METER Group, Inc.) was used to measure wind speed, air temperature, atmospheric pressure, relative humidity (RH), and solar radiation at 0.5 m above the ground surface every 30 seconds. The ATMOS 41 could measure wind speed from 0 to 30 m/s with an accuracy of ± 0.3 m/s, air temperature from -50 to 60 °C with an accuracy of ± 0.6 °C, atmospheric pressure from 50 to 110 kPa with an accuracy of ± 0.1 kPa, RH from 0 to 100% with an accuracy of $\pm 0.1\%$, and solar radiation from 0 to 1750 W/m² with an accuracy of $\pm 5\%$ W/m². Measured meteorological data were used to estimate the atmospheric resistance (R_{at}). The measured wind speed during the experiment is shown in Fig. C. 1. Three soil moisture/temperature sensors (5TM, METER Group, Inc.) were installed at predesigned locations to measure soil moisture and temperature at the topsoil layer every 30 seconds. The depth of measured soil moisture and temperature was 0.1m BGS. The

5TM could measure volumetric soil moisture (VWC) from 0 to 100 % with an accuracy of $\pm 2\%$ VWC and soil temperature from -40 to 50 °C with an accuracy of ± 1 °C. Measured soil moisture and temperature were used to estimate the soil resistance (R_s) and the diffusion coefficient in the soil (D). The weather sensor and soil moisture and temperature sensors were connected to a ZL6 data logger (METER Group, Inc.) for data storage.



(a)



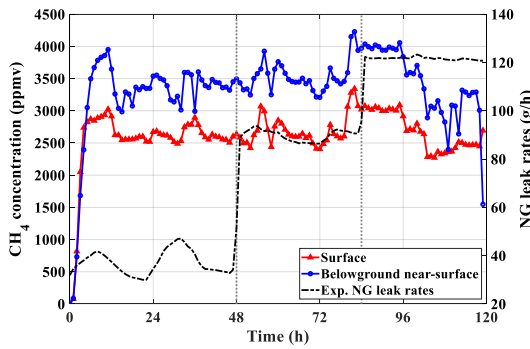
(b)

Fig. 2. 1. (a) The controlled NG leak rates in the field-scale 5-day experiment. The gray dotted lines represent the time when the released gas increased to the next level. (b) Plain view of experimental testbed and sensor layout. The PVC pipeline (gray line) and emission point (red star) were at 0.91 m BGS. The ATMOS 41 sensor (green square) was set up in the northeast of the testbed. Three 5TM sensors (black squares) were installed in the northeast, southeast, and northwest of the testbed.

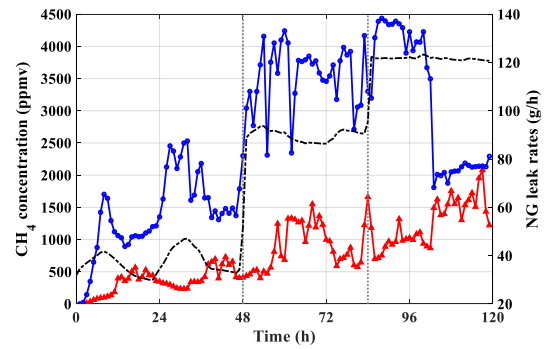
2.3 Results

2.3.1 Surface and BNS CH₄ Concentrations and Plumes

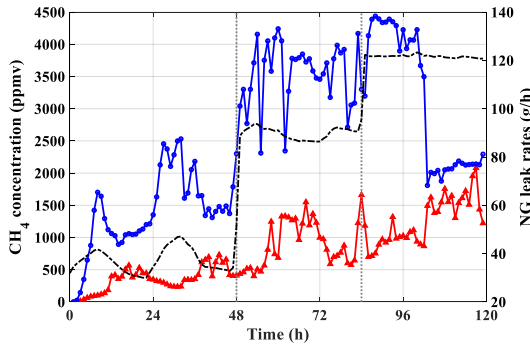
The measured surface and BNS CH₄ concentrations at distances from 0 m to 4 m (Fig. 2. 2) showed increasing trends with the increase of controlled gas leak rates. With the increase of measured distance from 0 m to 4 m, the range of variation of measured surface and BNS CH₄ concentrations decreased. During the experiment, the highest averaged surface and BNS CH₄ concentrations were detected at 0 m, which was directly above the leak point, with 2668 ppmv and 3219 ppmv (Fig. 2. 2a). The averaged BNS CH₄ concentrations were higher than averaged surface CH₄ concentrations ranging from 20% to 486% within a monitoring radius of 4 meters.



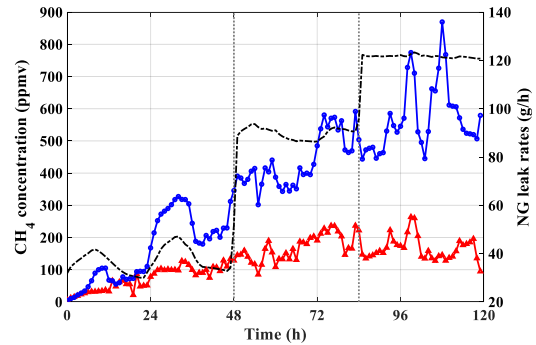
(a)



(b)



(c)



(d)

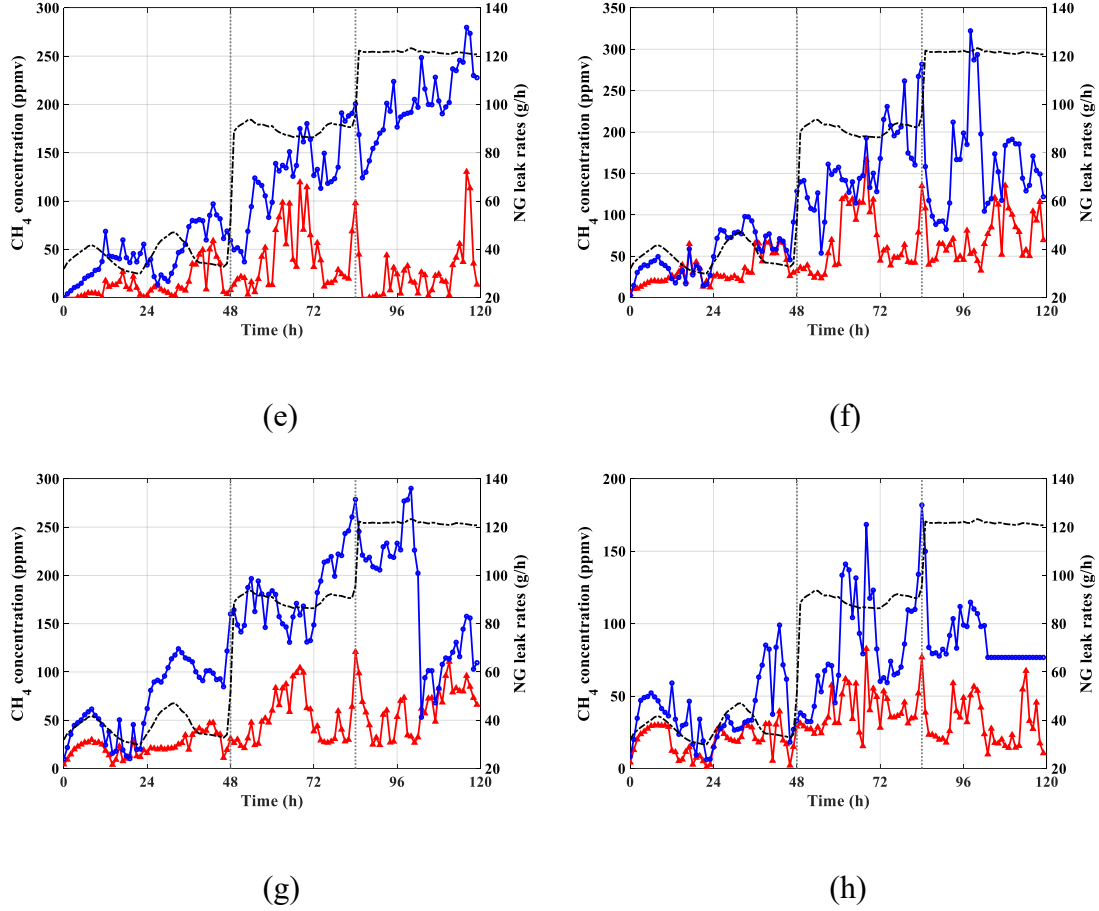
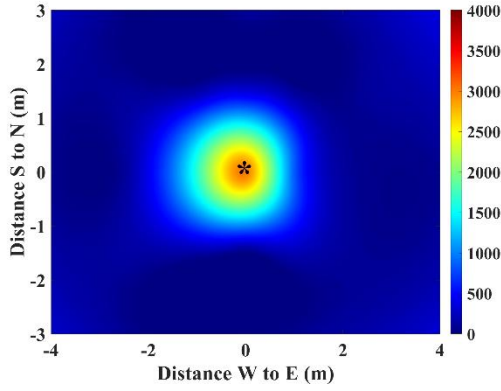


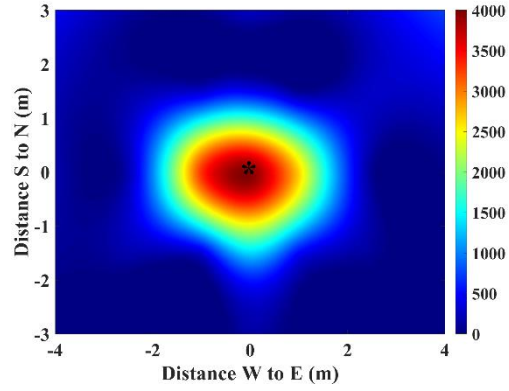
Fig. 2.2. Measurements of maximum surface and BNS CH_4 concentrations at (a) 0, (b) 1, (c) 1.5, (d) 1.8, (e) 2.5, (f) 2.9, (g) 3, and (h) 4 m from the leak point. The red line presents surface methane concentration, while the blue line indicates BNS CH_4 concentrations. The BNS CH_4 concentration in (h) shows a constant value from hour 104 due to the detection issue of the sensor. The dashed line presents the controlled NG leak rates (g/h). The gray dotted lines present the time when the released gas increased to the next level.

Fig. 2.3 displays the variation of the spatial distribution of CH_4 plumes measured at the surface (Fig. 2.3a, 3c, and 3e) and BNS (Fig. 2.3b, 3d, and 3f) when the averaged leak rate was increased from 89 g/h to 121 g/h between hour 84 and hour 86. The surface and BNS CH_4 concentrations decreased from 0 m to the boundary of the testbed. Furthermore, the surface and BNS CH_4 plumes extended from the leak point to the boundary of the testbed. The plume on the surface CH_4 plume extended approximately 1 m from the leak source, while the BNS CH_4 plume

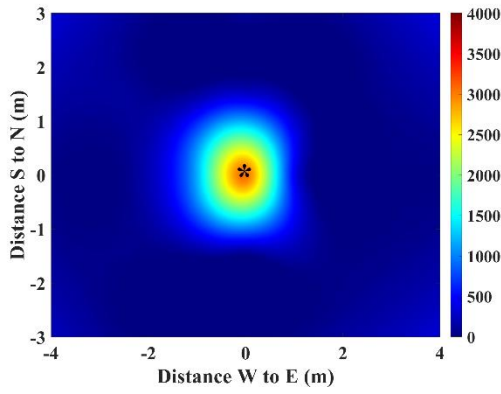
extended approximately 2 m from the source. The overall surface CH₄ expressions are also lower than the overall BNS CH₄ expressions.



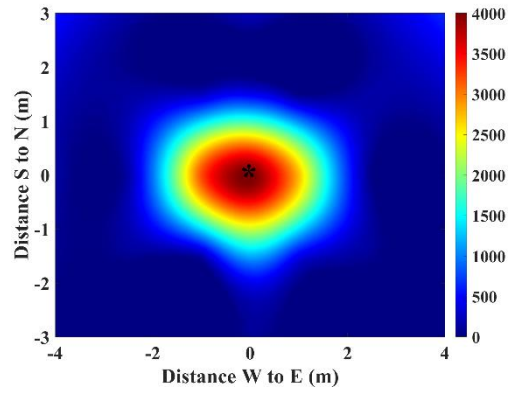
(a)



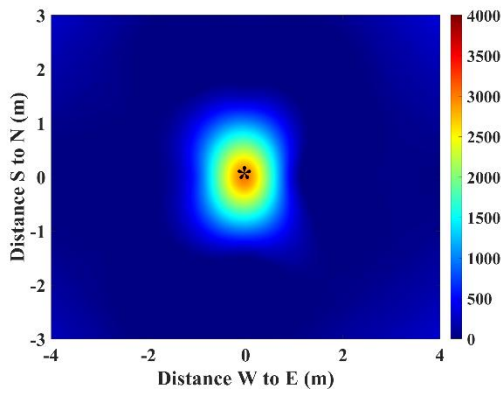
(b)



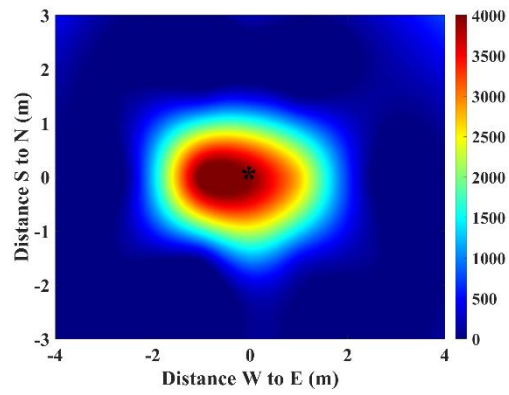
(c)



(d)



(e)



(f)

Fig. 2. 3. Top view of observed surface (a, c, and e) and BNS (b, d, and f) CH₄ expression (ppmv) from hour 84 to hour 86. The controlled gas leak rate increased from 89 g/h to 121 g/h during this period. The star marker (*) in the contour presents the location of the leak point.

2.3.2 Surface and BNS CH₄ Fluxes

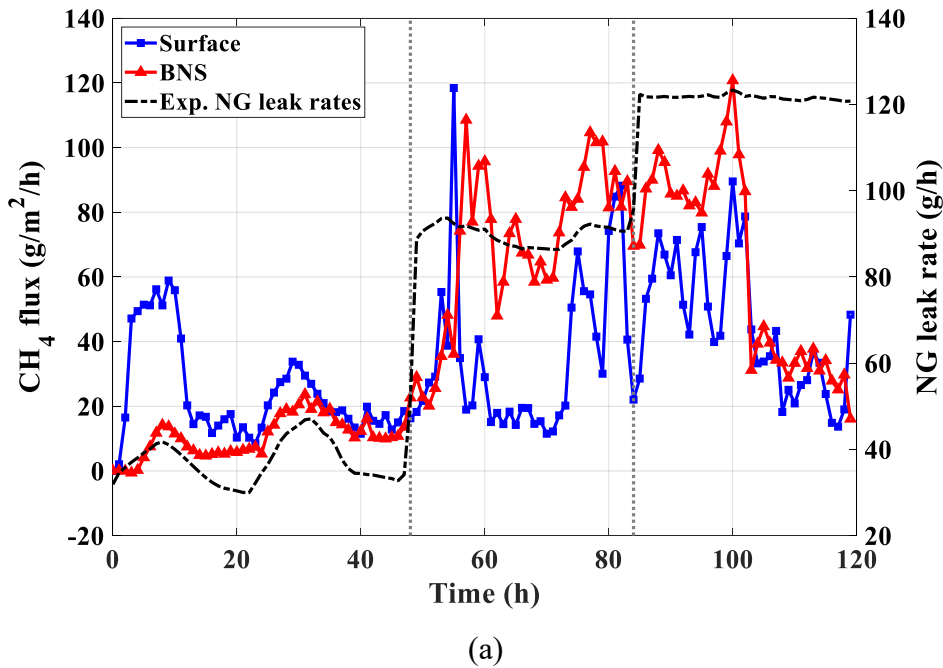
The estimated total surface (F_s) and BNS CH₄ fluxes (F_{ns}) summing surface and BNS CH₄ fluxes (Eq. 2.2 and Eq. 2.8) are shown in Fig. 2. 4a. The estimated atmospheric and soil resistances are shown in Fig. A.2. The averaged surface CH₄ flux was initially higher than the averaged BNS CH₄ flux by 14 g/m²/h prior to the NG leak rates increased. However, as the leak was increased from 37 g/h to 89 g/h at hour 48 and from 89 g/h to 121 g/h at hour 84, the averaged BNS CH₄ flux was higher than the averaged surface CH₄ fluxes by 31 g/m²/h and 16 g/m²/h, respectively. In addition, at hour 102, averaged surface and BNS CH₄ fluxes decreased to 34 g/m²/h and 38 g/m²/h, respectively.

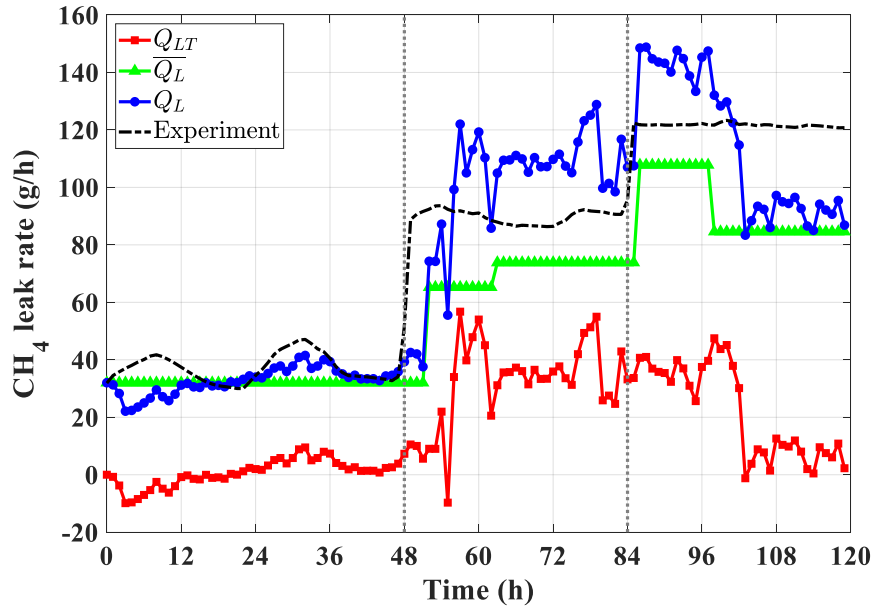
2.3.3 Modeled Non-steady NG Leak Rates

The estimations of steady-state NG leak rate ($\overline{Q_L}$), transient changes in NG leak rate (Q_{LT}), and modeled non-steady NG leak rates (Q_L) are presented in Fig. 2. 4b. The steady-state underground NG leak rate ($\overline{Q_L}$) increased from 32 g/h to 106 g/h from hours 52 to 85, while decreasing to 85 g/h at hour 97 with the increase of the experimental NG leak rates from 37 g/h to 121 g/h. Furthermore, the average transient NG leak rate (Q_{LT}) was 2 g/h until hour 56 and then suddenly increased to 37 g/h at hour 57 until hour 102. However, the average transient NG leak rate decreased to 8 g/h from hour 102 to hour 120. By combining steady ($\overline{Q_L}$) and transient (Q_{LT}) underground NG leak rates, the averaged modeled NG leak rates (Q_L), were obtained with 33 g/h, 98 g/h, and 114 g/h in levels 1, 2, and 3, respectively. Two increased trends of the modeled non-

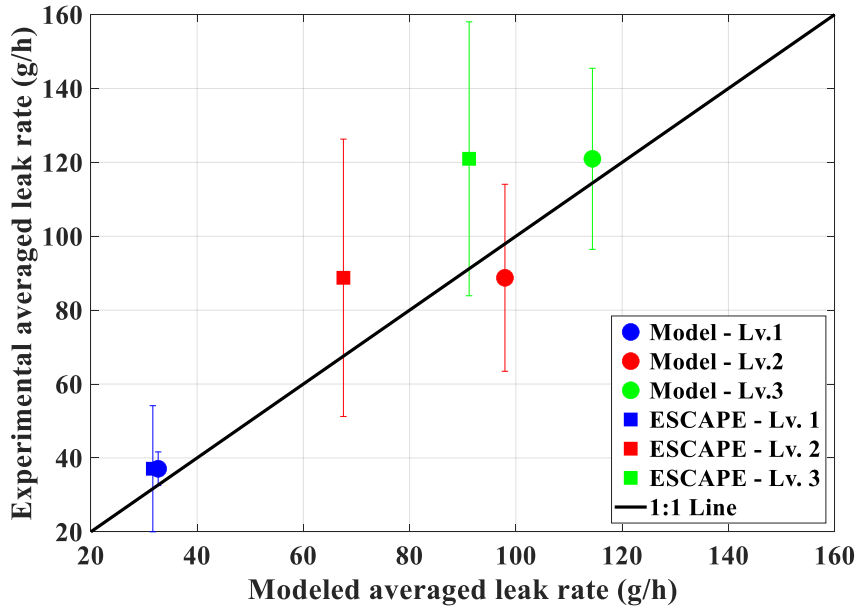
steady NG leak rates occurred at hour 53 and hour 85, while a decreased trend appeared from hour 102 to hour 120 in level 3 and retained an averaged NG leak rate of 94 g/h.

Comparison between the true NG leak rates and modeled NG leak rates generated by the original and modified ESCAPE model indicates that the overall modeled non-steady NG leak rates from the modified ESCAPE model were in better agreement ($R^2=0.77$ and $m=0.99$) than the leak rate from the original ESCAPE model ($R^2=0.45$ and $m=0.77$). This was also supported by the lower standard deviations and differences observed between the modeled and true NG leak rates at each gas leak scenario, as shown in Fig. 2. 4c. The differences between the modeled NG leak rates from the modified ESCAPE model and the true NG leak rates ranged from 5.7% to 11.9% for three NG leak rate scenarios. However, the modeled NG leak rates by the original ESCAPE model presented differences from 14.6% to 24.6%. Furthermore, the standard deviations of NG leak rates in the original ESCAPE model are from 17 g/h to 37 g/h, while those in the modified ESCAPE model are from 5 g/h to 25 g/h (Table 2. 1).





(b)



(c)

Fig. 2. 4. (a) The variations of estimated surface and BNS CH_4 fluxes with the controlled NG leak rates (black dashed line) during experiments. The gray dotted lines presented the time when the released gas increased to the next level. (b) The comparison between the estimated transient NG leak rates (Q_{LT}) (red circle line), average steady-state NG leak rates ($\overline{Q}_L$) (green triangles), and the modeled non-steady NG leak rates (Q_L) (blue circle line). (c) A comparison between the

experimental and modeled averaged NG leak rate from the modified (circles) and original (squares) ESCAPE model in each NG leak scenario. The black line presents the 1:1 line.

Table 2. 1. A summary of the estimated non-steady NG leak rate from both the ESCAPE and the modified ESCAPE model in each NG leak rate scenario. The "difference" column indicates the percentage difference between the experimental and modeled total leak rate.

NG release rate level		Experimental averaged leak rate (g/h)	Modeled averaged leak rate (g/h)	Difference (%)
ESCAPE	Lv. 1	37 ± 5	32 ± 17	14.6
	Lv. 2	89 ± 7	68 ± 38	23.9
	Lv. 3	121 ± 4	91 ± 37	24.6
Modified ESCAPE	Lv. 1	37 ± 5	33 ± 5	11.9
	Lv. 2	89 ± 7	98 ± 25	10.7
	Lv. 3	121 ± 4	114 ± 24	5.7

2.3.4 Different Number of Measured Locations

There were 8 different measured locations in the controlled gas release experiment (Fig. 2. 2). The changes in the NRMSE with the increase of measured locations from 2 to 8 in each gas leak rate level is illustrated in Fig. 2. 5. The decreased trend of NRMSE occurred at all leak rate levels as the number of measured locations increased from 2 to 8. The NRMSE decreased from 4.13 to 0.19 with the leak rate at Level 1, from 2.53 to 0.28 with the leak rate at Level 2, and from 1.14 to 0.2 with the leak rate at Level 3. Furthermore, the NRMSE with leak rates at Levels 2 and 3 were gradually higher than that at Level 1 as the number of measured locations increased from 3 to 5, respectively.

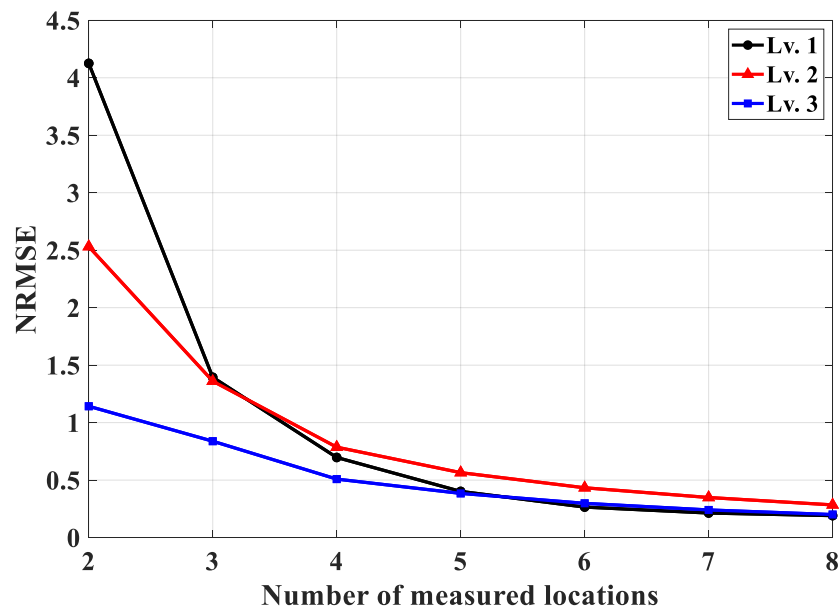


Fig. 2. 5. The NRMSE with the selected number of measured locations from 2 to 8 in the modified ESCAPE model during the leak rate at Levels 1 to 3.

2.4 Discussion

2.4.1 Transport of Surface and BNS CH₄

The surface and BNS CH₄ plume areas increased and expanded as the NG leak rate increased, with CH₄ preferentially migrating from the leak point towards the testbed boundary (Fig. 2. 3). The large difference between the surface and BNS CH₄ plumes indicates that the BNS CH₄ plume area developed much faster and over a greater distance than the surface CH₄ plume area. Thus, the surface CH₄ expression may not be suitable for describing the evolution of the BNS CH₄ expression. Furthermore, the observed difference between the estimated total surface and BNS CH₄ fluxes (Fig. 2. 4a) indicates that the transportation of CH₄ between the surface and BNS layers was in an unsteady state. Hence, the measurement of the BNS CH₄ should be considered when trying to understand the non-steady gas migration of CH₄ from the subsurface to the atmosphere.

The inverse relationship observed between the variations of atmospheric resistance and the changes in surface CH₄ flux (Fig. C. 3) suggests that an increase in atmospheric resistance decreased the transportation of CH₄ from the surface to the atmosphere. A comparison between soil resistances, soil moisture, and BNS CH₄ fluxes (Fig. C. 4) suggests that high soil moisture induced low soil resistance to enhance the transportation of the BNS CH₄ flow. The elevated BNS CH₄ flux is a result of an increase in CH₄ concentration in soil due to low soil resistance. Based on the variation of atmospheric and soil resistances in Fig. A.1, the atmospheric resistance was higher than the soil resistance from hours 84 to 86, with an average value of 0.10 s/m and 0.04 s/m, respectively. Thus, the slight differences in the CH₄ plume on the surface may be due to high atmospheric resistance but low soil resistance in the transportation of CH₄ during this period.

During the experiment, the soil resistance decreased from 0.13 s/m to 0.04 s/m when the leak rate increased from the first level to the second level for 9 hours (from hour 48 to hour 57).

Subsequently, it remained at an average value of 0.04 s/m until the end of the experiment (Fig. A.1). This decrease in soil resistance facilitated the transportation of CH₄ flow from the BNS to the surface, resulting in higher BNS CH₄ fluxes than surface CH₄ fluxes from hour 57 to hour 102. However, although the soil resistance remained at a low value of 0.04 s/m from hour 102 to hour 119, the BNS CH₄ fluxes decreased during this period. This decrease may have been induced by the occurrence of precipitation from hour 81 to hour 94 (Fig. C. 5). The precipitation during this period did not significantly change soil moisture at the depth of 0.1 m but retained an average value of 0.11. Therefore, we speculated that the precipitation during this period may have caused the BNS (at a depth of 0.05 m) to approach full saturation, resulting in more lateral gas migration than vertical gas migration.

Comparing calculated surface and BNS CH₄ fluxes can provide indications of the response time that released NG from the pipeline reached the surface and belowground surface (Fig. C. 6). For instance, the apparent increase in BNS CH₄ flux at hour 51 suggests that the underground NG reached the BNS 3 hours after the leak rate was increased. There were five response times when increases in BNS CH₄ flux occurred at hours 51, 62, 85, and 97. These increases suggest that the underground NG leak rates may have increased before these times. However, compared to the BNS CH₄ flux, the change in surface CH₄ flux after hour 71 showed an almost continuous increase from hour 71 to hour 97, making it difficult to determine the possible time of change in underground NG leak rates. Therefore, these results emphasize the importance of determining BNS CH₄ fluxes in quantifying underground NG leak rates.

2.4.2 Modeled Non-steady Underground NG Leak Rates

The fluctuation of the transient underground NG leak rate (Fig. 2. 4b) reveals the CH₄ emission suppression (-) and promotion (+) caused by atmospheric and soil conditions. Furthermore, the time lag between the true NG leak rate and the modeled NG leak rate may serve as an indicator of the average travel time of CH₄ migration from the pipeline to the surface and BNS. For instance, the increase in the modeled NG leak rate at hour 57 indicates that the leaked NG may spend 9 hours reaching the CH₄ detectors. The decrease in modeled NG leak rates after hour 102 may be attributed to the reduction in BNS fluxes due to the lateral BNS gas migration by precipitation between hour 81 to hour 94. The improvements in the standard deviation and differences in modeled non-steady NG leak rates by the modified ESCAPE model (Fig. 2. 4c and Table 2. 1) indicate the importance of BNS soil properties and gas migration in the quantification of non-steady NG leak rates. The decrease in the difference in the modeled non-steady NG leak rates indicates that the modified ESCAPE model could properly capture the non-steady variations of NG leak rates in a high leak rate scenario.

A significant difference between the modified and original ESCAPE model is that the former incorporated BNS CH₄ measurements and time-varying soil properties (such as soil moisture and temperature) in the inversion algorithm for quantifying underground NG leak rates. This improvement not only advanced the performance of modeled non-steady NG leak rates with lower differences and standard deviations but also provided a significant indication that soil properties and BNS CH₄ measurements should be carefully considered in the detection and quantification of underground NG leak rates.

2.4.3 Number of Measured Locations in the Modified ESCAPE Model

The decrease in NRMSE at each leak rate scenario (Fig. 2. 5) indicates modeled non-steady NG leak rate agreed well with the true NG leak rate as the number of measured locations increased. When the number of measured locations increased to 4, the NRMSE dropped below 1 at Levels 1 to 3. Thus, the recommended number of measured locations was 4 within a radius of 4 meters. However, the NRMSE values with the leak rates at Levels 2 and 3 were slightly higher than that at Level 1 as the number of measured locations increased. The slight difference may be attributed to uncertainties in measurements and simulation as gas leak rates increased from Level 1 to 3. These results suggest that a larger number of measured locations may lead to a more accurate estimation of non-steady gas leak rates, but there may be limitations due to uncertainties in the model simulations and measurements.

2.5 Conclusions

Intending to estimate non-steady state CH₄ leak rates over time, the present study developed and tested a model based on the concept of coupling soil and atmospheric resistances, key environmental parameters, and limited belowground and surface CH₄ concentration measurements. Experimental observations demonstrate BNS CH₄ concentrations 20% to 486% higher than the vertically equivalent surface CH₄ concentrations within the lateral surface expression of the NG plume (radius of 4 m). Elevated concentrations varied based on distance from the leak location and environmental variability (e.g., atmospheric stability and wind conditions). Furthermore, with an increase in the gas leak rate from 37 to 89 g/h, a significant variation in the average BNS CH₄ concentration was observed within 3 hours of the increase. However, changes to the surface CH₄ concentrations during this period were not present due to the dominant influence of atmospheric variability on surface concentrations. When the controlled NG leak rate increased from 37 to 121 g/h, the belowground plume area expanded first, extending approximately two times farther than that of the surface presentation of the leak, demonstrating the elevated subsurface migration prior to surface indication. The significant differences observed indicate that BNS CH₄ concentration is an important factor in leak rate estimates as the surface expression does not necessarily define the belowground plume location/behavior. The modified ESCAPE model incorporates soil and atmospheric resistance to estimate both the steady and non-steady state NG leak rate. The estimated non-steady underground NG leak rate not only agreed well with experimental NG leak rates ($m=0.99$ and $R^2=0.77$) but also captured the response time in the detection and the evolution of the gas leakage after the gas leak rate increased. The performance of the model improved when the leak rate was in the low and moderate NG leak rate categories (i.e., from 37 to 121 g/h). These results show that integrating the belowground soil

characteristics and gas measurements with the atmospheric variability could advance the quantification of non-steady underground NG leak rates. The scenario analysis of measured locations indicates that four locations are needed to estimate underground non-steady NG leak rates using the low-cost, near-real-time CH₄ detector network. In conclusion, the proposed low-cost near-real-time CH₄ detector network and the modified ESCAPE model offer an innovative tool for the industry to assess risk and address and potentially prevent gas leakage incidents.

Chapter 3. Influence of Soil Properties and Soil Aeration Design on Subsurface Methane Removal²

Abstract

Elevated methane (CH₄) concentrations in the vadose zone following natural gas (NG) pipeline leaks present environmental and safety hazards. Soil aeration is commonly used to mitigate subsurface CH₄, but conventional designs rarely consider soil properties, leading to variable CH₄ mass removal efficiency (Re_{MCH4}) and aeration duration. To quantify how soil characteristics and aeration system parameters jointly control Re_{MCH4} , we conducted controlled soil aeration experiments at the Methane Emission Technology Evaluation Center at Colorado State University and integrated measurements with a modified multiphase, multicomponent transport model. Over 100 scenario simulations were performed to evaluate Re_{MCH4} and the time required to reduce CH₄ concentrations below 0.005 vol.% across varying soil types, water saturations, bar hole configurations, and vacuum pressure (P_b). Experimental Re_{MCH4} showed that a rapid depletion near bar holes occurs during early aeration when transport was advection dominated, followed by slower removal from less accessible pore space when transport became diffusion-limited. The intrinsic permeability and soil water saturation controlled plume capture. Wet conditions enhanced capture, whereas low-permeability soils prolonged removal. Bar hole number and spacing relative to the initial plume control airflow distribution. Misalignment reduces Re_{MCH4} by 20% to 30% through airflow bypass and competition. Moderate P_b enhances local advection and improves removal, whereas further increases create diminishing returns. Optimized designs achieve 97 to

² This chapter is based on a manuscript in preparation, which is entitled “Influence of Soil Properties and Soil Aeration Design on Subsurface Methane Removal” by Jui-Hsiang Lo, J. R. R. Navodi Jayarathne, Daniel Zimmerle, Kathleen Smits

98% Re_{MCH_4} within 60 min, whereas suboptimal configurations substantially delay cleanup. These findings highlight the importance of integrating soil characteristics into system design to maximize subsurface CH_4 mitigation and improve pipeline safety through NG soil aeration.

3.1 Introduction

Elevated concentrations of natural gas (NG) in the vadose zone following subsurface pipeline leaks pose persistent environmental and public safety risks. Methane (CH_4), the primary component of NG, can migrate through unsaturated soils, accumulate in confined spaces, and contribute to greenhouse gas emissions if not effectively removed. As aging pipeline infrastructure operates in increasingly urbanized environments, reliable mitigation requires predictive understanding of gas transport and removal in the vadose zone under site-specific soil conditions. Soil aeration is a widely implemented method to remove trapped NG from the vadose zone after leaks are identified. This approach typically involves the installation of boreholes, commonly referred to as bar holes, near confirmed or suspected leak locations. Gas migrates from the surrounding soil toward these bar holes through passive venting or vacuum-assisted aeration. The aerated gas is captured for treatment or directly released to the atmosphere in accordance with site-specific regulatory constraints. The aeration process is repeated with additional bar holes until subsurface CH_4 concentrations are reduced below established safety thresholds.

Despite its widespread use, NG soil aeration often exhibits various removal efficiency and concentration rebound, in which CH_4 levels rise above acceptable limits following an initial reduction. These outcomes can prolong mitigation efforts, increase operational costs, and introduce uncertainty in cleanup timelines. A primary reason for these inefficiencies is the mismatch between aeration system design and site-specific subsurface conditions that govern gas migration and mass transfer (American Gas Association, 2023; Sarabia, 2019; E. Six, 2014; Spectrum News, 2019; U.S. Environmental Protection Agency, 2019). Key design and operational parameters, including bar hole spacing and number, aeration flow rate, applied vacuum pressure, and operating duration, are commonly selected using generalized or empirical guidelines that do not explicitly account for

soil heterogeneity or gas transport behavior. As a result, aeration performance can vary substantially across sites with similar system configurations but differing soil properties.

In current field practice, bar holes are typically installed above the pipeline and distributed based on the inferred extent of the subsurface NG plume, site access constraints, and removal objectives. Gas removal is achieved through passive aeration over several days or through active aeration using vacuum pumps to enhance advective transport. Subsurface CH₄ concentrations are monitored to assess progress toward safety targets. While these practices form the basis of standard mitigation guidance (Pipeline and Hazardous Materials Safety Administration, 2017), they do not explicitly incorporate soil properties that control gas permeability, effective diffusion, and moisture-dependent flow resistance. Consequently, sites with low-permeability soils or elevated water saturation can experience limited gas mobility and prolonged aeration durations. For example, in Georgetown, Texas, NG venting continued for more than 30 days without achieving non-hazardous concentrations. Post-incident analyses attributed the prolonged cleanup to low intrinsic permeability and elevated water content that restricted gas transport (Sarabia, 2019; E. Six, 2014; Spectrum News, 2019). Such cases underscore the need to quantify how soil physical properties and moisture conditions influence aeration effectiveness.

Relatively few experimental or numerical studies have systematically examined the coupled effects of soil properties and aeration system design on subsurface CH₄ removal. Conceptual guidance can be drawn from soil vapor extraction (SVE), a well-established vadose-zone remediation technology for volatile organic contaminants. Both SVE and NG soil aeration rely on mass transfer of gas-phase constituents followed by advective and diffusive transport toward extraction points such as wells or bar holes (Digiulio, 1992; Fischer et al., 1998; Suthersan et al., 1999; U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1995).

However, substantial differences in operational scale, duration, and driving forces limit the transferability of SVE-based design approaches to NG soil aeration. SVE systems typically operate for months to years and treat areas on the order of 900–4000 m² (U.S. Environmental Protection Agency, 1998), whereas NG soil aeration is deployed at localized leak sites to reduce gas concentrations in the vadose zone within hours to days. In addition, SVE systems generally apply relatively low pressure drawdowns relative to atmospheric pressure, typically 0.05 to 0.1 atm, and often incorporate active air injection to enhance contaminant removal. In contrast, NG soil aeration can use substantially larger pressure drawdown relative to atmospheric pressure (e.g., 0.9 atm), and may rely solely on aeration at bar holes. These differences imply distinct gas transport dynamics, mass-transfer limitations, and rebound mechanisms that conventional SVE design assumptions may not capture. While SVE concepts provide a useful organizing framework, NG soil aeration requires modeling approaches that explicitly account for short operational timescales, large pressure drawdown, and strong sensitivity to soil heterogeneity and moisture conditions.

Numerical modeling offers a practical means to isolate key controls on NG removal under controlled conditions and to guide field implementation. Although direct modeling studies of NG soil aeration are limited, gas transport models developed for SVE applications provide a physical basis for extending such analyses to NG mitigation scenarios (Barnes, 2003; Barnes & White, 2006; Benson, 2011; Harper et al., 2003; V. T. Nguyen et al., 2013; Scientific Software Group, 2011; U.S. Army Corps of Engineers, 2002). As in SVE, soil physical properties are expected to exert primary control on aeration performance by governing advective and diffusive gas transport. Soil texture and structure influence permeability and tortuosity. Coarse-grained soils (e.g., sand) can support more rapid gas migration than fine-grained soils (e.g., silt loam), whereas increasing water saturation reduces air-filled porosity and gas permeability, thereby limiting CH₄ transport.

In layered systems, permeability contrasts can promote gas entrapment and contribute to rebound after aeration.

Motivated by these considerations, this study combines controlled field-scale experiments with a modified multiphase, multicomponent transport model (Deepagoda et al., 2016; Gao et al., 2021) to investigate subsurface CH₄ migration and mass removal during NG soil aeration under varying soil conditions and system designs. We hypothesize that CH₄ removal efficiency, radius of influence, and rebound behavior are governed by soil physical properties and their interaction with aeration design and operational parameters. Six controlled field-scale experiments were conducted to characterize subsurface CH₄ behavior during aeration and to evaluate model performance. Using the modified model, 108 scenario simulations were performed to systematically assess CH₄ mass removal efficiency, radius of influence, and aeration duration across representative sand and silt loam conditions and system configurations. In this study, dry and wet near-surface soil conditions are compared only within the tested range of saturation, plume geometry, and aeration configuration. The improved removal observed under wet near-surface conditions is interpreted as a boundary-condition effect on airflow pathways and plume capture, not as a general indication that wetter soils are easier to remediate. The results provide quantitative guidance for site-specific NG soil aeration design by linking soil properties and operating conditions to CH₄ removal performance, with implications for more efficient mitigation and improved safety outcomes.

3.2 Methods

3.2.1 Controlled Soil Aeration Experiments

Controlled field-scale soil aeration experiments were conducted to obtain measurements for evaluating NG soil aeration performance and validating the numerical model. Experiments were conducted at the Methane Emissions Technology Evaluation Center (METEC), Colorado State University (Fort Collins, CO, USA), which supports controlled NG releases under monitored atmospheric, surface, and subsurface conditions. A rural, grass-covered testbed was selected for the soil aeration experiments. Testbed construction details are provided in (Jayarathne et al., 2024; Jayarathne, Kolodziej, et al., 2022a). The testbed soil was classified as sandy loam based on laboratory grain-size analysis. A controlled leak source was installed at a depth of 0.91 m below ground surface to release NG at prescribed rates and to establish subsurface CH₄ plume prior to aeration (Fig. 3. 1). Subsurface CH₄ concentrations were monitored using six non-dispersive infrared CH₄ sensors (INIR-ME100, SGX Sensortech Inc.) installed at depths of 0.3, 0.6, and 1.8 m and horizontal distances of 1 to 3.6 m from the leak point. Data were recorded at 5 s intervals. Co-located soil moisture and temperature sensors (TEROS 10 and 11, and 5TM, METER Group, Inc.) were used to track hydrothermal conditions during the experiments. Details of sensors can be found in Appendix A.3.

The soil aeration system consisted of pre-drilled bar holes connected to venturi-based purgers (Appendix B.3) that were supplied by a high-pressure air compressor through a manifold (Fig. 3. 2). Details of purgers that were used in this study can be found in Appendix B.3. Bar holes were spaced approximately 1.5 m apart. In each scenario, only selected holes were activated, and the remaining holes were sealed. Aeration was initiated by operating the venturi-based purgers to achieve an average pressure drawdown of 5 psi relative to atmospheric pressure at the active bar

holes, resulting in a maximum total extraction flow rate of 0.25 m³/min per purger. Six experimental scenarios were conducted (Table 3. 1) to evaluate the effects of near-surface water saturation and bar hole number. For each scenario, NG was released for 8 h at leak rates of 0.3 to 0.7 kg/h (8 to 20 SLPM) to establish a quasi-stable subsurface plume (Gao et al., 2021; Jayarathne et al., 2024; Ulrich et al., 2019). The leak was terminated prior to initiating aeration.

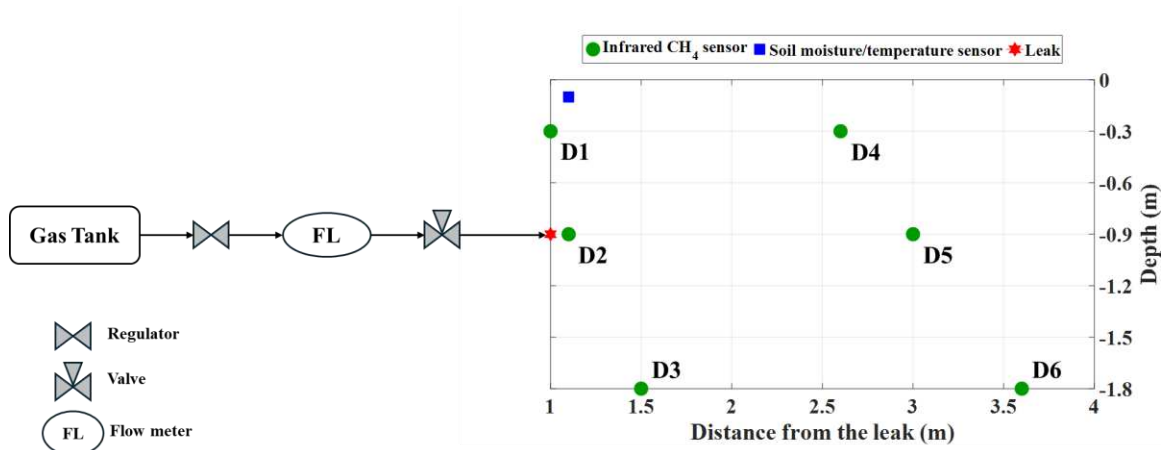


Fig. 3. 1. Schematic of subsurface sensors used in the controlled soil aeration experiments. Compressed NG is delivered from the gas tank to a leak. A pressure regulator, flow meter, and control valve control the leak rate. Six non-dispersive infrared methane sensors (INIR-ME100, green circles) were installed underground to monitor subsurface CH₄ concentrations. Soil moisture and temperature at the INIR-ME100 locations are monitored by soil moisture and temperature sensors. A near-surface soil-moisture/temperature sensor (5TM) at 0.1 m depth (blue square) recorded near-surface soil moisture and temperature. The black arrow denotes the direction of NG flow, and the x-axis indicates horizontal distance from monitoring locations (D1 to D6) to the leak.

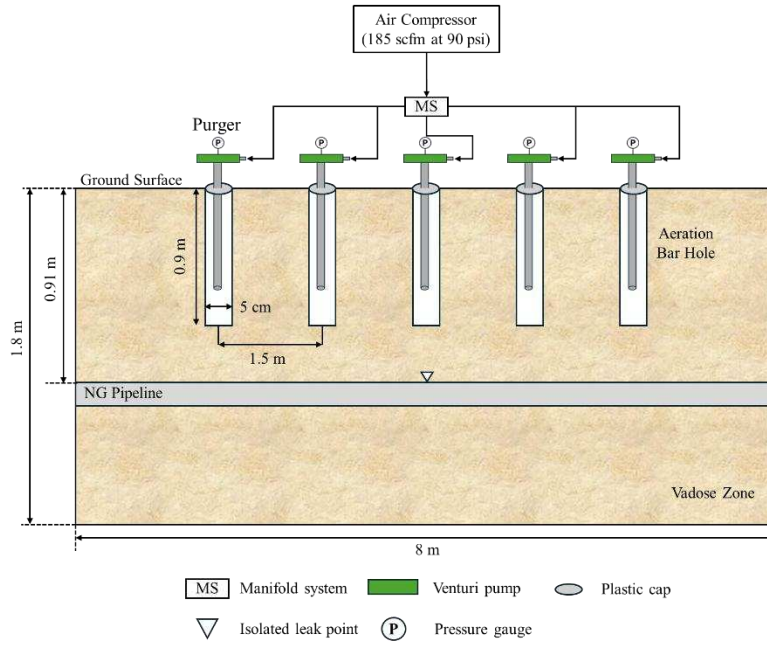


Fig. 3. 2. Cross-sectional schematic of the soil aeration system with multiple purgers and aeration bar holes in the controlled experiments. Purgers and bar hole locations ranged from 1 to 5, depending on the selected experimental scenarios in Table 3. 1. Each aeration bar hole was drilled to a depth of 0.9 m (3 ft), with a diameter of 5 cm (2 in.), and installed at an average spacing of 1.5 m (5 ft). This schematic illustrates a configuration with three purgers. The NG pipeline was buried at 0.91 m below the ground surface. The air compressor delivered a total compressed airflow of 185 SCFM at 90 psi, which was distributed to each purger through the manifold system. Each purger generates a vacuum pressure of approximately 5 psi (0.3 atm) at the bar hole during aeration to remove gas from the vadose zone. The pressure gauge of the purger was used to monitor the vacuum pressure. The plastic cap of the purger was used to seal the top of the bar hole to prevent air from entering the bar hole. The white triangle denotes the isolated leak point.

Table 3. 1. Experimental scenarios and operation strategies of aeration in controlled experiments. “D” is used to present the dry soil condition. “WS” is applied to describe the wet near-surface condition.

Scenario #	Experimental Scenarios	Number of Aeration Bar Holes	Averaged Leak Rate kg/h (SLPM)	Aeration Duration (hours)	Average Saturation (S_w) ^a
S1	Dry soil (D)	1	0.7 (20)	1	0.1
S2	Wet near-	1	0.4 (10)	2	0.8

	surface (WS)				
S3	Dry soil (D)	3	0.3 (8)	5	0.1
S4	Wet near-surface (WS)	3	0.4 (10)	1.3	0.8
S5	Dry soil (D)	5	0.4 (10)	1.8	0.1
S6	Wet near-surface (WS)	5	0.4 (10)	1	0.8
a. The average saturations were calculated using measured soil moisture at a depth of 10 cm below the ground surface and porosity.					

3.2.2 Numerical Simulation

A two-dimensional, two-phase (water and gas) and two-component (CH_4 and air) transport model (Gao et al., 2021) was used to simulate the CH_4 removal from the vadose zone during NG soil aeration under varying soil conditions and system designs (Fig. 3. 3). The solid phase was treated as unreactive, rigid, and incompressible. Soil properties were assumed homogeneous and isotropic, and simulations were conducted under isothermal conditions. Simulations were conducted in a two-dimensional Cartesian vertical domain measuring 40 m in the horizontal direction and 5 m in the vertical direction. The primary bar hole was located above the leak point, and additional bar holes were placed symmetrically at prescribed spacing at a depth of 0.9 m.

The water saturation field was prescribed and held constant during aeration because aeration durations were short relative to water redistribution timescales. Dissolution of CH_4 into pore water was neglected because its aqueous solubility is low relative to the gas phase mass under the modeled conditions (Gao et al., 2021). The leak source was terminated prior to aeration to represent a post-repair scenario.

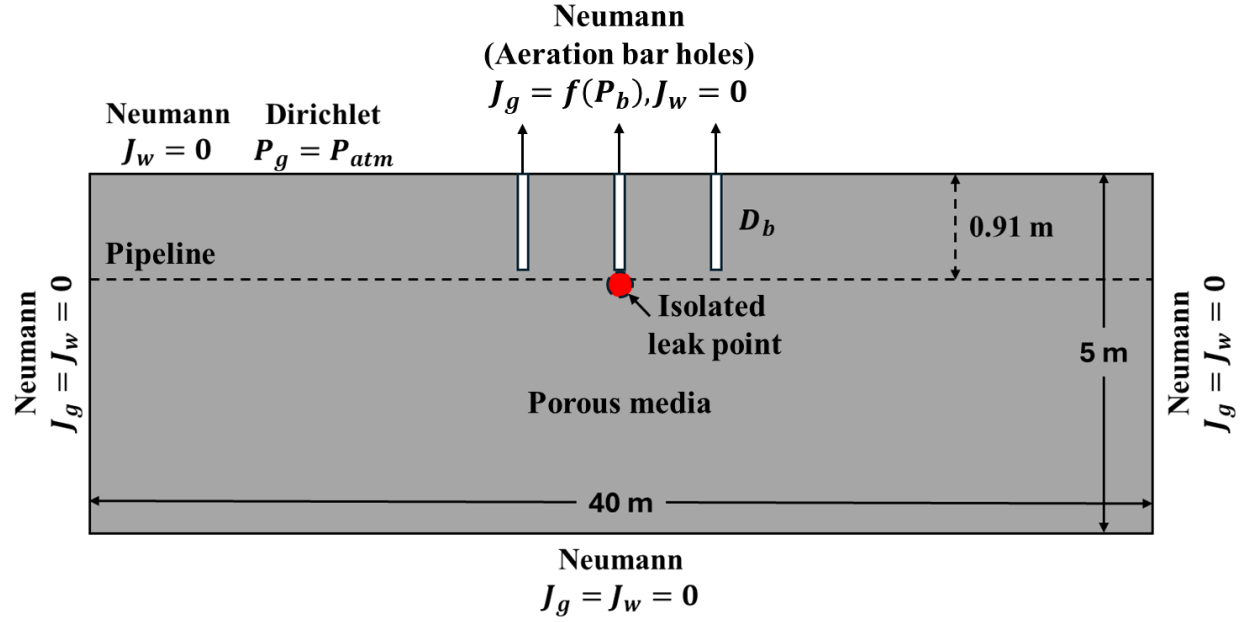


Fig. 3. 3. Two-dimensional conceptual model of soil aeration. The white rectangles represent aeration bar holes. J_w and J_g indicate water and gas flux, respectively. No-flux boundary conditions are applied on all outer sides ($J_g = J_w = 0$). The gas flux (J_g) at the aeration bar hole describes the aerated gas flux from the soil into the aeration bar hole based on the vacuum pressure (P_b). The gas flux is treated as constant at the interface between the soil and the aeration bar holes. Each bar hole is 3 cm in diameter and 0.9 m deep (D_b). The dashed line indicates the NG pipeline, and the red circle illustrates an isolated leak point. P_g describes the gas pressure, while P_{atm} is atmospheric pressure. Three bar holes are shown here for illustration. The actual number varies across simulation cases.

Governing equations for two-phase flow and CH_4 transport follow Gao et al. (2021), enabling us to quantify how soil properties and aeration design jointly control gas migration and removal. Mass conservation for the gas and water phases is given by:

$$\phi \frac{\partial(\rho_i S_i)}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}_i) = 0 \quad \text{Eq. 3. 1}$$

where the subscript i represents the liquid water (w) and gas (g) phases, ϕ is the porosity of the soil (-), ρ_i is the density of the fluid in i phase (kg/m^3), S_i is the saturation of fluid in i phase, and $\mathbf{u}_i$ is the Darcy velocity of fluid in i phase (m/s), defined as:

$$\mathbf{u}_i = -\frac{K_{in}k_{ri}}{\mu_i}(\nabla P_i + \rho_i \mathbf{g}) \quad \text{Eq. 3. 2}$$

where k is the intrinsic permeability of soil (m^2), k_{ri} is the relative permeability of fluid in i phase (-), μ_i is the viscosity of the fluid in i phase ($\text{Pa}\cdot\text{s}$), P_i is the pressure of fluid in i phase (Pa), and $\mathbf{g}$ is the gravitational acceleration (m/s^2). The relationship between capillary pressure, saturations of gas and aqueous phases, and relative permeability is described by the van Genuchten model (van Genuchten, 1980).

Gas phase transport of CH_4 is described by:

$$\phi \frac{\partial(\rho_g w_{\text{CH}_4} S_g)}{\partial t} + \nabla \cdot (\rho_g w_{\text{CH}_4} \mathbf{u}_g) - \nabla \cdot [D_{\text{CH}_4}^* \nabla(\rho_g w_{\text{CH}_4})] = 0 \quad \text{Eq. 3. 3}$$

where w_{CH_4} is the mass fraction of CH_4 (-) and $D_{\text{CH}_4}^*$ is the effective diffusion coefficient tensor of CH_4 in the vadose zone (m^2/s), which is estimated by Millington and Quirk's (1961) equation.

Boundary conditions for gas flow and CH_4 transport are shown in Fig. 3. 3. At the ground surface, gas pressure was set to atmospheric pressure (P_{atm}). At the bar hole boundary, aeration was represented using the manufacturer purger specifications, and internal flow within the bar hole was not simulated. No gas flux was imposed on the lateral and bottom boundaries to minimize boundary losses. For the water phase, the saturation was prescribed and held constant during aeration. The initial saturation profile was defined assuming hydrostatic equilibrium. For CH_4 transport, the bar hole boundary was treated as an outlet. At the ground surface, an open boundary condition was applied with an inflow CH_4 mass fraction set to the atmospheric background value. For outflow at the ground surface, a convective outflow condition with zero diffusive flux was imposed. A zero diffusive flux was imposed the lateral and bottom boundaries to minimize boundary losses (Nguyen et al., 2013).

3.2.2.1. Soil characteristics and design parameters of soil aeration

Soil characteristics impact subsurface CH₄ migration and removal efficiency. Sand with high permeability promotes rapid gas movement and effective CH₄ removal, while silt loam with low permeability restricts airflow and reduces removal efficiency. Therefore, sand and silt loam were selected as representative soils in the numerical simulations. The silt loam is used as a representative lower-permeability soil condition under the present Darcy-based transport assumptions and is not intended as a general representation of clay-rich soils. Soil water saturations (S_w) were set to 0.2, 0.4, and 0.6 on the surface, with a fixed bottom saturation of 0.3. The van Genuchten model was used to relate relative permeability to saturation, and soil temperature was held constant at 20 °C. Physical and hydraulic properties were obtained from Gao et al. (2021) (Table 3.2).

Key design parameters included applied vacuum pressure (P_b) and bar hole deployment. P_b was used to calculate based on industry purger specifications, ranging from 0 to 0.9 atm (0 to 13 psi) relative to standard atmospheric pressure (1 atm, 14.7 psi). A pressure of 0 atm represents passive aeration, where CH₄ migration occurs solely by natural diffusion. Simulation scenarios were divided into three cases based on the number and spacing of aeration bar holes (Table 3.2). Case #1 used a single bar hole above the leak, while Cases #2 and #3 used three bar holes spaced symmetrically at 1 m and 5 m, respectively.

Table 3. 2. Physical and hydraulic properties used in numerical simulations for representative sand and silt loam, including porosity (ϕ), residual soil water saturation (S_r), van Genuchten parameters, and intrinsic permeability (k). Values were derived from laboratory measurements (Gao et al., 2021) and literature to represent contrasting higher- and lower-permeability soil conditions under

present transport model (Bonazountas & Wagner, 1984; Clapp & Hornberger, 1978; Gao et al., 2021).

Soil type	ϕ	S_r	α (cm ⁻¹)	n	m	k (m ²)
Sand	0.35	0.034	0.158	3.58	0.72	2.90E-11
Silt loam	0.48	0.053	0.067	4.17	0.76	3.28E-14

Table 3. 3. Summary of bar hole configurations used in simulations. Case #1 includes a single bar hole positioned directly above the leak. Cases #2 and #3 include two additional bar holes, symmetrically placed around the central hole at 1 m and 5 m spacing, respectively, to evaluate the effects of bar hole number and spacing on CH₄ removal efficiency.

Case #	Number of Bar Holes	Spacing between Bar Holes (m)
1	1	0
2	3	1
3	3	5

A total of 108 numerical simulations were conducted, varying two soil types, six vacuum pressures, three surface saturations, and three bar hole deployments to evaluate how soil characteristics and system design influence CH₄ removal during NG soil aeration. All simulations ran for 60 minutes, reflecting typical field aeration durations. Model initialization details are provided in Appendix D.1. The simulation of Case #1 in sand at $S_w = 0.2$ and $P_b = 0.9$ atm served as a benchmark for comparative analysis across scenarios. Aeration performance was evaluated using subsurface CH₄ migration behavior, mass removal efficiency, and the time to reach the target concentration threshold (Johnson et al., 1990; Kuo, 2014; U.S. Army Corps of Engineers, 2002). The following section describes the methods for estimating each indicator.

3.2.3 Evaluation of Soil Aeration Performance

3.2.3.1 Mass removal efficiency

Mass removal efficiency of CH₄ (Re_{MCH_4}) quantifies the effectiveness of soil aeration in removing residual CH₄ from the vadose zone:

$$Re_{M_{CH_4}}(t) = \frac{M_{0CH_4} - M_{CH_4}(t)}{M_{0CH_4}} \quad \text{Eq. 3. 4}$$

To facilitate comparison across scenarios, the normalized residual CH₄ mass ($M_{CH_4}^*$) represents the fraction of remaining CH₄ in the vadose zone during aeration:

$$M_{CH_4}^*(t) = \frac{M_{CH_4}(t)}{M_{0CH_4}} \quad \text{Eq. 3. 5}$$

where $M_{CH_4}(t)$ (g) is the residual CH₄ mass in the vadose zone at time t (min), and M_{0CH_4} (g) is the initial residual CH₄ mass in the vadose zone.

3.2.3.2 Aeration Duration

Aeration duration is typically determined based on a site-specific basis, safety thresholds, environmental requirements, and project objectives. Based on Johnson et al. (1990), we used cumulative mass removal and residual contaminant levels to define operational duration. In NG aeration practice, operations oftentimes continue until the CH₄ concentration at the bottom of the bar hole is below 0.005 vol.% (50 ppmv). Because CH₄ removal varies spatially, the normalized residual CH₄ mass ($M_{CH_4}^*$, Eq. 3. 5) was used to evaluate the aeration duration across all simulation scenarios consistently.

3.3 Results and Discussion

In this section, the comparison between modeled and experimental CH₄ subsurface removal efficiency is used to investigate the model performance. The flux-based transport indicator is used to demonstrate that the model can capture the gas migration during aeration. The simulated belowground CH₄ migration behavior is used to evaluate the mass removal efficiency and required aeration duration across three bar hole configurations (Cases #1 to #3) in both coarse- and fine-grained soils under varying soil water saturation levels. Details of Cases #1 to #3 can be found in Table 3.2. Case #1 in sand serves as the benchmark scenario, providing a reference point for assessing the effects of additional bar holes and soil conditions on CH₄ removal performance.

3.3.1 Experimental Subsurface CH₄ Migration Behavior

Fig. 3. 4a, c, and e show observed subsurface CH₄ concentrations for the single bar hole aeration (S1) during active aeration. Measured CH₄ concentrations were spatially interpolated to generate concentration fields. Only half of the cross-section is shown because symmetry about the leak point is assumed under homogeneous soil conditions. Prior to aeration ($T = 0$ min), the subsurface CH₄ plume extends approximately $x = 3$ m laterally from the leak point (Fig. 3. 4a). Because the leak point is located directly beneath the bar hole, CH₄ concentrations decrease toward the bar hole location along the horizontal transect. After 30 min of active aeration, the 0.005 vol.% concentration contour moves from $x = 3.0$ m to approximately $x = 2.8$ m (Fig. 3. 4c). At the monitoring location ($x = 2$ m, depth = 0.75 m), CH₄ concentration increases from near zero to 0.1 vol.%, indicating lateral migration of gas toward the bar hole during aeration.

After 60 min of aeration, further depletion of the subsurface CH₄ plume is observed near the bar hole (Fig. 3. 4e). At the same monitoring location ($x = 2$ m, depth = 0.75 m), CH₄ concentration

decreases from 0.1 vol.% to approximately zero, indicating net removal at this depth over the first hour of aeration. In contrast, elevated CH_4 concentrations persist near the surface above this location, indicating that depletion is not uniform with depth. This pattern suggests that CH_4 removal initiates near the base of the bar hole where pressure gradients and advective fluxes are strongest, and then progresses upward and outward as aeration continues.

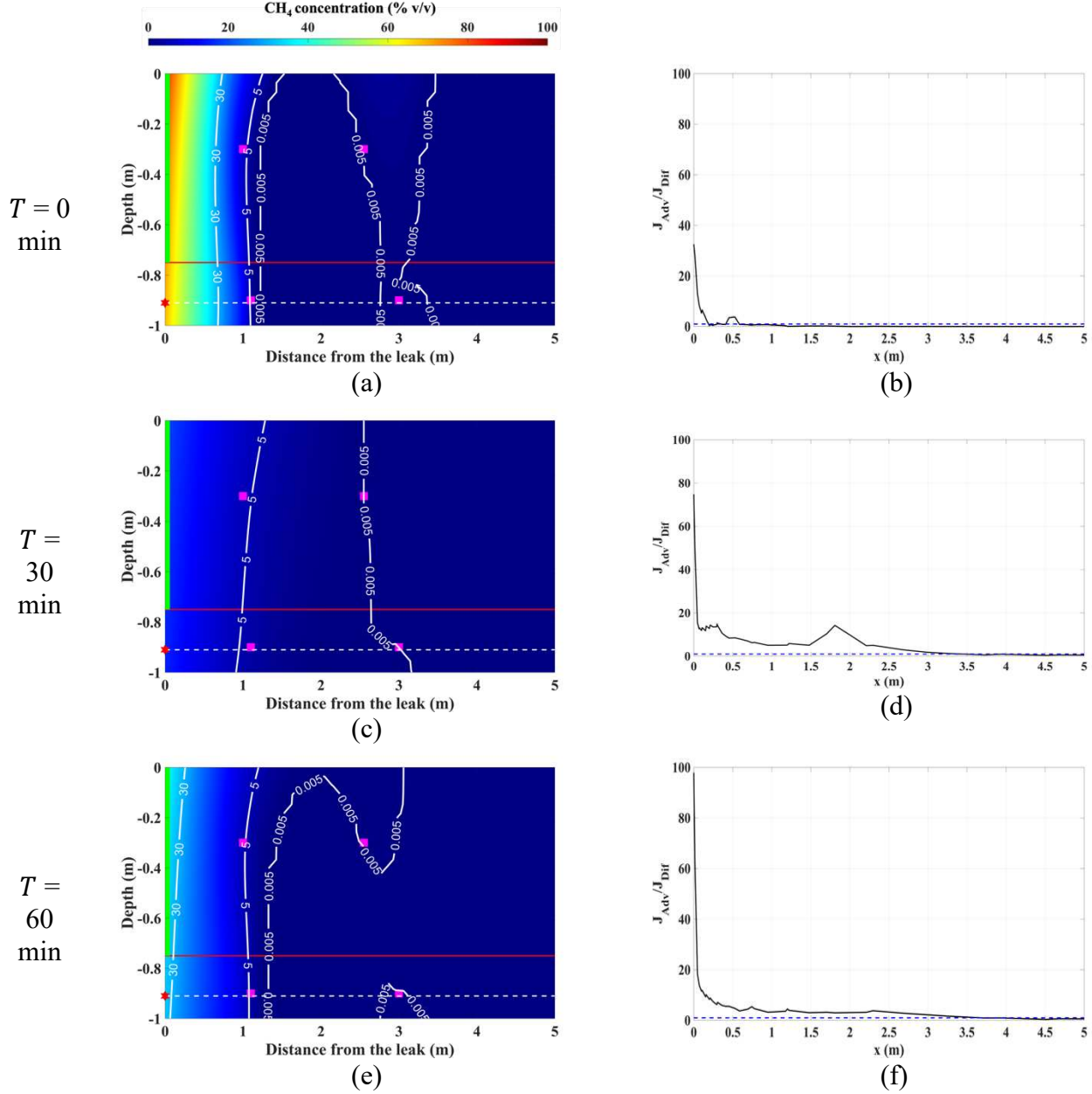


Fig. 3. 4. Observed subsurface CH₄ concentrations (a, c, and e) and modeled transport indicator (J_{Adv}/J_{Dif}) during soil aeration for a single bar hole. J_{Adv} indicates the subsurface CH₄ advective flux (kg/m²/min). J_{Dif} describes the subsurface CH₄ diffusive flux (kg/m²/min). Left panels show interpolated CH₄ concentration distributions derived from subsurface CH₄ measurements. The purple squares indicate the locations of CH₄ sensors. The green bar at $x = 0$ m denotes the bar hole location, the red star indicates the isolated leak point, and the white dashed line marks the pipeline. Right panels (b, d, and f) present a modeled J_{Adv}/J_{Dif} , evaluated along a horizontal transect at the depth of 0.75 m (red line). Values of J_{Adv}/J_{Dif} higher than 1 indicate advection-dominated transport, whereas values lower than 1 indicate diffusion-dominated transport. The blue dashed line indicates $J_{Adv}/J_{Dif} = 1$.

3.3.2 Model Performance Against Experimental Measurements

Fig. 3. 4b, d, f show the modeled transport indicator (J_{Adv}/J_{Dif}), which indicates whether gas transport is dominated by advection or diffusion. J_{Adv}/J_{Dif} greater than 1 indicates advective dominance, whereas values less than 1 indicate diffusion-dominated transport. At $T = 0$ min, elevated J_{Adv}/J_{Dif} values occur immediately adjacent to the bar hole (Fig. 3. 4b), indicating advective dominance driven by pressure gradients following leak shutoff. After 30 min of aeration, J_{Adv}/J_{Dif} increases near $x = 2$ m (Fig. 3. 4d), consistent with observed CH₄ migration toward the bar hole and the associated increase in concentration at this location. By $T = 60$ min, J_{Adv}/J_{Dif} decreases substantially from approximately 18 to 5 (Fig. 3. 4f), corresponding to declining CH₄ concentrations and reduced advective flux as local gas mass is depleted. At both $T = 30$ and 60 min, J_{Adv}/J_{Dif} remains greater than 1 from the bar hole to approximately $x = 3.4$ m, indicating advection-dominated transport over this distance. This extent represents an effective aeration radius of approximately 3.4 m for the controlled experiment and is consistent with the modeled radius of influence ($R_I = 3.3$ m). R_I is defined as the distance from the bar hole to the advection-

diffusion transition boundary. The corresponding R_I for $S_w = 0.2$ under a vacuum pressure of 5 psi relative to atmospheric pressure is shown in Fig. D. 2.

Fig. 3. 5 compares measured and modeled subsurface CH_4 removal efficiencies for six operational scenarios. The model reproduces the primary variability in removal efficiency observed in the experiments, with an overall R^2 of 0.78. Scenarios with wet near surface conditions (S2, S4, and S6) show high CH_4 removal efficiencies, with both measurements and simulations approaching 100% removal. This agreement indicates that the model captures the dominant gas transport behavior under wet near-surface conditions. Elevated water saturation limits near-surface air short-circuiting, redirecting gas flow toward the bar holes, and enhancing plume lateral capture and CH_4 removal. This result should be interpreted as an effect of boundary condition on airflow pathways and plume capture, rather than as a general indication that wetter soils are intrinsically easier to remediate.

In drier scenarios, modeled removal efficiencies are slightly higher than measured values, particularly for configurations with fewer bar holes. Nevertheless, the model reproduces the observed trend of increasing removal efficiency with increasing bar hole number. The differences are consistent with the persistence of diffusion-dominated regions in dry soils, where large air-filled pore volumes and heterogeneity promote preferential flow paths adjacent to poorly aerated domains. As CH_4 is depleted along these preferential pathways, gas entrapped in smaller or less connected pores can diffuse back toward the bar holes, contributing to rebound. Additional factors may also contribute to differences under dry conditions. The applied vacuum pressure (0.3 atm) and aeration flow rate may have been insufficient to fully remove accumulated CH_4 within the experimental duration. In addition, CH_4 sensor installation within vertical plastic casings limited detection to gas adjacent to or below the sensors and did not directly capture upward CH_4 migration,

which can be more obvious in dry soils. Overall, the comparison in Fig. 3. 5 demonstrates that the model provides a physically consistent representation of subsurface CH₄ removal across a range of soil moisture conditions and aeration configurations. Rather than reproducing absolute removal efficiencies under all conditions, the model captures the dominant controls on subsurface CH₄ removal and reliably predicts scenario-to-scenario trends associated with soil moisture and aeration design.

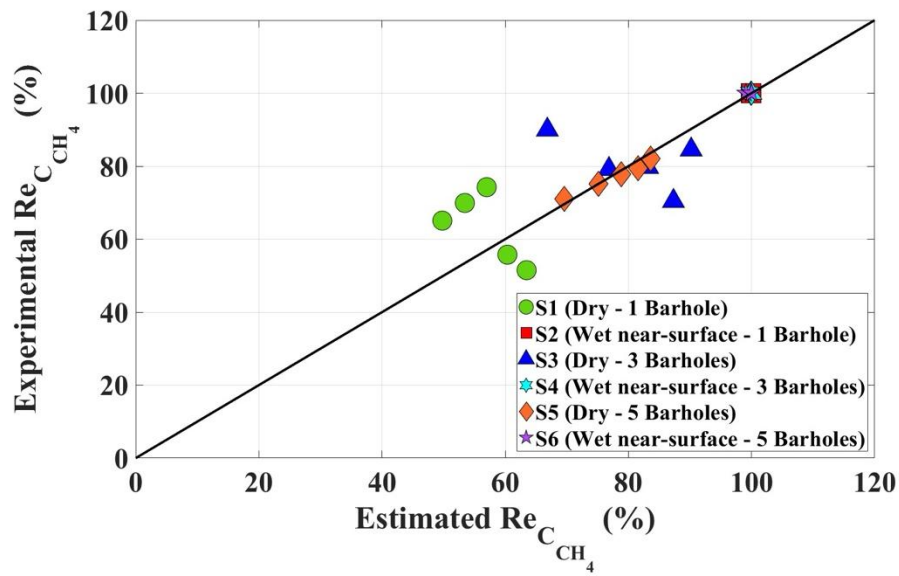


Fig. 3. 5. Comparison of simulated and experimental local CH₄ removal efficiency (Re_{CH_4}) for the six experimental scenarios. Re_{CH_4} is estimated with a vacuum pressure of 0.3 atm (5 psi) and an average plume diameter of 2.6 m. The overall agreement between estimations and observations shows $R^2 = 0.78$. The black line presents a 1:1 line.

The following sections show belowground CH₄ migration behavior, CH₄ mass removal efficiency, and aeration duration for Cases #1 to #3 under dry soil and wet near-surface conditions. These results are used to understand the impacts of soil conditions and the design of soil aeration on subsurface CH₄ removal.

3.3.3 Modeled Subsurface CH₄ Transport During Aeration

Fig. 3. 6 shows the temporal evolution of modeled CH₄ plumes in the vadose zone during 60 min of aeration for Cases #1 to #3 in sand at $S_w = 0.2$ under vacuum pressure 0.9 atm (13 psi). Corresponding results for silt loam are shown in Fig. S2. Prior to aeration ($T = 0$ min), CH₄ shows a bulb-shaped plume in all cases (Fig. 3. 6a, d, g), reflecting buoyancy-driven upward migration and lateral and downward diffusion when advective flow is negligible (Deepagoda et al., 2016).

After 30 min of aeration, CH₄ plumes decrease in all configurations (Fig. 3. 6b, 6e, and 6h), although removal efficiency varies with bar hole layout. Case 1 with a single bar hole presents the lowest residual CH₄ mass, with approximately 10% residual CH₄ mass. Case 2 includes three bar holes aligned with the initial plume and shows a more spatially uniform depletion pattern, with approximately 14% residual CH₄ mass. In Case 2, overlapping aeration zones promote lateral CH₄ migration between bar holes (Fig. 3. 6e). In contrast, Case 3 presents the lowest removal, with approximately 48% residual CH₄ mass remaining after 30 min. The residual plume persists near the central bar hole, indicating inefficient plume capture due to wide spacing and misalignment between the bar hole layout with the initial gas distribution. After 60 min of aeration, Cases 1 and 2 achieve approximately 98% CH₄ removal, whereas Case 3 retains approximately 30% of the initial CH₄ mass.

A wider or uniformly distributed initial plume was not simulated because it would represent an idealized design scenario rather than the field-observed and model-initialized residual CH₄ distribution (Gao et al., 2021; Jayarathne et al., 2024) considered in this study. The residual plume at the start of aeration was spatially nonuniform and concentrated near the plume core. Therefore, the purpose of the present simulations is not to demonstrate that more bar holes always increase removal efficiency, but to evaluate how bar hole layout interacts with realistic plume geometry.

The results indicate that multiple bar holes are effective only when their capture zones overlap the high concentration CH_4 region; otherwise, induced airflow can bypass the plume and draw lower- CH_4 air, reducing effective removal.

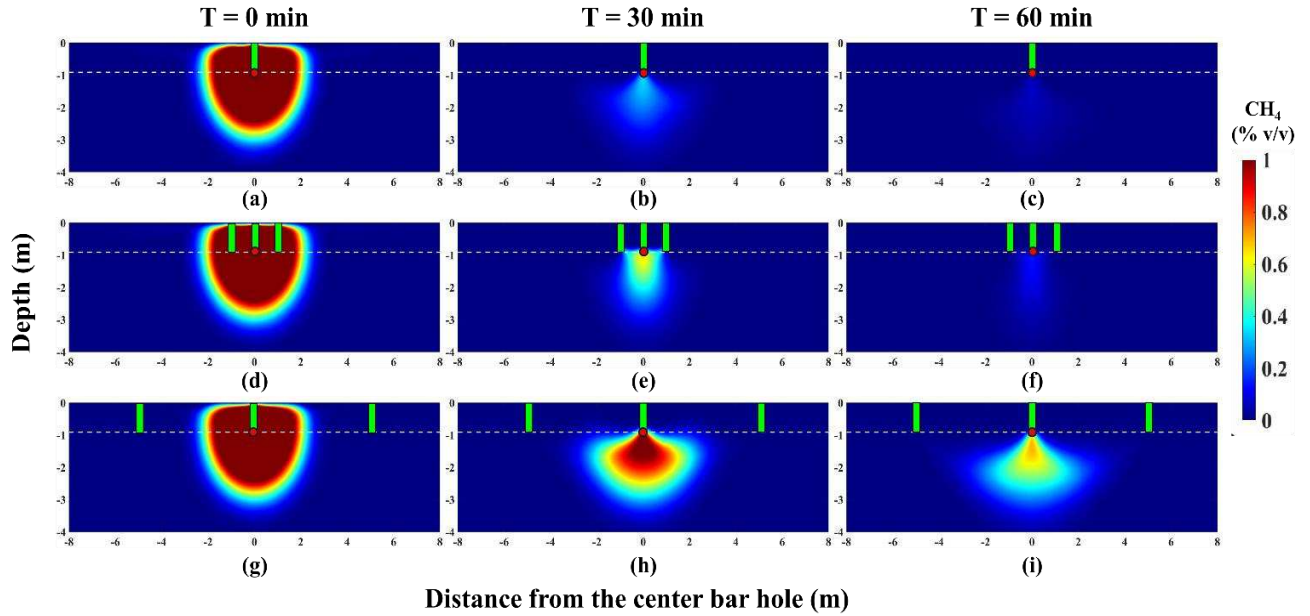


Fig. 3. 6. Cross-section plots of the belowground residual CH_4 concentrations in sand ($S_w = 0.2$) for Cases #1 to #3 before ($T = 0$ min) and during ($T = 30$ and 60 min) soil aeration. The CH_4 plume at $T = 0$ min (a, d, and g) indicates the initial distribution of CH_4 before aeration. Green squares indicate the locations of aeration bar holes: a single bar hole in Case #1 (a–c), three bar holes with 1 m spacing apart in Case #2 (d–f), and three bar holes with 5 m spacing in Case #3 (g–i). All bar holes operate at a vacuum pressure of 0.9 atm. The white dashed line marks the pipeline at 0.91 m depth. The red circle denotes the isolated leak point. The color bar represents CH_4 concentration by volume (vol.%).

The balance between advective and diffusive fluxes governs gas transport behavior. In highly permeable soils under large pressure gradients, CH_4 transport is initially advection dominated and transitions toward diffusion dominated behavior as pressure gradients decay. Horizontal and vertical advective (F_{Adv}) and diffusive (F_{Dif}) fluxes for Case #1 in sand and silt loam at $S_w = 0.2$

and vacuum pressure ranging (P_b) ranging from 0 to 0.9 atm are shown in Fig. D. 4 and Fig. D. 5. Corresponding results for Cases #2 and #3 are provided in Fig. D. 5 to Fig. D. 8. For the single-bar hole configuration, F_{Adv} near the bar hole is approximately two orders of magnitude greater than F_{Dif} but decreases rapidly within approximately 2 m of the bar hole, beyond which diffusion dominates CH₄ transport. The location of this transition depends on the applied vacuum pressure. When no drawdown is applied ($P_b = 0$ atm), transport near the bar hole is dominated by diffusion.

Near the bar hole, vertical and horizontal F_{Adv} show similar magnitudes in sand and silt loam. However, the silt loam with low permeability requires larger pressure gradients to reach comparable flow rates in. In contrast, F_{Dif} is consistently higher in silt loam than in sand, reflecting stronger residual CH₄ concentration gradients caused by restricted airflow. On average, vertical and horizontal F_{Dif} in silt loam exceed that in sand by 148% and 80%, respectively, indicating that diffusion plays a more significant role during prolonged aeration in low permeable soils.

In multiple bar hole configurations, peak F_{Adv} occurs near each bar hole, and vertical fluxes exceed horizontal fluxes due to stronger vertical pressure gradients. However, compared to the single bar hole case, peak F_{Adv} values are reduced because of airflow interference between adjacent bar holes. This interference limits advective transport, increases reliance on diffusion, and results in higher residual CH₄ concentrations. Therefore, the effect of adding bar holes depends on whether the spacing improve plume capture without causing excessive overlap and airflow interference. Effective bar hole spacing should expand plume coverage to avoiding excessive airflow interference between bar holes, improving removal efficiency and reducing aeration duration.

3.3.4 Mass Removal Efficiency of CH₄

CH₄ mass removal efficiency ($Re_{M_{CH_4}}$) is strongly controlled by soil properties and aeration system design. Fig. 3. 7 shows the normalized residual CH₄ mass ($M_{CH_4}^*$) and $Re_{M_{CH_4}}$ for Case #1 (single bar hole, $S_w = 0.2$) in sand and silt loam across vacuum pressure values relative to atmospheric pressure (P_b) ranging from 0 to 0.9 atm. Increasing P_b results in a rapid decrease in residual CH₄ mass in both soils. At $P_b = 0.9$ atm, $M_{CH_4}^*$ decreases by 98% in sand and 96% in silt loam (Fig. 3. 7a, c), whereas no pressure drawdown is applied ($P_b = 0$ atm) results in negligible CH₄ removal (<0.01%). Correspondingly, $Re_{M_{CH_4}}$ reaches approximately 98% at $P_b = 0.9$ atm in both soils, compared to approximately 79% at $P_b = 0.1$ atm (Fig. 3. 7b, d). Differences between sand and silt loam soils reflect contrasts in permeability and porosity. Higher permeability in sand allows greater airflow and more efficient CH₄ transport, whereas silt loam restricts advective flow and prolongs removal.

The relationship between $Re_{M_{CH_4}}$ and P_b is distinctly nonlinear. At $P_b = 0.9$ atm, 90% and 87% of total CH₄ mass in sand and silt loam, respectively, are removed within the first 30 min of aeration, whereas the remaining 30 min contribute only an additional 8 to 10% removal. Similar behavior is observed at lower vacuum pressure values. Increasing P_b from 0.1 to 0.3 atm increases final $Re_{M_{CH_4}}$ by approximately 11%, whereas increasing P_b from 0.7 to 0.9 atm increases by only approximately 1%. These results indicate diminishing returns at high vacuum pressure because rapid early depletion of accessible CH₄ limits further removal during later stages of aeration.

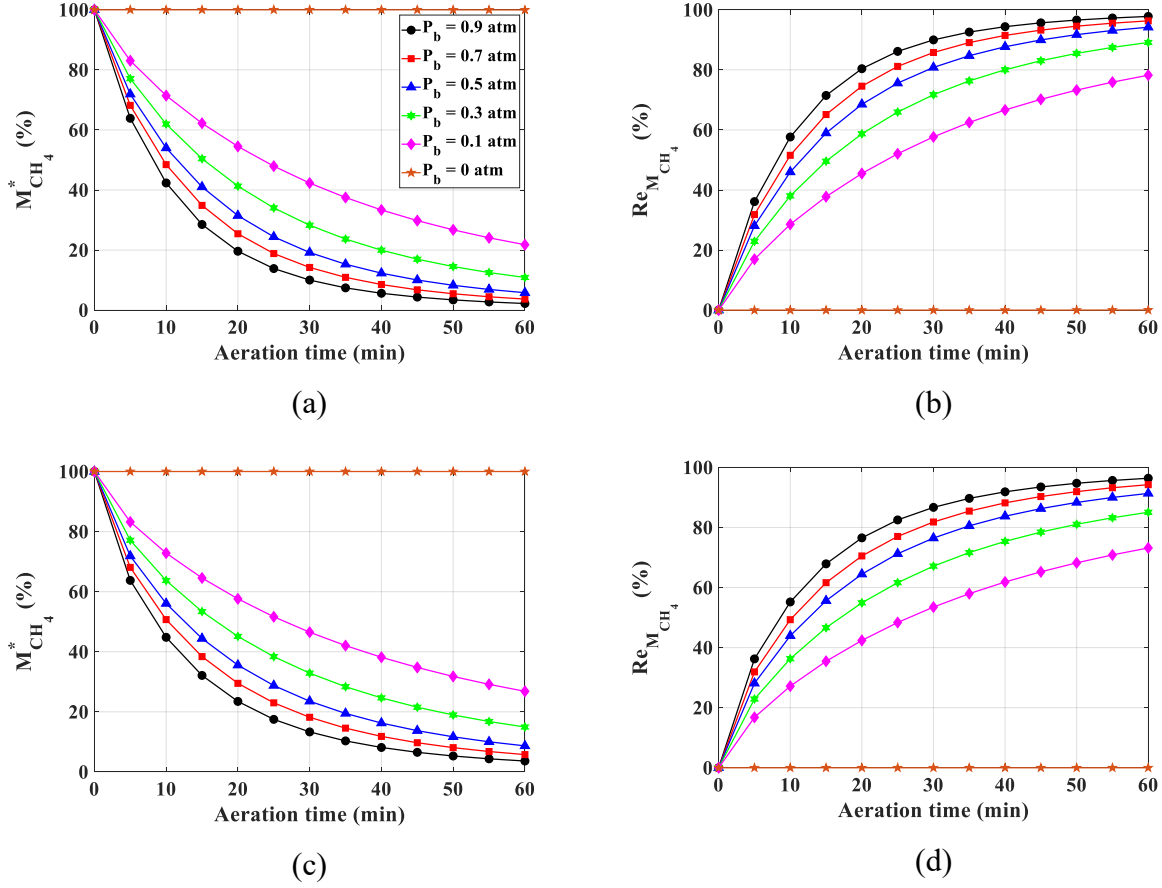
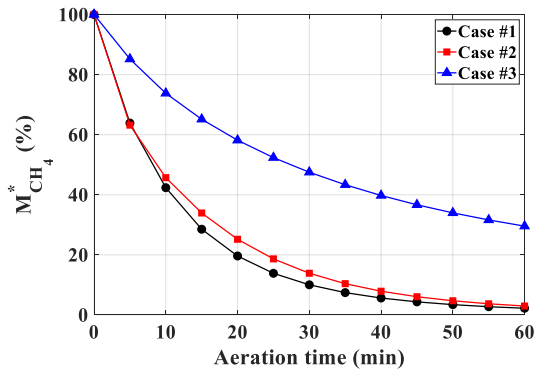


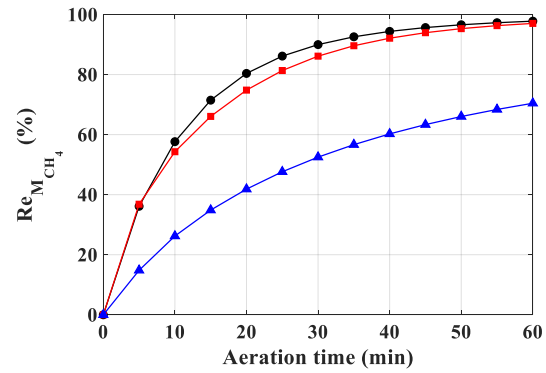
Fig. 3. 7. Simulated normalized residual CH_4 mass ($M_{\text{CH}_4}^*$) and mass removal efficiency of CH_4 ($Re_{M_{\text{CH}_4}}$) for Case #1 (a single bar hole and $S_w = 0.2$) in (a and b) sand and (c and d) silt loam under vacuum pressures ranging from 0 to 0.9 atm. Results are shown along a horizontal transect 0.9 m below the ground surface.

Fig. 3. 8 compares $M_{\text{CH}_4}^*$ and $Re_{M_{\text{CH}_4}}$ for Cases #1 to #3 in sand and silt loam at $S_w = 0.2$ under a vacuum pressure of 0.9 atm relative to atmospheric pressure. After 60 min of aeration, Case #1 achieves the highest removal efficiency (98%), followed by Case #2 (97%), whereas Case #3 removes 70% of the initial CH_4 mass. Under these conditions, the initial plume length (approximately 3 m) is smaller than modeled R_l for all cases in both sand (3.4 m) and silt loam (3.2 m) soils, indicating that a single bar hole is sufficient to capture the plume. Therefore, adding additional bar holes primarily introduces airflow interference rather than increasing removal

efficiency. In Case #2, bar hole spacing (1 m) is smaller than both R_I and the initial plume length, so the bar holes are located within the plume and directly contribute to CH₄ removal. As a result, $Re_{M_{CH_4}}$ is approximately 1% lower than that of Case #1. In contrast, bar holes in Case #3 are spaced 5 m apart and located outside the initial gas plume, which causes airflow to bypass subsurface CH₄ regions and reduces removal efficiency to 70%. These findings do not indicate that multiple bar holes are ineffective. Instead, they show that additional bar holes improve removal only when their capture zones overlap the residual CH₄ plume. In the simulations, the initial plume length was smaller than the modeled R_I , so one centrally located bar hole was sufficient to capture most of the residual CH₄. Under this condition, adding bar holes did not substantially increase plume capture because of airflow interference or bypass, particularly when the added bar holes were located outside the high-concentration plume region. Therefore, bar-hole number alone should not be used as the design criterion. Effective multiple bar hole design requires spacing and alignment relative to both the R_I and the geometry of the residual CH₄ plume.



(a)



(b)

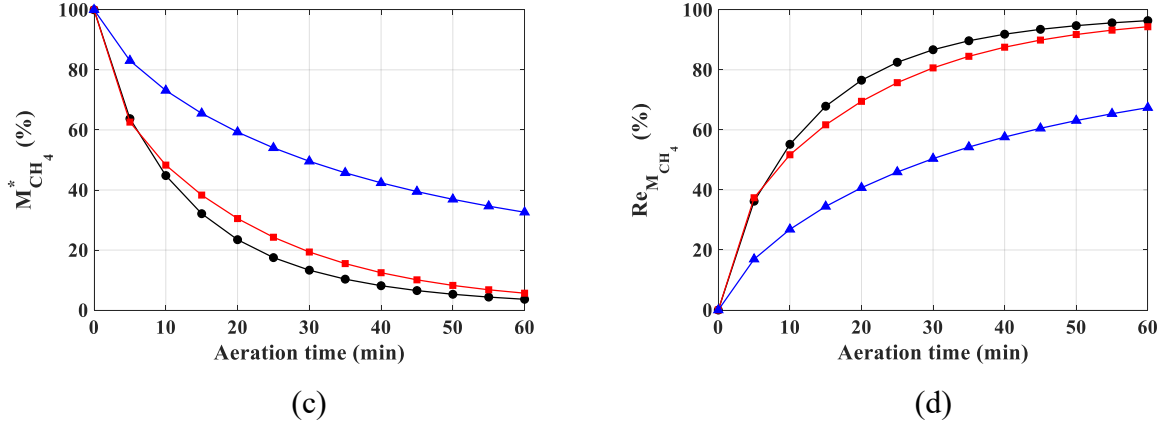


Fig. 3. 8. Simulated normalized residual CH₄ mass ($M_{CH_4}^*$) and mass removal efficiency of CH₄ ($Re_{M_{CH_4}}$) for Cases #1 (a single bar hole), #2 (three bar holes spaced 1 m apart), and #3 (three bar holes spaced 5 m apart) (a and b) sand and (c and d) silt loam with vacuum pressures of 0.9 atm and soil water saturation of 0.2.

3.3.5 Aeration Duration to Reach Removal Goals Based on Removal Efficiency

Normalized residual CH₄ mass ($M_{CH_4}^*$; Fig. 3. 8) was used to estimate the aeration duration required to achieve a 90% removal target, defined $M_{CH_4}^* = 0.1$. In the sand at $S_w = 0.2$ under a vacuum pressure of 0.9 atm relative to atmospheric pressure, Case #1 reaches 90% removal within approximately 30 min, while Case #2 requires about 35 min due to airflow interference between adjacent bar holes. Case #3 fails to achieve the 90% target within 60 min, retaining approximately 29% of the initial CH₄ mass due to plume bypassing. These results further demonstrate that appropriate bar hole number and spacing are critical for minimizing aeration duration and achieving efficient CH₄ removal from the vadose zone.

3.3.6 Study Limitations

Although this study provides new insights into how soil properties and aeration system design control subsurface CH₄ removal, several limitations should be acknowledged. The experimental results were obtained under controlled field scale conditions and may not fully represent site heterogeneity, stratification, or multiple release scenarios encountered at real sites. In addition, aeration was conducted over short periods (60 min or less), and CH₄ sensor placement was limited to discrete depths and lateral positions. As a result, the measurements may not resolve near surface concentration gradients or preferential flow pathways. Model limitations include simplified representation of soil intrinsic permeability, porosity, and gas phase connectivity, which may reduce predictive accuracy for highly heterogeneous soils or soils with elevated water saturation. In addition, the two-dimensional transport model used in this study is intended to resolve the dominant cross-sectional controls on subsurface CH₄ migration and removal during soil aeration, including plume capture and the interaction between bar-hole spacing and induced airflow, rather than to reproduce the full three-dimensional geometry of field sites. As a result, irregular plume shapes, off-plane spreading, subsurface infrastructure, and asymmetric boundary conditions may further influence gas transport and removal in ways not fully represented here. Therefore, the present results should be interpreted as mechanism-based cross-sectional insights under the tested conditions, while fuller three-dimensional site complexity remains a subject for future work. Despite these constraints, the combined experimental and modeling approach provides a mechanistic basis for interpreting soil aeration performance and for informing site specific design.

3.4 Conclusions

This study integrated controlled field scale NG soil aeration experiments with a two phase, two component transport model to quantify how subsurface soil properties and aeration system design jointly control CH₄ removal in the vadose zone. Experimental observations revealed consistent patterns of subsurface CH₄ migration and depletion during aeration. These patterns included initial plume contraction toward the bar hole followed by net mass removal. Specifically, the 0.005 vol.% CH₄ concentration contour migrated from 3.0 m to 2.8 m within the first 30 min of aeration, indicating advection driven migration toward the extraction point prior to depletion.

Modeled results reproduced the observed transport behavior and removal efficiencies, supporting the use of the model for scenario-based evaluation of NG soil aeration performance. Scenario simulations demonstrate that subsurface CH₄ removal follows a two-stage process. During the early stage of aeration, strong pressure gradients near bar holes induce advection dominated transport and result in rapid CH₄ mass removal. As aeration progresses, removal rates decline and transport becomes diffusion limited as remaining CH₄ is entrapped in less connected pore spaces. Under a vacuum pressure of $P_b = 0.9$ atm relative to atmospheric pressure, residual CH₄ mass decreased by approximately 90% in sand and 87% in silt loam within the first 30 min. Only an additional 8 to 10% was removed during the subsequent 30 min, indicating diminishing returns at large, applied pressure drawdown. Bar hole configuration strongly influenced removal efficiency through plume capture, airflow interference, and bypass. Removal was maximized when the radius of influence encompassed the residual plume, whereas bar holes placed outside the plume promoted bypass and reduced removal efficiency.

Flux-based indicators (J_{Adv}/J_{Dif}) and the modeled radius of influence (R_I) show that gas transport is advection dominated near bar holes and transitions to diffusion dominated behavior

with distance. This behavior is consistent with an R_f of approximately 3.3 m for the single bar hole configuration. Intrinsic permeability and water saturation govern gas phase connectivity and the spatial extent of induced pressure gradients, thereby controlling the balance between advective and diffusive transport. Compared with sand soil, restricted airflow in silt loam promotes diffusion dominated transport during later stages of aeration, leading to slower CH_4 mass removal during prolonged operation and increasing the likelihood of rebound after aeration. These results indicate that rebound is a predictable outcome of diffusion dominated transport in poorly connected pore domains rather than a failure of aeration systems.

The variation of R_f with soil water saturation and vacuum pressure further indicates that increasing bar hole density can be more effective than increasing pressure drawdown alone. Bar hole placement and spacing should therefore be designed with respect to both soil properties and the geometry of the subsurface gas plume. When bar holes overlap the plume, CH_4 removal efficiencies of 97% to 98% can be achieved within 60 min. In contrast, bar holes placed outside the plume promote airflow bypass and competition, which substantially reduces removal performance. Importantly, aggressive aeration strategies, such as excessive pressure drawdown or excessive use of bar holes, do not linearly improve removal and can reduce efficiency through airflow interference. Furthermore, aeration duration required to reach safety based removal targets is highly sensitive to system configuration. Optimized bar hole placement achieved greater than 90% CH_4 removal within approximately 30 min to 35 min. In contrast, suboptimal designs required substantially longer durations or did not meet removal targets within the same timeframe.

Overall, this study demonstrates that subsurface CH_4 removal during NG soil aeration is governed by coupled interactions among soil properties, moisture conditions, applied pressure drawdown, and bar hole deployment. The integrated experimental and modeling framework

provides actionable guidance for aeration design at a given site and emphasizes plume aligned bar hole placement and optimization of vacuum pressure rather than aggressive overdesign. These findings support more efficient CH₄ mitigation, reduced cleanup times, and improved risk reduction across a range of subsurface conditions.

Chapter 4. A Reduced-Order Framework for the Design and Operation of Natural Gas Soil Aeration at Pipeline Leak Sites³

Abstract

Subsurface accumulation of natural gas (NG) following pipeline leaks presents a significant explosion hazard and requires rapid and effective methane (CH₄) removal. Although soil aeration is widely used for NG mitigation, current practice relies largely on generalized guidance and operator experience, with limited quantitative support for aeration system design and operation. This study developed a reduced-order, physics-based framework that translates complex subsurface gas transport behavior into a field-applicable engineering tool for evaluating CH₄ mass removal efficiency, aeration duration, and bar-hole spacing and bar-hole configuration. The framework was derived by reducing high-fidelity multiphase transport simulation outputs into a reduced-order evaluation framework that linked to observable site conditions, including soil moisture, plume size, vacuum pressure, and soil type. Comparisons with controlled field-scale experiments in sandy loam soils show that the framework reasonably reproduces observed subsurface CH₄ removal behavior across six representative NG soil aeration scenarios ($R^2 = 0.74$), supporting rapid screening-level engineering assessment during NG leak response. Results further demonstrate that elevated CH₄ concentrations may persist near the surface even after localized depletion, underscoring the importance of plume-wide monitoring and proper bar-hole placement within the affected zone. Overall, the framework provides operators with a quantitative basis for selecting aeration duration, vacuum pressure, and bar-hole spacing and number based on site-

³ This chapter is a subject of the paper currently under review at *Gas Science and Engineering*, which is entitled “A reduced-order framework for the design and operation of natural gas soil aeration at pipeline leak sites” by Jui-Hsiang Lo, J. R. R. Navodi Jayarathne, and Kathleen Smits

specific conditions and removal objectives. By linking site-specific conditions to aeration performance, the approach improves the efficiency, consistency and effectiveness of NG soil aeration while supporting enhanced pipeline safety.

4.1 Introduction

Subsurface accumulation of natural gas (NG) following pipeline leaks poses an immediate safety hazard because methane (CH_4), the primary component of NG, is combustible within an ignitable range of approximately 5–15% CH_4 by volume. Utilities commonly use soil aeration to remove subsurface NG and reduce subsurface CH_4 concentrations to acceptable levels. Although NG soil aeration is widely applied in practice, field experience shows that subsurface CH_4 removal is often slow and inefficient, with elevated concentrations persisting despite prolonged aeration. A well-documented example occurred in Georgetown, Texas, where aeration continued for more than thirty days without achieving the target safety threshold (Sarabia, 2019; Spectrum News, 2019). These observations suggest that current NG soil aeration practices are often not matched to site-specific soil conditions or plume behavior, underscoring the need for a reliable and quantitative framework for NG soil aeration design and operation.

NG soil aeration is conducted by drilling a series of holes in the ground, referred to as aeration bar holes, near the identified or suspected leak location. These bar holes provide pathways for passive venting whereby residual NG migrates by natural diffusion and may also be connected to a vacuum pump to actively induce airflow toward the bar hole. Active aeration enhances pressure-induced advective transport, drawing CH_4 from surrounding soil pores toward the bar holes, after which the extracted gas is either collected or discharged according to site-specific regulatory requirements. Aeration operations are typically repeated with additional bar holes or extended operating time (hours to days) until subsurface CH_4 concentrations fall below the approved safety threshold. In practice, aeration performance is generally assessed using residual CH_4 concentrations measured within bar holes rather than extracted CH_4 flux. Despite the apparent simplicity of this process, field performance remains inconsistent because current practices rely

largely on generalized operational guidance, without quantitatively accounting for NG plume geometry, residual CH₄ distribution, soil characteristics (e.g., soil type, texture, moisture saturation), or removal objectives.

Although NG soil aeration is widely used and recognized as standard practice (Pipeline and Hazardous Materials Safety Administration, 2017), its design and operation remain poorly understood from a quantitative perspective. Existing NG industry guidance primarily provides qualitative observations, noting that wet or frozen ground can impede gas removal and prolong aeration duration. Other industry reports similarly indicate that soil type and moisture influence removal efficiency by reducing air permeability and restricting NG migration (E. Six, 2014; R. Six, 2007). However, these insights remain largely descriptive, and the quantitative relationship linking site conditions and aeration system performance is not well established. Field-scale observations of NG soil aeration are particularly limited, especially those relating subsurface CH₄ transport behavior to aeration design and removal performance. The lack of quantitative field-scale datasets has limited the development of field-applicable engineering methods that incorporate soil characteristics, plume geometry, and operational constraints into NG soil aeration design.

Related research in environmental remediation, particularly soil vapor extraction (SVE), provides useful insight into the physical processes that govern subsurface gas removal (Carroll et al., 2012; Hutzler & Murphy, 1988; Kuo, 2014; Sun et al., 2023; Suthersan et al., 1999; U.S. Army Corps of Engineers, 2002; U.S. Environmental Protection Agency, 1995). SVE uses pressure-induced airflow to remove volatile contaminants from the vadose zone. Extensive SVE studies have shown that soil air permeability, soil moisture, and surface sealing strongly control advective gas transport and removal efficiency. System parameters such as well spacing, extraction flow rate, and applied vacuum pressure govern the effective radius of influence and cleanup duration. These

findings underscore the importance of linking site-specific soil conditions to appropriate system configuration and operation. However, SVE applications typically involve long-term remediation of relatively large contaminant plumes, which differs substantially from short-term NG soil aeration within highly localized plumes and oftentimes urgent response conditions. Consequently, SVE principles can inform, but cannot directly define NG soil aeration design and operation.

Gas transport in the vadose zone is governed by coupled advective and diffusive processes that strongly influence the efficiency of subsurface gas removal. Advective transport generated by imposed pressure gradients governs bulk gas movement and removal from the soil. Effective CH₄ removal requires sustained contact between advective airflow and residual gas within soil pores (Armstrong et al., 1994; U.S. Army Corps of Engineers, 2002). Soil intrinsic permeability and air permeability strongly control the magnitude of advective transport. Increasing soil moisture saturation reduces gas-phase connectivity and restricts airflow pathways, thereby limiting pressure propagation and accessible treatment zones. Under low-permeability or poorly connected conditions, airflow preferentially bypasses less accessible regions, where gas transport is controlled by diffusion (Høier et al., 2009; Yoon et al., 2009). These diffusion-controlled regions can also contribute to rebound behavior, whereby CH₄ concentrations increase once active aeration is stopped, as gas migrates from less accessible pore spaces back into advective flow zones. These processes control removal efficiency, radius of influence, and aeration duration, while also explaining the sensitivity of NG soil aeration to soil texture, moisture, and subsurface heterogeneity (Armstrong et al., 1994; Carroll et al., 2012; Høier et al., 2009).

Multiphase transport models have improved understanding of contaminant migration (Benson, 2011; Joss & Baehr, 1995; V. T. Nguyen et al., 2013; Scientific Software Group, 2011). However, the computational complexity of these models limits their use in rapid field decision-making. To

overcome this challenge, SVE practice has adopted simplified analytical approaches that capture dominant physical processes while remaining practical for field-scale engineering assessment. A notable example is the framework developed by Johnson et al. (1990), which relates measurable site conditions to system variables such as venting flow rate, removal flow rate, bar-hole number and spacing, and cleanup duration. These simplified methods have been applied successfully in field-scale SVE operations (Kuo, 2014; U.S. Army Corps of Engineers, 2002). Despite their utility, existing simplified approaches in SVE cannot be directly applied to NG soil aeration because NG leak sites involve fundamentally different leak geometries, shorter operational timescales, transient gas migration patterns, and emergency-response objectives. These differences highlight the need for a reduced-order, physics-based framework specifically developed for NG soil aeration and capable of quantitatively linking measurable field parameters to subsurface CH₄ removal performance.

The objective of this study is to develop a reduced-order, physics-based framework for evaluating NG soil aeration design and operation. Building on conceptual advances from simplified SVE models (Johnson et al., 1990), this framework links measurable field parameters to quantitative estimates of CH₄ removal efficiency, aeration duration, and bar-hole deployment. The approach is intended as a screening-level engineering tool that uses field-obtainable inputs to support rapid decision-making during NG leak response. Controlled field-scale experiments were conducted under representative NG aeration conditions to evaluate framework performance across contrasting soil conditions and bar-hole configurations. By combining experimental observations with reduced-order physical formulations, the framework provides practical estimates of aeration performance, including required aeration duration, bar-hole number and spacing, plume coverage, and removal efficiency. The framework provides utility with a screening-level method for

improving aeration effectiveness, identifying conditions where additional monitoring or modeling may be required, and supporting more efficient NG leak mitigation. The following sections outline the theoretical basis of the approach and illustrate its application to field-scale NG soil aeration.

4.2 Methods

4.2.1 Controlled Field Experiments

Controlled field experiments were conducted to collect measurements under representative site and operating conditions for the evaluation of the proposed reduced-order framework. While performance evaluation metrics are described later, this section introduces the experimental testbed, soil aeration system, and experimental scenarios. The experiments were designed to represent realistic NG soil aeration conditions across contrasting operating scenarios rather than statistically replicated trials under identical conditions.

A 5-day field-scale soil aeration experiment was conducted at the Methane Emissions Technology Evaluation Center (METEC) at Colorado State University, Fort Collins, Colorado, USA. METEC consists of underground pipeline testbeds designed to simulate NG leak scenarios at selected emission rates under diverse atmospheric, surface, and subsurface conditions. The facility includes testbeds with varying surface covers, soil types, and moisture. For this study, experiments were conducted in a rural, grass-covered testbed containing sandy loam soil. Additional details regarding the testbed design can be found in Jayarathne, Kolodziej, et al. (2022a) and Jayarathne et al. (2024). Within the approximately 40 m long and 10 m wide test area, a leak point was installed at a depth of 0.91 m below ground surface to represent a NG leak from a distribution pipeline and to comply with standard soil cover requirements for NG distribution mains (49 C.F.R. § 192.327, 2025). A cross-sectional schematic of the selected testbed

infrastructure is shown in Fig. 4. 1. NG for simulating the leak was delivered via a 0.635 cm polytetrafluoroethylene (PTFE) tubing connected to a 0.635 cm vent screen, all enclosed in a 10 cm gravel-filled wire cube to prevent clogging. Compressed NG (85 to 95% CH₄) was supplied from 145 L cylinders and released at controlled rates of 10 standard liters per minute (SLPM) using regulators, solenoid valves, and precision orifices. Several environmental and CH₄ concentration sensors were installed to continuously monitor soil moisture, soil temperature, and subsurface CH₄ concentration. Infrared methane sensors (INIR-ME100, SGX Sensortech, Inc.) outfitted with custom-designed encasements were used to measure subsurface CH₄ concentrations during aeration. These sensors were calibrated and used in previous studies (Jayarathne, Kolodziej, et al., 2022a, 2022b). In this study, a total of six INIR sensors were strategically installed at depths of 0.3 m, 0.6 m, and 1.8 m below the ground surface, positioned laterally at distances ranging from 1.0 m to 3.6 m from the leak point. Data was recorded at 5-second intervals. INIR sensors were calibrated prior to the aeration experiments to ensure measurement accuracy and consistency across locations. Subsurface CH₄ measurements were collected along a single monitored cross-section. For interpreting subsurface CH₄ migration and removal behavior, the testbed was treated as a laterally homogeneous system, with emphasis placed on cross-sectional plume response rather than fully resolved three-dimensional plume evolution. These measurements were used to evaluate changes in subsurface CH₄ concentrations during aeration under representative operating scenarios.

Soil moisture and soil temperature were measured using TEROS 10 and TEROS 11 sensors (METER Group, Inc.) co-located with the INIR sensors at each depth at 10-minute intervals. Soil moisture and temperature sensors (TEROS and 5TM, METER Group, Inc.) were used to measure soil moisture and temperature with soil moisture accuracy of ± 3 % and temperature with ± 0.5 °C.

Measurements were recorded every 10 minutes using ZL6 dataloggers (METER Group, Inc.). The soil type at the testbed was determined as sandy loam based on the laboratory testing (57% sand, 29% silt, and 14% clay). Soil properties of sandy loam using Rosetta 3 (Zhang & Schaap, 2017) based on the soil composition (Table 4. 1).

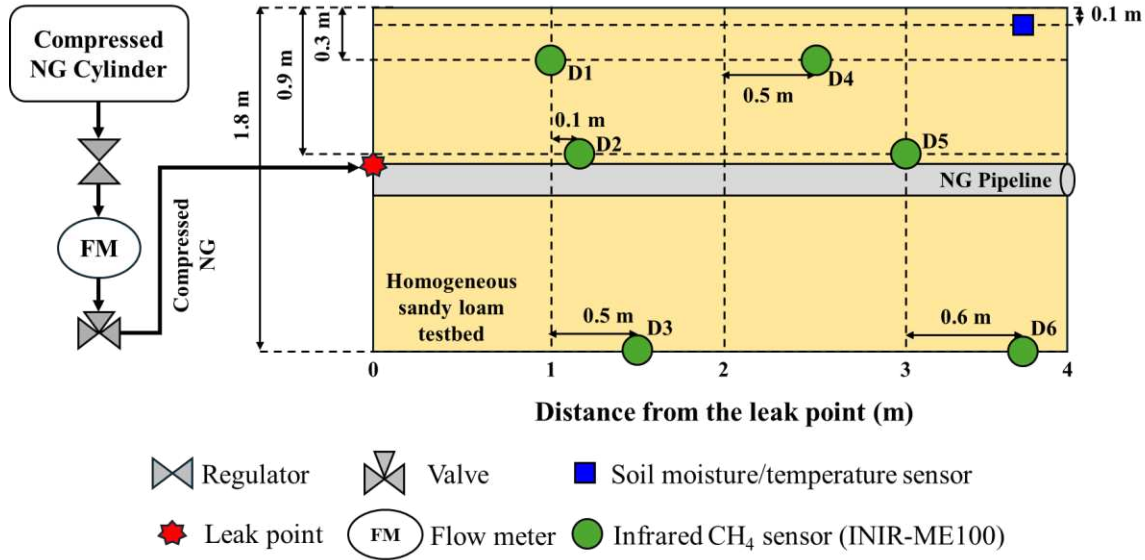


Fig. 4. 1. Vertical cross-sectional schematic of the soil aeration testbed and instrumentation. Compressed NG was delivered from a gas cylinder to the subsurface leak point through a pressure regulator, flow meter, and control valve that controlled the leak rate. Six infrared CH₄ sensors (INIR-ME100, green circles) were installed along the monitored cross-section to monitor subsurface CH₄ concentrations. A soil-moisture/temperature sensor (5TM; blue square) at a depth of 0.1 m recorded near-surface soil moisture and temperature. The black arrow denotes the direction of NG flow, and horizontal distances are shown relative to the leak point.

Table 4. 1. Physical and hydraulic properties used in numerical simulations for sandy loam, including porosity (ϕ), residual soil water saturation (S_r), van Genuchten parameters, and soil permeability (k)

Soil type	Porosity ϕ (cm ³ cm ⁻³)	Intrinsic permeability k (m ²)	Residual water saturation S_r (cm ³ cm ⁻³)	van Genuchten parameters ^a		
				α (cm ⁻¹)	n	m
Sandy loam	0.39	4.53×10^{-9}	0.1	0.027	1.45	0.31

^a Obtained from Rosetta 3 based on the soil composition from the laboratory testing (57% sand, 29% silt, and 14% clay).

The soil aeration system consists of bar holes, purgers, and a high-pressure air compressor (Fig. 4. 2). Due to hard subsurface conditions at the testbed, all bar holes were pre-drilled and sealed prior to experiments to ensure a consistent bar-hole configuration across experimental scenarios. According to the designs of soil aeration in the NG industry, aeration bar holes are typically from 1.3 to 7.6 cm (0.5 to 3 inches) in diameter and are installed several inches above the pipeline, which is generally buried at depths of 0.5 to 1.2 m (1.5 to 4 feet). The vacuum pressure applied for soil aeration varies from 0 to 0.9 atm (0 to 13 psi) at the aeration bar hole. The spacing between bar holes is between 1.5 and 3 m (5 to 10 feet), and the total number of aeration bar holes at the site varies depending on the investigated size of the subsurface NG plume. Therefore, in this study, each aeration bar hole was drilled to 0.9 m (3 ft) depth with a 5 cm (2 inches) diameter and installed on an average 1.5 m (5 ft) spacing starting next to the leak point.

For each experimental scenario, only the selected bar holes were activated and connected to purgers, while the remaining pre-drilled bar holes were kept sealed with plastic caps. Each active bar hole was connected to one purger. For scenarios with multiple active bar holes, the purgers were operated simultaneously through the manifold system. These design choices reflect realistic field constraints and allow evaluation of CH₄ transport and removal. In field applications, one or more purgers connected to an air compressor are used to generate a localized vacuum at the aeration bar hole to extract subsurface CH₄ from the soil. Five purgers were used in the experiments and connected to the air compressor through a manifold system. The air compressor supplied compressed air to the manifold at 185 scfm and 90 psi. When the compressed air reached the purger, it generated a vacuum through the venturi pump on the top of the purger. Each active purger was equipped with a pressure gauge to monitor the operating vacuum pressure during aeration.

The aeration flow rate was estimated from the purger design curve based on the measured vacuum pressure. At the average vacuum pressure of 0.3 atm (5 psi), the estimated aeration flow rate was 0.25 m³/min (9 scfm) per active purger. For screening-level design calculations, the total aeration flow rate was estimated by multiplying this flow rate by the number of active purgers, resulting in a maximum total aeration flow rate of 1.27 m³/min (45 scfm) for five active purgers. During aeration, CH₄ concentrations near the center bar-hole outlet were monitored using a MIRA Strato gas analyzer (Aeris Technologies, Inc.) as a field indicator of aeration progress. Fig. 4. 2 shows the orientation of the bar holes relative to the leak point, and the purger-air compressor system used in the controlled experiments.

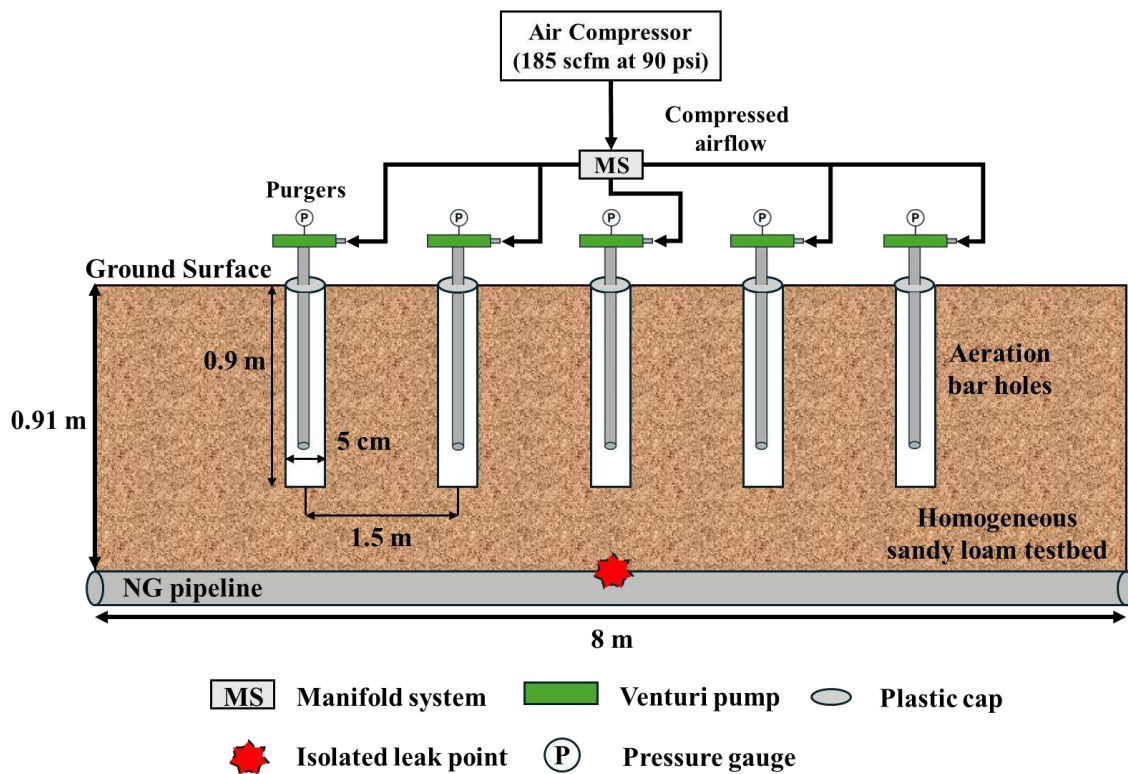


Fig. 4. 2. Vertical cross-sectional schematic of the soil aeration system used in the controlled experiments. The system consisted of an air compressor, manifold system (MS), purgers, and aeration bar holes installed above the NG pipeline within the homogeneous sandy loam testbed.

Depending on the experimental scenario (Table 4. 2), the number of active purgers and aeration bar holes ranged from one to five. Each aeration bar hole was drilled to a depth of 0.9 m, with a diameter of 5 cm, and approximately 1.5 m apart. This schematic illustrates a five-purger/bar-hole configuration. The air compressor supplied approximately 185 SCFM of compressed airflow at 90 psi, which was distributed to each purger through the manifold system. Vacuum pressure at each bar hole was generated using a venturi pump installed on the purger, producing an average pressure drawdown of approximately 0.3 atm (5 psi) on the top of each purger. Pressure gauges are used to monitor vacuum pressure during aeration. The dashed red star indicates the subsurface leak location.

Controlled experiments were conducted with six different aeration scenarios as shown in Table 4. 2. The experiments were performed by releasing NG for 8 hours at average CH₄ leak rates ranging from 0.3 to 0.7 kg/h (8 to 20 SLPM) to develop a stable underground NG plume (Gao et al., 2021; Jayarathne et al., 2024; Ulrich et al., 2019). The leak was terminated prior to starting the aeration. To operate soil aeration under different surface soil water saturation conditions, the surface of the testbed was watered to create a saturated near-surface condition. The condition is referred to as a “water cap” in this study and is represented by the “Wet near-surface (WS)” scenarios in Table 2. The experiments conducted under dry soil conditions are named as “Dry soil (D)” scenarios. The soil water saturation was 0.1 in dry soil and approximately 0.8 in the water cap scenario. In addition to soil water saturation, the main difference between experimental scenarios was the number of aeration bar holes, ranging from 1 to 5, and the aeration duration (1 to 6 hrs).

Table 4. 2. Experimental scenarios and operation strategies of aeration in controlled experiments. “D” is used to present the dry soil condition. “WS” is applied to describe the wet near-surface condition.

Scenario #	Experimental scenarios	Number of active aeration bar holes and purger locations	Averaged leak rate kg/h (SLPM)	Aeration duration (hours)	Near-surface saturation (S_w) ^a
1	Dry soil (D)	1	0.7 (20)	1	0.1
2	Wet near-surface (WS)	1	0.4 (10)	2	0.8
3	Dry soil (D)	3	0.3 (8)	5	0.1
4	Wet near-surface (WS)	3	0.4 (10)	1.3	0.8
5	Dry soil (D)	5	0.4 (10)	1.8	0.1
6	Wet near-surface (WS)	5	0.4 (10)	1	0.8

^a Near-surface saturation was calculated using measured soil moisture at a depth of 10 cm below the ground surface and porosity.

4.2.2 Reduced-Order Framework for Field-Scale NG Soil Aeration

The proposed reduced-order framework was developed by translating outputs from a physics-based multiphase transport simulations into a field-applicable engineering method for NG soil aeration. The framework expresses dominant subsurface gas transport behavior using simplified relationships that rapidly estimate CH₄ removal performance, aeration duration, and bar-hole configuration from measurable site and operational inputs. Fig. 4. 3 summarizes the framework and outlines the sequence of inputs required to design and operate NG soil aeration in the field. The framework begins with site characterization and concludes with recommended aeration design and operation parameters, providing a consistent and transparent basis for guiding aeration decisions under varying site conditions. Using field-obtainable inputs, the framework estimates key engineering parameters, including CH₄ removal efficiency, required aeration duration, bar-hole number and spacing, and recommended bar-hole layout, which are typically difficult to determine directly during field operations.

Within the framework, the subsurface CH₄ plume is approximated as an elliptical cylinder. Plume area is estimated from the measured lateral plume boundary, while the plume thickness is approximated using the leak depth (D. H. D. Bass, 1993; U.S. Army Corps of Engineers, 2002). During aeration, induced airflow is assumed to contact a fraction of the target CH₄ plume, representing a dimensionless airflow contact efficiency factor (η) ranging from 0 to 1 (Hutzler et al., 1990; U.S. Army Corps of Engineers, 2002). A value of $\eta = 1$ represents the upper-bound condition in which airflow fully contacts the target plume, whereas $\eta < 1$ represents incomplete contact resulting from airflow bypass, soil heterogeneity, or poorly connected pore regions. For screening-level calculations, the base-case analysis assumes $\eta = 1$ to estimate the maximum potential removal capacity under idealized conditions. This assumption does not imply complete airflow contact under field conditions. Instead, it provides a first-order engineering estimate suitable for rapid field decision-making.

Although the simplified soil venting approaches developed for SVE cannot be directly applied to NG soil aeration due to the different spatial scales, transient behavior, and operational time frames involved, they provide a physically consistent foundation for assessing the performance of the reduced-order framework presented in this study. Therefore, the framework retains only the dominant first-order relationships among airflow, soil conditions, and CH₄ removal performance, as identified from the underlying multiphase transport simulations. To maintain field applicability, the required inputs are limited to parameters that can be readily obtained on-site, avoiding reliance on laboratory testing or complex numerical simulations. This enables rapid screening-level assessment and practical application during NG leak response operations.

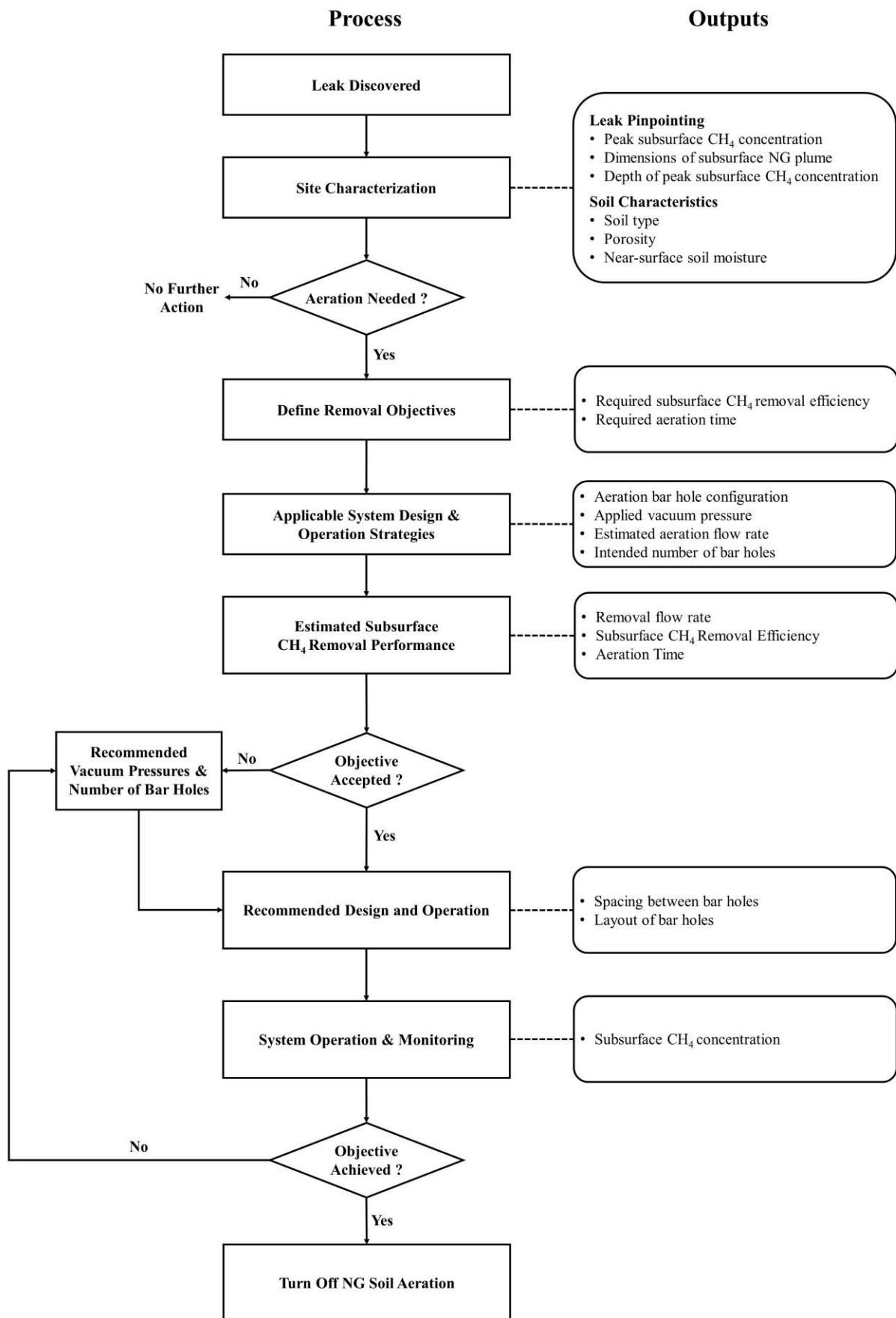


Fig. 4. 3. Conceptual framework of the reduced-order approach for field-scale NG soil aeration design and operation. The framework integrates site characterization and operation inputs to estimate subsurface CH₄ removal performance, bar-hole number and spacing, aeration duration, and recommended bar-hole deployment.

Site characterization

Whenever subsurface leaks are detected or suspected, a site characterization is conducted to provide the basic information required to determine whether NG soil aeration is needed and to offer the initial inputs for the reduced-order approach. The site characterization includes leak pinpointing and soil characteristics. At a leak site, initial leak pinpointing can identify the approximate thickness and the qualitative extent of the subsurface CH₄ plume. In addition to plume geometry, the CH₄ concentration distribution is required, especially the peak concentration, to determine if NG soil aeration is required. If subsurface CH₄ concentrations exceed safety thresholds or the estimated gas plume cannot dissipate naturally, the NG soil aeration needs to be implemented to mitigate the potential hazard.

Soil characteristics are another critical component in the site characterization. These include soil type, porosity (ϕ), and near-surface water saturation (S_w), which control the mass of subsurface CH₄, affect the soil relative permeability to subsurface gas transport, and impact the overall subsurface CH₄ removal performance. The near-surface saturation was measured at approximately 10 cm below the ground surface. S_w is a field-measurable input used for screening-level assessment and represents near-surface water saturation rather than an average saturation across the full plume depth. In this study, S_w was calculated using soil moisture measurements collected at approximately 0.1 m below ground surface. When moisture measurements with depth are available, S_w may be replaced with a representative plume-scale saturation to refine the

estimated CH₄ volume (Eq. 4. 2). The subsurface NG plume is approximated as an elliptical cylinder, with the horizontal plume area (A_e) from the distances between the location of the highest CH₄ concentration and the plume boundary defined by near-zero CH₄ readings (Eq. 4. 1). The total volume of subsurface CH₄ (V_{CH_4}) can be estimated by multiplying the ellipsoidal surface area by the thickness of CH₄ plume (z_{CH_4}) and the volume of gas in the soil (Eq. 4. 2). The mass of CH₄ (M_{CH_4}) can be estimated by multiplying V_{CH_4} by the measured CH₄ concentration (C_{CH_4}) (Eq. 4. 3).

The outputs from site characterization define the site conditions needed to evaluate the subsurface CH₄ mass and determine whether soil aeration is required. These outputs transition directly into the next step, which defines aeration objectives. The objectives specify the required subsurface CH₄ removal efficiency and aeration duration. This process from site characterization to aeration objectives mirrors the sequence shown in the flowchart and ensures a clear linkage between initial site data and subsequent design and operational decisions.

$$A_e = \pi \frac{L_a}{2} \frac{L_b}{2} \quad \text{Eq. 4. 1}$$

$$V_{CH_4} = A z_{CH_4} \phi (1 - S_w) \quad \text{Eq. 4. 2}$$

$$M_{CH_4}(t) = V_{CH_4} C_{CH_4}(t) \quad \text{Eq. 4. 3}$$

where L_a and L_b are the full major and minor axis lengths of the elliptical plume, measured through the location of peak CH₄ concentration between zero-concentration plume boundaries.

Define Removal Objectives

Once NG soil aeration is selected as the mitigation approach, the next step is to define the removal objectives that the aeration system is intended to achieve. These objectives include the targeted subsurface CH₄ removal efficiency and the maximum allowable aeration duration, which

together establish the quantitative criteria that guide aeration design and operation. Removal objectives are determined using the outputs from site characterization, including estimated plume geometry and peak subsurface CH₄ concentration.

Within the proposed framework, two performance metrics are used to evaluate aeration effectiveness: overall CH₄ mass removal efficiency ($Re_{M_{CH_4}}$, %) and local CH₄ removal efficiency ($Re_{C_{CH_4}}$, %). The overall CH₄ mass removal efficiency ($Re_{M_{CH_4}}$) is defined as the ratio of the removed CH₄ mass to the initial subsurface CH₄ mass (Eq. 4. 4). The metric $Re_{C_{CH_4}}$ is calculated from the reduction in CH₄ concentration measured at a monitored location (Eq. 4. 5). The $Re_{M_{CH_4}}$ incorporates concentration distribution, plume geometry, soil properties, and the total accumulated CH₄ mass, providing a site-scale measure of aeration performance. This metric is used to evaluate whether sufficient subsurface CH₄ removal has been achieved to satisfy safety and regulatory objectives.

In contrast, $Re_{C_{CH_4}}$ provides the relative reduction in subsurface CH₄ concentration at a specific location during aeration and is primarily used to assess field-observed aeration progress. Since it is based on concentration measurements at a single point, it is sensitive to local flow conditions, bar-hole configuration, and near-field gas transport behavior. Moreover, it is used to evaluate whether the applied vacuum pressure and aeration flow rate are effectively influencing the target region of the plume. Low or stagnant local CH₄ removal efficiency ($Re_{C_{CH_4}}$) may indicate insufficient advective flow, poor bar-hole placement, or restrictions in soil permeability near the monitoring location. Furthermore, the $Re_{C_{CH_4}}$ helps identify rebound behavior or persistence of a localized or entrapped gas plume. An increase in the local CH₄ concentration after aeration may indicate ongoing release from soil pores or delayed diffusion from low-permeability zones.

Therefore, while $Re_{M_{CH_4}}$ describes the total progress toward site-level removal goals, the $Re_{C_{CH_4}}$ provides spatially resolved insight into the effectiveness of aeration at specific locations, enabling operators to evaluate performance limitations, adjust system configuration, and refine the aeration strategy as needed.

$$Re_{M_{CH_4}}(t) = \frac{M_{0CH_4} - M_{CH_4}(t)}{M_{0CH_4}} \quad \text{Eq. 4. 4}$$

$$Re_{C_{CH_4}}(t) = \frac{C_{0CH_4} - C_{CH_4}(t)}{C_{0CH_4}} \quad \text{Eq. 4. 5}$$

where t is the time during aeration (min), M_{0CH_4} (g) is the initial CH_4 mass, $M_{CH_4}(t)$ (g) is the CH_4 mass at time t , $C_{CH_4}(t)$ (ppmv) is the measured CH_4 concentration at time t , and C_{0CH_4} (ppmv) is the measured initial CH_4 concentration.

The aeration duration defines the period when subsurface CH_4 is removed from the subsurface to meet the removal objectives. In practice, the allowable aeration duration is determined primarily by the operator because the duration of field activities is constrained by site access, safety considerations, and other site-specific conditions. As a result, the required aeration duration varies from site to site and is established early in the planning process as part of the overall removal objective. However, although aeration duration is determined by operators, it can be evaluated using site-specific design parameters and the expected performance of the aeration. The relationship among overall subsurface CH_4 mass, achievable removal flow rate, and bar-hole configuration provides a basis for estimating whether the specified aeration duration is adequate to reach the targeted removal efficiency. The method for estimating aeration duration using the applicable design and operational parameters is presented in the following section.

As a result, the required subsurface CH_4 removal efficiency and allowable aeration duration serve as the removal objectives for the reduced-order approach. They outline the essential link

between site characterization and system design, enabling the calculation of the removal performance to meet the aeration goals and providing the basis for evaluating whether specific design and operational strategies are feasible under actual field conditions.

Applicable System Designs & Operational Strategies

Once the removal objectives are defined, the next step is to identify the applicable aeration design and operational strategies that can be implemented under field conditions. This step reflects the practical options available to the operator and establishes the controllable parameters governing NG soil aeration performance. These parameters form the basis for evaluating the expected CH₄ removal efficiency, aeration duration, and plume coverage.

The primary design and operational parameters include bar-hole configuration, applied vacuum pressure, estimated aeration flow rate, and the number of active bar holes. Bar-hole configuration defines the diameter, depth, spacing, and layout of the aeration bar holes. In this study, bar-hole dimensions were selected based on the controlled experimental design. Applied vacuum pressure was controlled by the aeration equipment (e.g., purger system) and the compressed air supplied by the air compressor. The induced vacuum pressure generated advective airflow toward the bar holes, promoting CH₄ removal from the subsurface. The aeration flow rate represents the expected volumetric airflow delivered through each bar hole under site-specific soil and operating conditions. In practice, this flow rate may be estimated using manufacturer design curves that relate vacuum pressure to achievable airflow. When pilot pressure testing is feasible, aeration flow rate may alternatively be estimated using Darcy's law and the van Genuchten model (Appendix E. 2). The intended number of aeration bar holes indicates the operational extent of the aeration system and directly influences the coverage and overall CH₄ removal performance. Because bar-

hole effectiveness depends on plume geometry and the radius of influence, the selected number and spacing of bar holes determine whether sufficient plume coverage can be achieved under field conditions. These parameters are iteratively adjusted within the framework until the target removal objectives are satisfied.

Estimated Subsurface CH₄ Removal Performance

The applicable design and operational parameters are used to evaluate the expected subsurface CH₄ removal performance. Key performance metrics include the removal flow rate, the subsurface CH₄ removal efficiency, and the aeration duration required to meet the removal objectives. The process for estimating the removal performance based on the design and operational parameters is presented in the following section.

Removal Flow Rate

The removal flow rate of CH₄ (RF_{CH_4}) (g/min) is the rate of CH₄ mass removed from soil per unit time through each aeration bar hole. This metric is the estimated mass-removal capacity of the aeration and is used to determine the number of bar holes required and the total aeration duration needed to achieve the defined removal objectives. The aeration flow refers to the volumetric airflow delivered by the aeration equipment at a bar hole and reflects the capacity of the applied vacuum pressure and the effectiveness of the aeration tool. In contrast, the RF_{CH_4} represents airflow that actively contributes to subsurface CH₄ removal by gas advection from the subsurface to the bar hole. While the aeration flow rate is determined primarily by operational factors such as vacuum pressure and soil permeability, the RF_{CH_4} depends on both the aeration

flow rate and the subsurface CH₄ concentration. As a result, the removal flow rate provides a more direct metric of removal performance and is the parameter used to evaluate whether the NG soil aeration can meet the required CH₄ removal targets.

The RF_{CH_4} incorporates both the subsurface CH₄ concentration (C_{CH_4} , g/m³) and the equipment-specific aeration flow rate (Q , m³/min) (Eq. 4. 6). For the reduced-order approach, the RF_{CH_4} is assumed to represent CH₄ mass transported homogeneously and radially toward the aeration bar hole within the contacted portion of the plume. Since the base-case calculation assumes complete airflow contact with the target plume and does not resolve mass transfer from poorly connected pore regions, the factor to adjust the effective removal flow rate is not included in calculation (i.e., $\eta = 1$ in Eq. 4. 6) (Kuo, 2014; U.S. Army Corps of Engineers, 2002). If the aeration duration (T_c) is limited, the acceptable CH₄ removal flow rate (RF_{CH_4acpt}) describes the minimum removal flow rate required at a bar hole to meet the aeration objective within the specified aeration duration. This value is calculated from the total volume of subsurface CH₄ (V_{CH_4}) and the target reduction in subsurface CH₄ concentration (Eq. 4. 7 and Eq. 4. 8).

$$RF_{CH_4} = \eta C_{CH_4} Q \quad \text{Eq. 4. 6}$$

$$RF_{CH_4acpt} = \frac{M_{Re}}{T_c} \quad \text{Eq. 4. 7}$$

$$M_{Re} = V_{CH_4}(C_{ini} - C_{target}) \quad \text{Eq. 4. 8}$$

where η (-) is the airflow contact efficiency factor, C_{CH_4} (ppmv) is the maximum subsurface CH₄ concentration (ppmv), C_{ini} (ppmv) is the initial maximum subsurface CH₄ concentration measured, Q (m³/min) is the aeration flow rate as specified by the design of the equipment, M_{Re} (g) is the estimated mass of accumulated CH₄ in soil, T_c (min) is the required aeration duration,

V_{CH_4} (m^3) is the volume of CH_4 in the soil (m^3), C_{target} (ppm) represents the target residual CH_4 concentration, which is set to 50 ppmv (0.005 vol.%) in this study. This value is an industry-informed operational target based on feedback from NG operators rather than a universal regulatory threshold and may be adjusted based on site-specific safety or operational requirements.

Subsurface CH_4 Removal Efficiencies

Within the framework, subsurface CH_4 removal efficiencies provide quantitative measures of NG soil aeration performance by evaluating reductions in both total subsurface CH_4 mass ($Re_{M_{CH_4}}$) and local CH_4 concentration ($Re_{C_{CH_4}}$). These metrics represent the fraction of the initial subsurface CH_4 mass and local CH_4 concentration removed during aeration and serve as primary metrics for assessing whether the defined removal objectives are being achieved. The formulations used to estimate CH_4 removal efficiencies are introduced in the objective-definition section (Eq. 4. 4 and Eq. 4. 5). The removal efficiency metrics integrate the combined effects of bar-hole configuration, applied vacuum pressure, and aeration duration on subsurface CH_4 removal performance. They are further used to identify diminishing removal rates and evaluate whether modifications to aeration design or operations, such as additional bar holes, adjusted spacing, or extended aeration duration, are needed to achieve target removal objectives. In this study, the overall CH_4 mass removal efficiency ($Re_{M_{CH_4}}$) is used as the primary decision-making metric for evaluating aeration system performance and guiding screening-level design decisions, including aeration duration, bar-hole number, spacing, and layout.

Aeration Duration

Aeration duration represents the duration required for NG soil aeration to achieve the target subsurface CH₄ removal objective. The applicable target threshold varies based on site-specific environmental conditions, operational requirements, and safety criteria. Common metrics used to evaluate aeration duration include cumulative CH₄ mass removal, aeration flow rate, CH₄ concentration in the extracted gas, composition of extracted gas, and residual CH₄ concentrations at the primary monitoring location (Johnson et al., 1990). In NG field practice, aeration typically continues until the monitored subsurface CH₄ concentration decreases to approximately 0 and 0.005 vol % (0 to 50 ppmv). Because C_{target} is a user-defined input, the estimated aeration duration can be recalculated for alternative site-specific endpoints. Within the reduced-order framework, aeration duration is estimated using the subsurface CH₄ mass (M_{Re}), the CH₄ removal flow rate (RF_{CH_4}), and the intended number of active bar holes (N_{bh_int}) (Eq. 4. 9). Aeration duration therefore reflects both the removal capability of the aeration system and practical operational constraints encountered under field conditions.

$$T_c = \frac{M_{Re}}{RF_{CH_4} \times N_{bh_int}} \quad \text{Eq. 4. 9}$$

Once the performance metrics have been evaluated, including the removal flow rate, subsurface CH₄ removal efficiency, and estimated aeration duration, the framework assesses whether the removal objectives have been reached. This evaluation compares estimated aeration performance against the target subsurface CH₄ removal efficiency and allowable aeration duration defined during the objective-definition step.

If the evaluated removal performance does not satisfy the defined removal objectives, the framework recommends adjustments to the aeration design and operational strategy, including

modifying the vacuum pressure, bar-hole number, and deployment. The relationships among vacuum pressure, bar-hole number, plume geometry, CH₄ removal efficiency, and aeration duration are represented using simplified contour diagrams that provide operators with rapid, field-applicable guidance for NG soil aeration design and operation. Based on the recommended vacuum pressure and bar-hole number, the framework then evaluates bar-hole spacing and layout to maximize plume coverage and improve CH₄ removal efficiency. By linking removal performance metrics to these adjustable design parameters, the framework offers a systematic and practical method for identifying field-applicable aeration strategies under varying site conditions. The following sections describe the evaluation of the bar-hole number (N_{bh}), spacing (S_{bh}), and layout.

Number of Aeration Bar Holes

The number of aeration bar holes (N_{bh}) is a key design parameter controlling the overall capacity of NG soil aeration to remove subsurface CH₄. It determines the extent of plume coverage and the number of active aeration locations to achieve the target removal objectives. Furthermore, N_{bh} directly influences the total CH₄ removal flow rate that can be achieved under site-specific soil and operating conditions.

Increasing the number of bar holes expands the effective aeration region and improves plume coverage, allowing pressure-driven airflow to reach a larger portion of the subsurface CH₄ plume. This generally enhances the mass-removal capacity by increasing the total CH₄ removal flow rate and reducing the time required to achieve the target removal efficiency. In contrast, an insufficient number of bar holes may result in incomplete plume coverage or insufficient removal flow rate, leading to prolonged aeration duration and reduced removal performance. Therefore, determining

the number of bar holes is essential for optimizing plume coverage, removal efficiency, and operational duration. Within the reduced-order framework, the recommended number of bar holes is estimated using the acceptable CH₄ removal flow rate and the maximum CH₄ removal flow rate achievable for a single bar hole (Eq. 4. 10). The value of $RF_{CH_4_{max}}$ is calculated using Eq. 6 and the maximum observed subsurface CH₄ concentration at the site.

$$N_{bh} = \frac{RF_{CH_4_{acpt}}}{RF_{CH_4_{max}}} \quad \text{Eq. 4. 10}$$

Recommended Design and Operation

The estimated CH₄ removal efficiency and aeration duration are compared against the targeted removal objectives to determine whether the proposed aeration design satisfies site requirements. If the predicted removal performance does not meet the specified objectives, system parameters, including the applied vacuum pressure, bar-hole number, spacing, or aeration duration, are adjusted and re-evaluated using the same performance estimation procedure. This iterative process continues until the predicted aeration performance agrees with the removal objectives. Once acceptable performance is achieved, the corresponding design parameters define the recommended aeration design and operation, including bar-hole spacing and layout.

Bar-Hole Spacing (S_{bh}) and Layout

Appropriate bar-hole spacing and layout are essential for minimizing plume coverages while minimizing overlap between adjacent aeration zones. If the spacing is too large, portions of the CH₄ plume may remain insufficiently aerated, reducing overall removal efficiency. In contrast, overly dense spacing can produce airflow interference and inefficient treatment coverage.

Therefore, bar-hole spacing (S_{bh}) is linked to both the subsurface plume geometry and the aeration area of an individual bar hole (A_{bh}).

Within the framework, the subsurface plume is approximated as an elliptical cylinder with its major axis aligned along the monitored cross-section. The effective aeration area of a single bar hole (A_{bh}) is estimated from the extracted gas volume associated with one bar hole during the target aeration period divided by the effective plume thickness (Eq. 4. 11) (U.S. Army Corps of Engineers, 2002). In this framework, A_{bh} represents an active aeration area derived from estimated CH_4 removal capacity rather than a radius of influence obtained from pressure testing, which is not routinely conducted during field-scale NG soil aeration. Therefore, A_{bh} is interpreted as an active removal area based on removal capacity for spacing and layout calculations.

Bar-hole layout is determined simultaneously with spacing and bar-hole number because these parameters collectively control plume coverage and uniformity of aeration. A hexagonal lattice arrangement is used to approximate near-uniform plume coverage while minimizing overlap between adjacent aeration zones (A_o). Within this geometric framework, S_{bh} corresponds to the center-to-center distance between bar holes (Eq. 4. 12). The coverage rate (CR) is a geometric indicator of the ratio of the effective covered area ($N_{bh}A_{bh} - A_o$) to the total plume area (A_{plume}) (Eq. 4. 13).

When an odd number of bar holes is required, one bar hole is placed at the plume centroid. Using the spacing derived from Eq. 4. 12 as the initial estimate, CR is calculated iteratively from the hexagonal layout, and S_{bh} is adjusted until CR reaches or exceeds 95% (Eq. 4. 14). The CR is used to reduce uncovered regions within the plume while avoiding unnecessarily dense bar-hole spacing and excessive overlap among adjacent aeration zones (U.S. Army Corps of Engineers, 2002). A sensitivity analysis using CR thresholds of 85%, 90%, 95%, and 99% is conducted to

evaluate its effect on estimations of bar-hole spacing and layout (Appendix E. 7). The results show that the 95% *CR* threshold provides a practical balance between plume coverage and efficient bar-hole deployment. Therefore, in this study, the 95% criterion is used as a practical engineering target for near-complete plume coverage in the screening-level spacing and layout analysis and should be interpreted as a study-specific design criterion for preliminary field planning rather than as a universal physical threshold or an established NG industry design standard.

In Eq. 4. 11, Q_{bh} represents the aeration flow rate assigned to an individual bar hole under the selected vacuum pressure. The effective aeration area (A_{bh}) is therefore calculated for a single bar hole and used as the basic active removal area for spacing and layout calculations. For multiple bar holes, the framework estimates total removal capacity using a first-order additive capacity assumption. This assumption does not explicitly resolve pressure redistribution, manifold losses, or pneumatic interference among adjacent bar holes during simultaneous operation.

$$A_{bh} = \frac{Q_{bh}T_c}{\eta\phi(1-S_w)z_{CH_4}} \quad \text{Eq. 4. 11}$$

$$S_{bh} = \sqrt{\frac{2A_{bh}}{\sqrt{3}}} \quad \text{Eq. 4. 12}$$

$$CR = \frac{N_{bh}A_{bh}-A_o}{A_{plume}} \quad \text{Eq. 4. 13}$$

$$\max CR(S_{bh}) \quad \text{subject to } CR(S_{bh}) \geq 95\% \quad \text{Eq. 4. 14}$$

where Q_{bh} (m^3/min) is the aeration flow rate of an individual bar hole, A_o is the overlap area between bar holes, and A_{plume} (m^2) is the area of the overall subsurface CH_4 plume based on the measurement of subsurface CH_4 concentration in the site characterization.

Once the aeration design is finalized, NG soil aeration can be implemented under the selected vacuum pressure and aeration duration. Subsurface CH_4 concentrations are continuously

monitored at selected locations to evaluate plume response and verify that the aeration is effectively reducing CH₄ concentrations within the targeted zone. Monitoring data are compared against the predicted removal performance to determine whether the removal objectives have been achieved.

The observed CH₄ concentrations are compared against the estimated removal performance to determine whether the removal objective has been achieved. If the monitored values do not meet the specified criteria, the performance data are used to reassess system behavior, and the design parameters are adjusted by adjusting the applied vacuum pressure, the number of bar holes, or the aeration duration. These amended parameters are re-evaluated through the performance estimation procedure, and the design is iteratively refined until the predicted performance reaches the removal requirements. When monitoring confirms that subsurface CH₄ concentrations have decreased below the target threshold (50 ppmv in this study), aeration may be terminated. After aeration is stopped, post-aeration CH₄ monitoring is conducted to evaluate residual CH₄ concentrations and potential rebound. Because the reduced-order framework does not explicitly simulate rebound dynamics, rebound assessment is incorporated as an operational monitoring step. If elevated or rebounding CH₄ concentrations are observed, the framework should be reapplied using updated plume conditions and revised operating parameters to reassess aeration duration, bar-hole number, spacing, and layout.

The framework described above integrates site characterization, aeration system design, performance estimation, and operational reassessment into a unified screening-level engineering approach for NG soil aeration. By linking measurable site conditions to physics-based performance estimates and field monitoring observations, the framework enables iterative evaluation and refinement of aeration performance under varying field conditions. The following section applies

the framework to controlled field experiments and simulated aeration scenarios to evaluate framework performance and demonstrate its practical application for NG leak response.

4.3 Results and Discussion

This section presents the results of the controlled NG aeration field experiments, according to the six scenarios outlined in Table 4. 2. The framework and respective Eq. 4. 1 to Eq. 4. 10 are used to estimate design and operational parameters, including the number of aeration bar holes and the required aeration duration. A comparison between estimated and experimental results is used to evaluate the framework. Analyses of the differences between estimated and observed removal performance provide insights that improve the practical design and operation of NG soil aeration systems.

4.3.1 Subsurface CH₄ Migration Behavior from Controlled Field Experiments

Before applying the reduced-order approach to field design and operation, it is important to understand the subsurface gas migration behavior observed in the controlled aeration experiments. Fig. 4. 4 and Fig. 4. 5 present the spatial distributions of residual CH₄ for all scenarios under dry soil conditions (S1, S3, S5) and wet near-surface conditions (S2, S4, S6) prior to aeration and during aeration at 30 and 60 minutes. The CH₄ concentration contours in Fig. 4. 4 and Fig. 4. 5 were generated using the interpolation v4 function in MATLAB based on measured subsurface CH₄ concentrations from gas sensors installed along the monitored cross-section. The v4 method provides biharmonic spline interpolation for two-dimensional scattered data and generates smooth surfaces suitable for visualizing cross-sectional CH₄ measurements. These contours are intended to visualize the cross-sectional CH₄ distributions during aeration. Only one side of the plume is shown because the bar-hole deployment was symmetric relative to the leak and aeration line.

At the beginning of aeration ($T = 0$ min), the CH₄ plumes show similar lateral and vertical distribution patterns in both soil conditions. In the wet scenarios (Fig. 4. 5a, Fig. 4. 5d, and Fig. 4.

5g), the plume shapes reflect buoyancy-driven upward migration and diffusion-driven lateral and downward spreading, consistent with (Deepagoda et al., 2016). However, the wet near-surface condition ($S_w=0.8$) produces substantially higher initial CH_4 concentrations, indicating that elevated surface water saturation restricts vertical gas migration and results in greater gas accumulation belowground. During aeration ($T = 30$ min), CH_4 concentrations decrease in all scenarios. The removal rate and spatial distribution of residual CH_4 are observed to be highly related to soil condition (dry vs wet) and bar-hole configuration. Under dry soil conditions, S1 and S3 show rebound or increase in gas concentration at $T = 30$ min (Fig. 4. 4b–c and Fig. 4. 4e–f), due to diffusion of CH_4 from adjacent, poorly aerated zones. In contrast, S5 demonstrates continued improvement in removal (Fig. 4. 4h–i) over time. Under wet near-surface conditions, rapid and efficient aeration is observed as the wet near-surface conditions enhance removal by redirecting gas laterally toward the aeration points. For example, S2 and S6 reach nearly complete removal by 30 minutes (Fig. 4. 5b and Fig. 4. 5h). S4 shows similar behavior, with CH_4 decreasing rapidly across the monitored domain (Fig. 4. 5e). By 60 minutes, residual CH_4 approaches zero in all wet scenarios (Fig. 4. 5c, Fig. 4. 5f, and Fig. 4. 5i). The change in the spatial distribution of residual CH_4 also indicates that although CH_4 at the bar-hole depth or specific monitored location may reach near-zero values, elevated concentrations may remain closer to the surface, emphasizing the need for spatially distributed monitoring rather than relying on a single measurement depth. For example, D2, the monitoring location closest to the isolated leak (Fig. 4. 1), indicated nearly complete removal in Fig. 4. 4h and Fig. 4. 5h. However, shallow CH_4 persisted above D2. Thus, relying on a single-point measurement would have resulted in a false assessment of removal effectiveness, reinforcing the need for multi-depth or spatially distributed monitoring during aeration operations.

Although the analysis of overall observed CH₄ removal performance provides design-level insight, evaluating the local removal efficiency (Re_{CH_4}) at a single monitoring location offers a rapid assessment of aeration performance under different soil saturations and bar-hole configurations (Appendix C. 4). Fig. C7 presents the observed Re_{CH_4} at D2 for all six scenarios with normalized aeration duration (t/t_0) to enable comparison among experiments with different aeration durations. In Fig. C7, the comparison among S1, S3, and S5 shows that increasing the number of bar holes improves local CH₄ removal efficiency (Re_{CH_4}) and mitigates rebound when spacing provides adequate coverage of the plume.

Overall, the results indicate that near-surface water saturation impacts the rate at which local CH₄ concentration removal efficiency (Re_{CH_4}) increases, whereas the number of bar holes largely governs the maximum removal efficiency achieved prior to rebound behavior. These findings demonstrate that effective NG soil aeration design and operation must account for site-specific soil conditions, particularly near-surface soil moisture and the number of bar holes needed to achieve sufficient plume coverage and CH₄ removal. Furthermore, the observed concentration rebound under dry soil conditions suggests that diffusion from less effectively aerated zones can continue to influence local CH₄ concentrations during and after active aeration. Therefore, post-aeration CH₄ monitoring and design reassessment remain important when elevated residual concentrations persist following shutdown. The reduced-order framework developed in this study is intended to provide screening-level estimates of removal efficiency and aeration design parameters rather than explicitly resolve transient rebound dynamics.

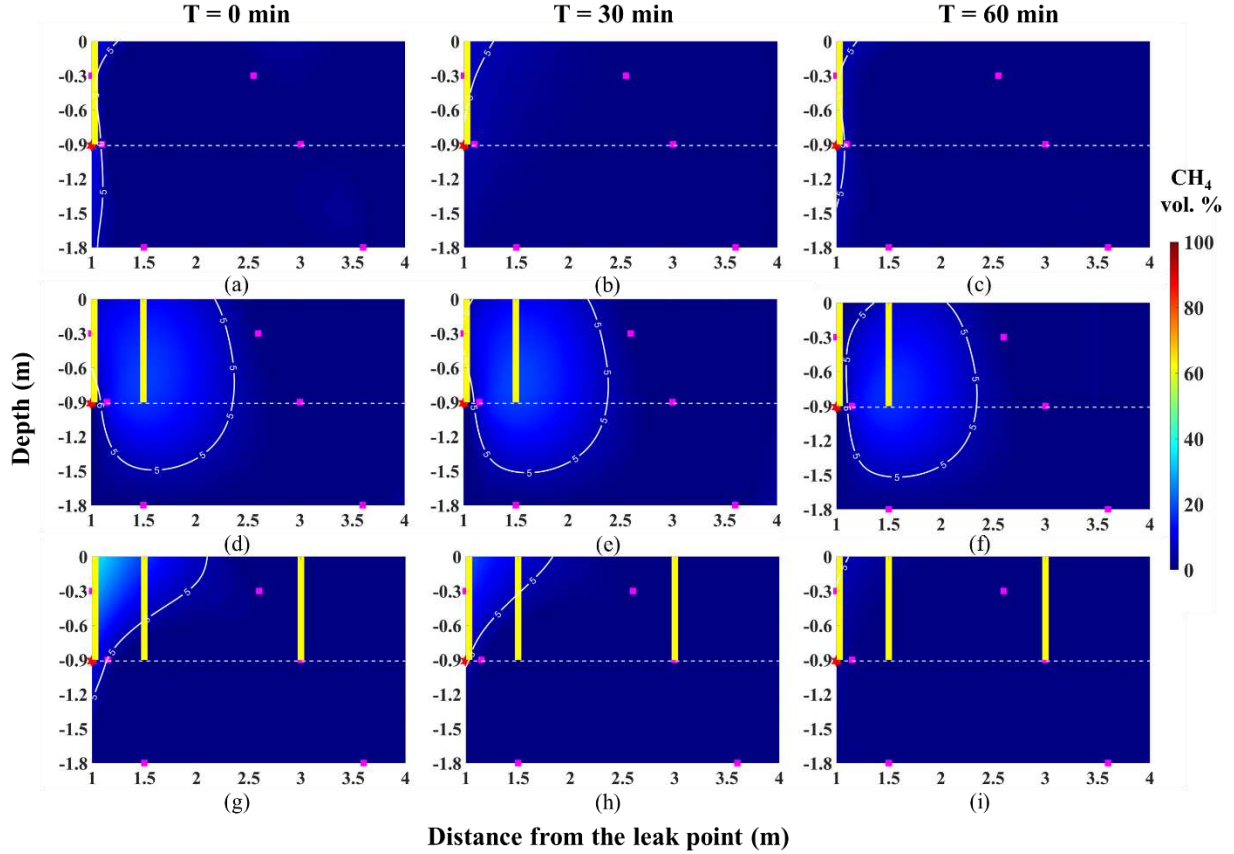


Fig. 4. 4. Cross-section plots of the spatial distribution of residual CH_4 during the first 60 min of soil aeration for S1 (a to c), S3 (d to f), and S5 (g to i) under dry soil conditions. S1, S3, and S5 represent dry soil scenarios with one, three, and five active aeration bar holes, respectively. The contours were generated from CH_4 concentrations measured by subsurface CH_4 sensors along the monitored cross-section and plotted as interpolated cross-sectional concentration fields. They represent cross-sectional CH_4 distribution response within the monitored domain rather than full three-dimensional plume evolution. Since the deployment of aeration bar holes is symmetric, the figure only shows the right side of the gas plume. The yellow bar in each figure presents the operated aeration bar hole during aeration. The white dashed line indicates the pipeline at a depth of 0.9 m at the testbed. The red star indicates the relative location of the isolated leak. The color bar shows CH_4 concentration in volume %. The pink squares represent the locations of INIR sensors. The average vacuum pressure at each aeration bar hole was 0.3 atm (5 psi).

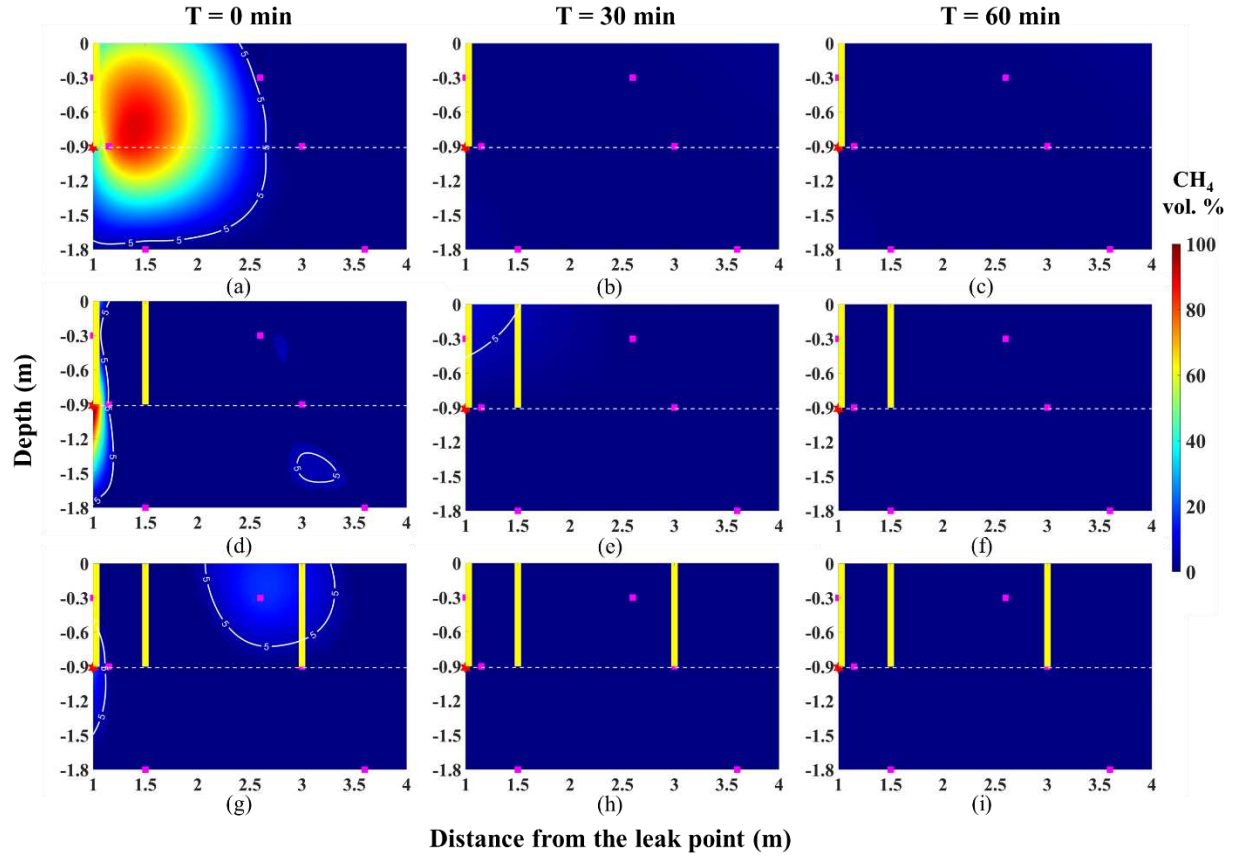


Fig. 4. 5. Cross-section plots of the spatial distribution of residual CH_4 during the first 60 min of soil aeration for S2 (a to c), S4 (d to f), and S6 (g to i). S2, S4, and S6 represent wet near-surface soil scenarios with one, three, and five active aeration bar holes, respectively. The contours were generated from CH_4 concentrations measured by subsurface CH_4 sensors along the monitored cross-section and plotted as interpolated cross-sectional concentration fields. They represent cross-sectional CH_4 distributions within the monitored domain rather than full three-dimensional plume evolution. Since the deployment of aeration bar holes is symmetric, the figure only shows the right side of the gas plume. The yellow bar in each figure presents the operated aeration bar hole during aeration. The white dashed line indicates the pipeline at a depth of 0.9 m at the testbed. The red star indicates the location of the isolated leak. The color bar shows CH_4 concentration in volume %. The pink squares represent the locations of INIR sensors. The average vacuum pressure at each aeration bar hole was 0.3 atm (5 psi).

4.3.2 Comparison of Framework Predictions Against Controlled Field Experiment Results

The experimental measurements were used to evaluate framework performance through a comparison of experimental and estimated CH₄ removal efficiencies across the six experimental scenarios (Fig. 4. 6). The approach was tested by applying the same soil water saturation and bar-hole configurations used in the experiments and evaluating whether the approach could capture the observed aeration behavior. This comparison evaluates screening-level removal performance and is not intended to fully reproduce time-dependent CH₄ concentration changes, including rebounds.

The estimated Re_{CH_4} shows reasonable trends with experimental Re_{CH_4} with an R^2 value of 0.74, indicating that the reduced-order approach captured the overall trend in CH₄ removal efficiency across the six experimental scenarios. In the wet near-surface scenarios (S2, S4, and S6), both the experimental and estimated removal efficiencies reached nearly complete removal (~100%). Under dry conditions, the reduced-order approach moderately overestimated Re_{CH_4} due to diffusion and incomplete plume removal from poorly aerated zones. The final experimental and estimated Re_{CH_4} are compared for each scenario (Table 4. 3). The largest differences were observed in the dry soil scenarios, with AE of 6.9%, 12.0%, and 15.6% for S1, S3, and S5, respectively. By contrast, the wet near-surface scenarios (S2, S4, and S6) showed zero final difference because both the experimental and estimated Re_{CH_4} reached complete removal. This result indicates strong agreement between the reduced-order approach and the field observations under wet near-surface conditions.

Under dry soil conditions (S1, S3, and S5), the reduced-order approach captures final Re_{CH_4} properly, demonstrating that the framework can estimate the Re_{CH_4} at the end of aeration. However, the approach does not reproduce the transient subsurface CH₄ concentration evolution,

including the early-time depletion and partial rebound observed in the experiments (Fig. C.1). These transient behaviors are induced by diffusion-dominated regions that persist in dry soils, where large air-filled pore volumes and soil heterogeneity create preferential pathways adjacent to poorly aerated domains (Armstrong et al., 1994; Carroll et al., 2012; Høier et al., 2009; Yoon et al., 2009). As CH_4 is removed from preferential flow paths, entrapped gas in smaller or disconnected pores diffuses back toward the bar hole, producing the observed rebound behavior.

Two additional factors contribute to the differences observed under dry soil conditions. First, the applied vacuum pressure of 0.3 atm and aeration flow rate of approximately 0.25 m³/min per bar hole may not have been sufficient to fully remove the accumulated CH_4 within the limited experimental duration. Second, measurement constraints associated with the INIR sensors may have influenced the comparison. The sensors were installed inside vertical plastic casings, limiting detection to CH_4 adjacent to or below the sensor and preventing direct measurement of upward CH_4 migration. This limitation is particularly important in dry soils, where vertical migration is more pronounced (Jayarathne, Kolodziej, et al., 2022b, 2022a).

The comparison further indicates that framework performance varies with soil moisture conditions. Within the tested range, stronger agreement was observed under wet near-surface conditions, whereas in dry soil scenarios, the experimental and estimated removal efficiencies showed larger differences. This contrast is consistent with field observations, in which wet near-surface conditions promoted more efficient lateral migration of CH_4 toward the aeration bar holes, while dry soil conditions showed fluctuating Re_{CH_4} in less effectively aerated zones.

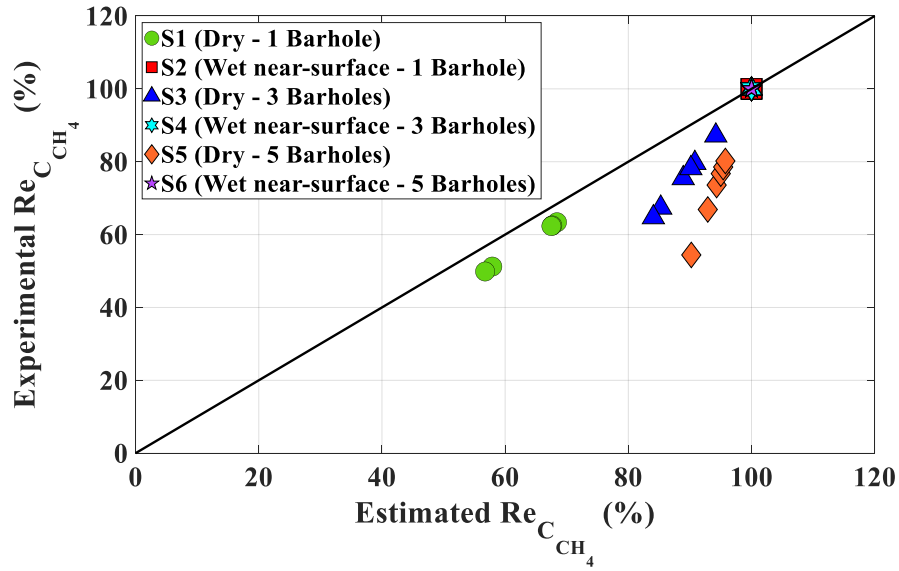


Fig. 4. 6. Comparison of estimated and experimental local CH_4 removal efficiency (Re_{CH_4}) for the six experimental scenarios. Re_{CH_4} is estimated using Eq. 4. 5 with a vacuum pressure of 0.3 atm (5 psi) and a plume diameter of 2.6 m. The overall agreement between simulations and observations shows $R^2 = 0.74$. The black line presents a 1:1 line.

Table 4. 3. Comparison of the observed and estimated Re_{CH_4} at the end of aeration experiment for the six experimental scenarios. Signed error (SE), absolute error (AE), and relative error (RE) were calculated using the final Re_{CH_4} at the end of each aeration experiment. “+” in SE indicates the overestimation.

	S1	S2	S3	S4	S5	S6
Observed final						
Re_{CH_4}	49.9	100	78.2	100	80.2	100
Estimated final						
Re_{CH_4}	56.7	100	90.1	100	95.8	100
SE	+6.8	0	+11.9	0	+15.6	0
AE	6.8	0	11.9	0	15.6	0
RE	13.8	0	15.3	0	19.4	0

4.3.3 Estimated Removal Performance

This section summarizes the removal performance predicted using the reduced-order approach, with maximum CH_4 removal flow rate, CH_4 mass removal efficiency, and required aeration duration to reach the target concentration. Across all indicators, vacuum pressure, bar-hole configuration, soil water saturation, and plume size control removal performance. These factors govern the advective airflow toward the aeration bar hole, the extent of plume coverage achieved by the aerated zone, and the subsurface CH_4 migration. Higher vacuum pressure enhances advective gas transport at each bar hole, while increases in the number of bar holes expand the effective aerated region, improving subsurface CH_4 plume coverage and overall removal flow rate. The model evaluation in this section focuses on the field-scale subsurface CH_4 removal response, while the estimation and interpretation of the maximum removal flow rate are provided in Fig. E1. Elevated near-surface water saturation suppresses upward CH_4 migration and promotes lateral gas movement toward the bar holes, improving $Re_{M_{\text{CH}_4}}$ (Fig. E3) but limiting the maximum achievable flow rate. Plume size further constrains aeration performance because larger plumes contain greater CH_4 mass and impose longer transport distances, resulting in lower achievable $Re_{M_{\text{CH}_4}}$ (Fig. E4) and longer aeration durations (Fig. E5).

Overall, the reduced-order approach reveals how vacuum pressure, bar-hole configuration, soil conditions, and plume size determine subsurface CH_4 removal performance. Variations in removal flow rate, overall CH_4 mass removal efficiency, and aeration duration are attributed to the same underlying physical mechanisms governing advective airflow and CH_4 transport distances. The summarized trends demonstrate how aeration performance can be controlled by adjusting vacuum pressure, bar-hole configuration, and aeration duration under site-specific constraints. Detailed results are presented in Appendices E. 3 to E. 5.

4.3.4 Recommended Design and Operation

The contour analyses in this section are used to extend the application of the reduced-order framework across practical ranges of water saturation, plume size, vacuum pressure, and bar-hole configuration. These analyses provide framework-based design estimates for screening-level field assessment and should be interpreted within the assumptions and parameter ranges evaluated in this study.

4.3.4.1 Estimated Number of Bar Holes

Fig. 4. 7 and Fig. 4. 8 present the estimated number of bar holes required to achieve the CH₄ removal target under varying plume sizes, vacuum pressures, and soil water saturation conditions. The results demonstrate clear dependencies between the number of bar holes and the controlling design and operational parameters. In general, the required number of bar holes increases with plume diameter and decreases as vacuum pressure increases. These relationships show the balance between the subsurface CH₄ mass that must be removed and the removal capacity provided by each bar hole.

The influence of vacuum pressure is evident for all plume sizes. At higher vacuum pressure, stronger induced airflow enhances the removal capacity of each bar hole, reducing the number of bar holes needed to reach the target removal. In contrast, when vacuum pressure is low, additional bar holes are required to compensate for the limited removal capability. This effect is particularly obvious for large subsurface CH₄ plumes. For example, at a plume diameter of 10 meters, aeration with a vacuum pressure of 0.2 atm requires multiple bar holes, while the same plume size can be managed with fewer bar holes when the vacuum pressure increases to 0.8 atm (Fig. 4. 8a).

Plume size also significantly controls the number of bar holes in NG soil aeration. Larger plumes contain greater subsurface CH₄ mass and longer transport distances to the aeration points, resulting in the need for a higher N_{bh} to reach specified removal objectives. For a plume diameter of 2 m, only one or two bar holes may be sufficient under moderate vacuum pressure (e.g., 0.3 atm). However, for plume diameters of 18 m, several bar holes are needed even under high vacuum pressure (e.g., 0.7 atm), illustrating the increased effort required to ensure adequate removal across a larger subsurface CH₄ plume. Soil saturation also affects the required bar-hole number. Wet near-surface conditions require fewer bar holes than dry soils because there is a higher $Re_{M_{CH_4}}$ per bar hole due to restricted vertical migration and enhanced lateral flow toward the aeration points. For example, at $L_{CH_4} = 6$ m (Fig. 4. 7c and Fig. 4. 7d), to reach the target removal objective with a vacuum pressure of 0.6 atm within 15 minutes, the wet near-surface conditions only require 2 bar holes, while dry soils need 5 bar holes. Therefore, fewer bar holes are required under wet near-surface conditions compared with dry soils at the same plume size and vacuum pressure.

These estimations highlight the importance of selecting appropriate combinations of bar-hole number and vacuum pressure based on measured plume dimensions and soil saturation. When only low vacuum pressure is available, achieving the target removal performance may require installing additional bar holes. However, when minimizing the number of bar holes is a priority, higher vacuum pressure or smaller plume sizes allow operators to meet removal goals with fewer bar holes. Thus, Fig. 4. 7 and Fig. 4. 8 provide a practical reference for field implementation by linking key site and operational parameters to the required number of bar holes in NG soil aeration.

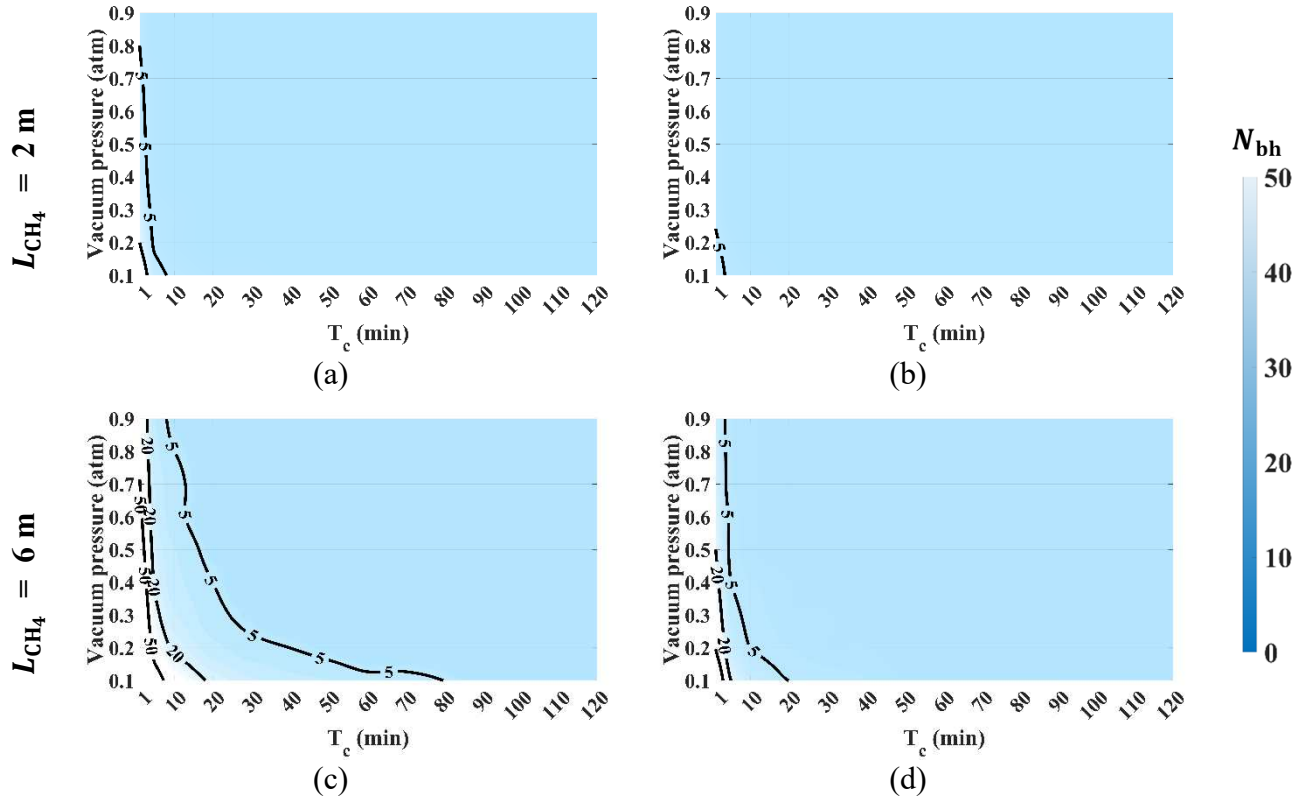


Fig. 4. 7. Estimated number of bar holes (N_{bh}) with vacuum pressure ranging from 0.1 to 0.9 atm and aeration duration (T_c) from 1 to 120 mins for different average diameters of CH_4 plume (L_{CH_4}). Panels (a, b) and (c, d) present $L_{CH_4} = 2$ and 6 m. The left contours (a and c) represent dry soil with $S_w = 0.1$, and the right contours (b and d) represent wet soil with an average water saturation of 0.80. N_{bh} is estimated using Eq. 4. 10.

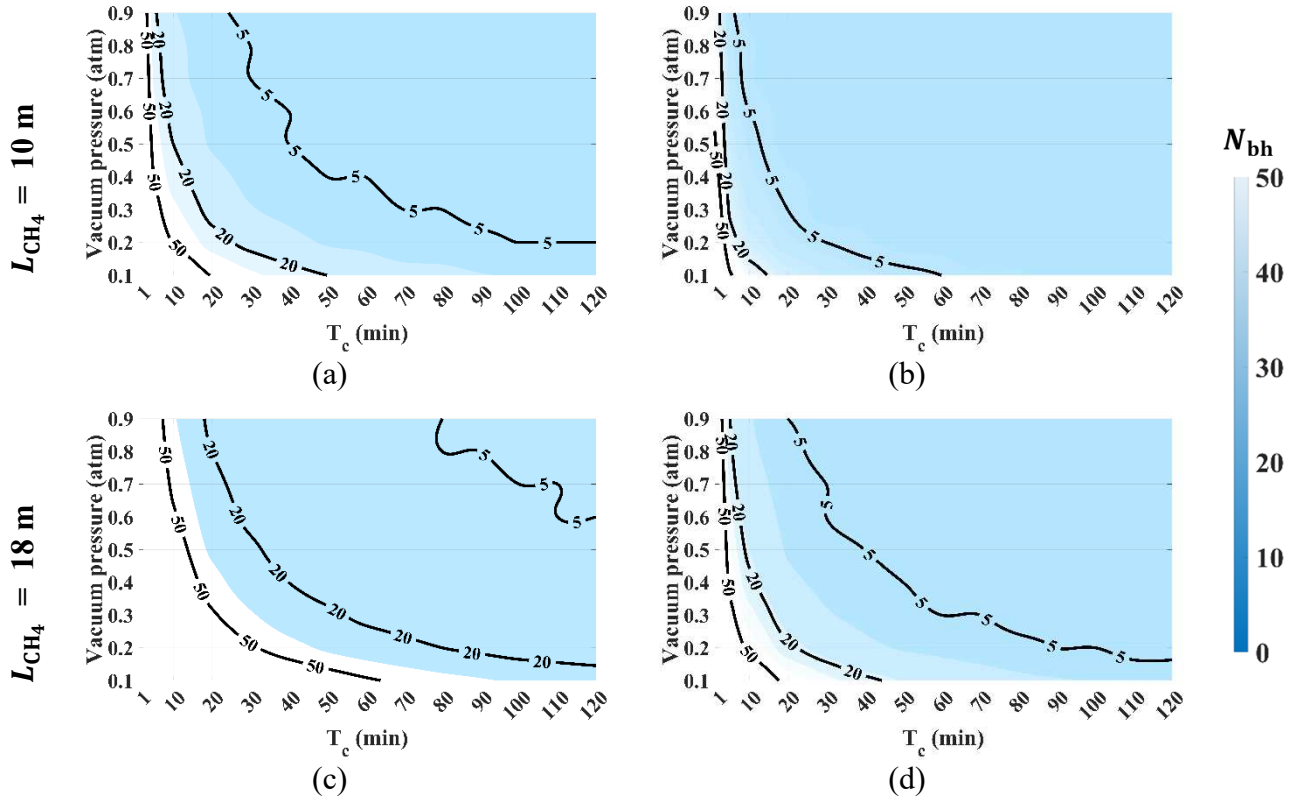


Fig. 4. 8. Estimated number of bar holes (N_{bh}) with vacuum pressure ranging from 0.1 to 0.9 atm and aeration duration (T_c) from 1 to 120 mins for different average diameters of CH₄ plume (L_{CH_4}). Panels (a, b), (c, d), (e, f), and (g, h) present $L_{CH_4} = 10$ and 18 m. The left contours (a and c) represent dry soil with $S_w = 0.1$, and the right contours (b and d) represent wet soil with an average water saturation of 0.80. N_{bh} is estimated using Eq. 4. 10.

4.3.4.2 Estimated Spacing between Bar Holes

This section presents the estimated spacing between bar holes (S_{bh}) for different numbers of bar holes under varying vacuum pressures and aeration duration at a fixed plume diameter of $L_{CH_4} = 2$ m (Fig. 4. 9 and Fig. 4. 10), as well as spacing variations across multiple plume sizes under a constant vacuum pressure of 0.3 atm (Appendix E. 6). In this framework, S_{bh} is selected as the largest spacing that still satisfied $CR \geq 95\%$. This criterion identifies the maximum spacing needed to maintain near-complete plume coverage while reducing overlap among removal zones.

For a fixed plume diameter, increasing the N_{bh} expanded the region where $CR \geq 95\%$ because the total removal area within the plume increased. However, the S_{bh} generally decreased as N_{bh} increased because more bar holes had to be distributed within the same plume domain while maintaining adequate overlap among adjacent aeration zones. The S_{bh} decreased from approximately 2.2 m to 1.5 m as N_{bh} increased from two to five. This result indicates that increasing N_{bh} improves plume coverage, but S_{bh} decreases because removal zones must maintain sufficient overlap to satisfy the 95% coverage criterion.

Vacuum pressure and near-surface soil moisture also affected S_{bh} . Higher vacuum pressure increased the removal capacity of a bar hole. Moreover, wet near-surface conditions promoted lateral gas movement toward the bar holes, increasing the coverage area. Under these conditions, larger spacing could still satisfy the 95% coverage criterion. However, if S_{bh} is too small, adjacent removal zones overlap excessively rather than improving layout efficiency. Therefore, the most efficient S_{bh} occurred near the $CR = 95\%$, where plume coverage was sufficient but unnecessary overlap was minimized. A sensitivity analysis using varying CR thresholds (85%-99%) is presented in Appendix E. 7 in SI.

Appendix E. 6 describes the variation in spacing across different plume diameters under a fixed vacuum pressure of 0.3 atm. Because the removal capacity of each bar hole remains constant at a fixed vacuum pressure, S_{bh} is primarily governed by N_{bh} positioned within the plume. The influence of T_c becomes important only when T_c is long enough for the effective aeration radius of each bar hole to extend beyond the plume boundary. At shorter T_c , increased T_c mainly enhances the coverage rate rather than changing the spacing itself. S_{bh} in dry soils is generally shorter than in wet near-surface soils because higher air-filled porosity reduces the effective aeration area, requiring shorter spacing to maintain adequate coverage.

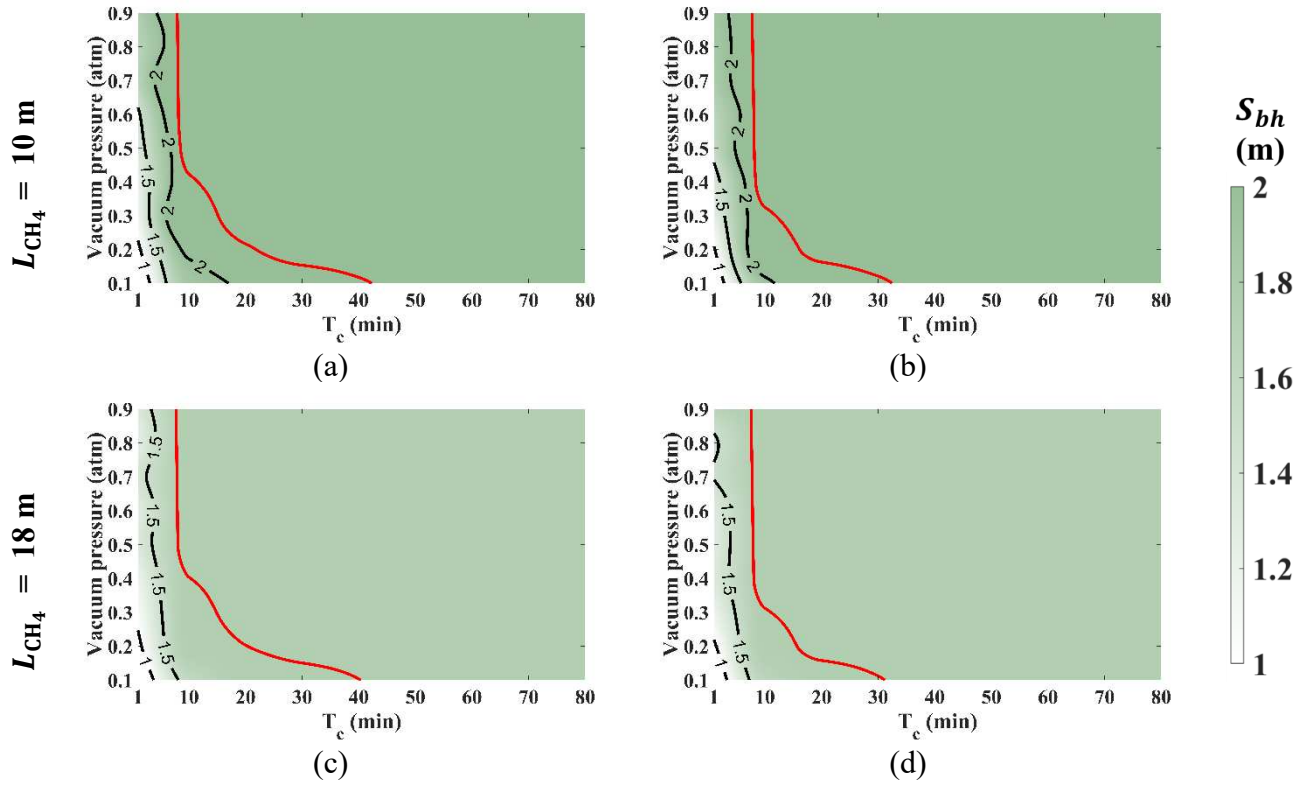


Fig. 4. 9. Estimated spacing between bar holes (S_{bh}) with vacuum pressure ranging from 0.1 to 0.9 atm and aeration duration (T_c) from 1 to 80 min for different numbers of bar holes (N_{bh}) and soil water saturations. Panels (a, b) and (c, d) present $N_{bh} = 2, 3, 4$, and 5. The left contours (a and c) represent dry soil with $S_w = 0.1$, and the right contours (b and d) represent wet soil with $S_w = 0.8$. All estimations are conducted with the average diameter of CH_4 plume of 2 m. The red solid line indicates $CR = 95\%$, which was used as the criterion for identifying sufficient plume coverage.

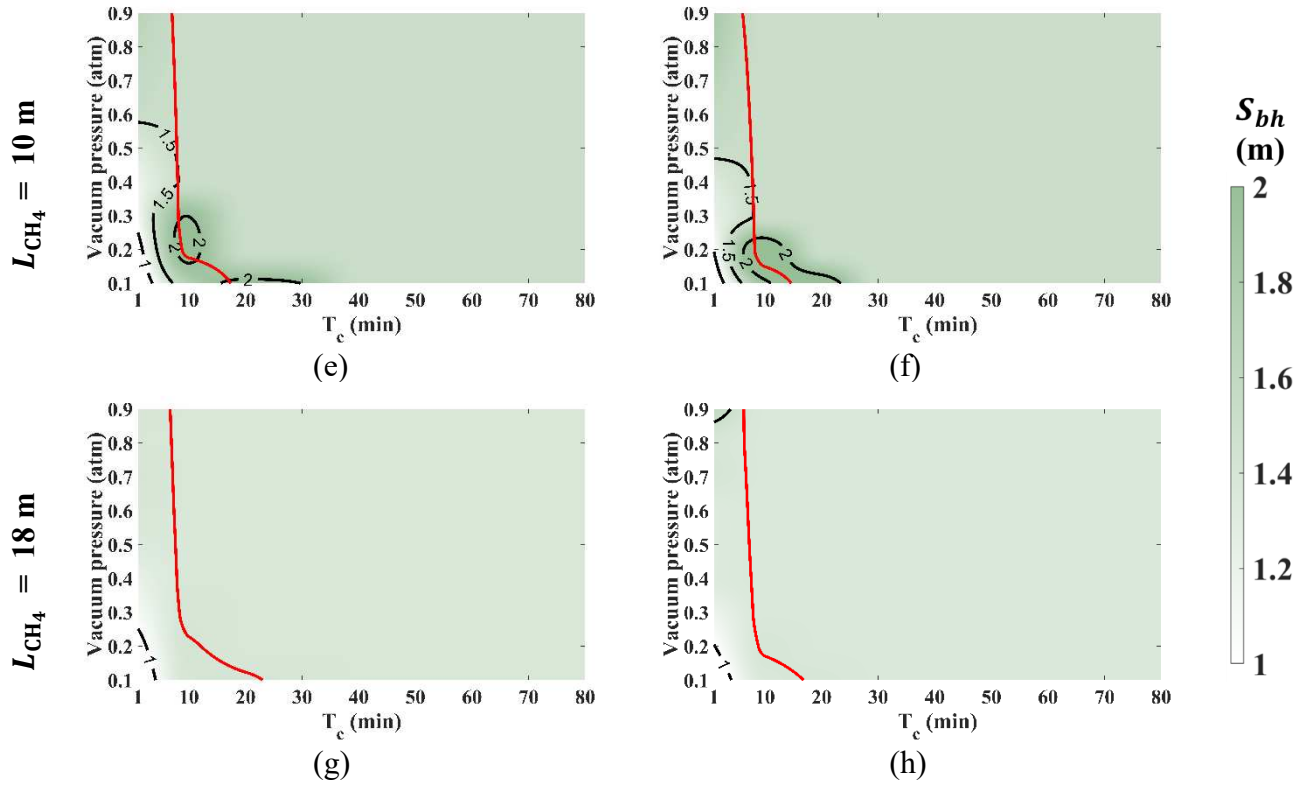


Fig. 4.10. Estimated spacing between bar holes (S_{bh}) with vacuum pressure ranging from 0.1 to 0.9 atm and aeration duration (T_c) from 1 to 80 min for different numbers of bar holes (N_{bh}) and soil water saturations. Panels (a, b) and (c, d) present $N_{bh} = 2, 3, 4$, and 5. The left contours (a and c) represent dry soil with $S_w = 0.1$, and the right contours (b and d) represent wet soil with $S_w = 0.8$. All estimations are conducted with the average diameter of CH_4 plume of 2 m. The red solid line indicates $CR = 95\%$, which was used as the criterion for identifying sufficient plume coverage.

4.3.4.3 Estimated Layouts of bar holes

Fig. 4.11 and Fig. 4.12 present the estimated layouts of bar holes for $N_{bh} = 2$ to 5 under identical aeration conditions ($L_{CH_4} = 2$ m, $T_c = 10$ min, and vacuum pressure of 0.3 atm) for both dry and wet near-surface soils. The optimal layouts are determined by identifying the bar-hole configurations that achieve at least 95% plume coverage with the corresponding spacing obtained from Section 4.3.4.2.

The results show that the optimal center-to-center spacing decreases as N_{bh} increases, while the coverage rate approaches complete plume coverage. This relationship indicates the geometric constraint that placing additional bar holes within a fixed subsurface gas plume requires smaller spacing to ensure sufficient overlap of the aeration zones. For a fixed N_{bh} , layouts under wet near-surface conditions achieve higher coverage and allow slightly larger optimal spacing than those in dry soil. This occurs because the higher soil water saturation increases the effective aeration area of each bar hole, enabling adequate coverage with a marginally wider spacing. Including a central bar hole in configurations with three or more bar holes improves symmetry and ensures that the plume center is fully aerated rather than leaving an uncovered zone near the core of the plume. This feature is particularly important for minimizing rebound that results from gas diffusion from the central region. For field applications, Fig. 4. 11 and Fig. 4. 12 provide a practical reference for selecting bar-hole layouts that reach the coverage target under specified aeration duration and vacuum pressure. Operators can use the layouts to determine whether a selected combination of spacing and bar-hole number will provide sufficient overlap to cover the measured plume while maintaining operational efficiency.

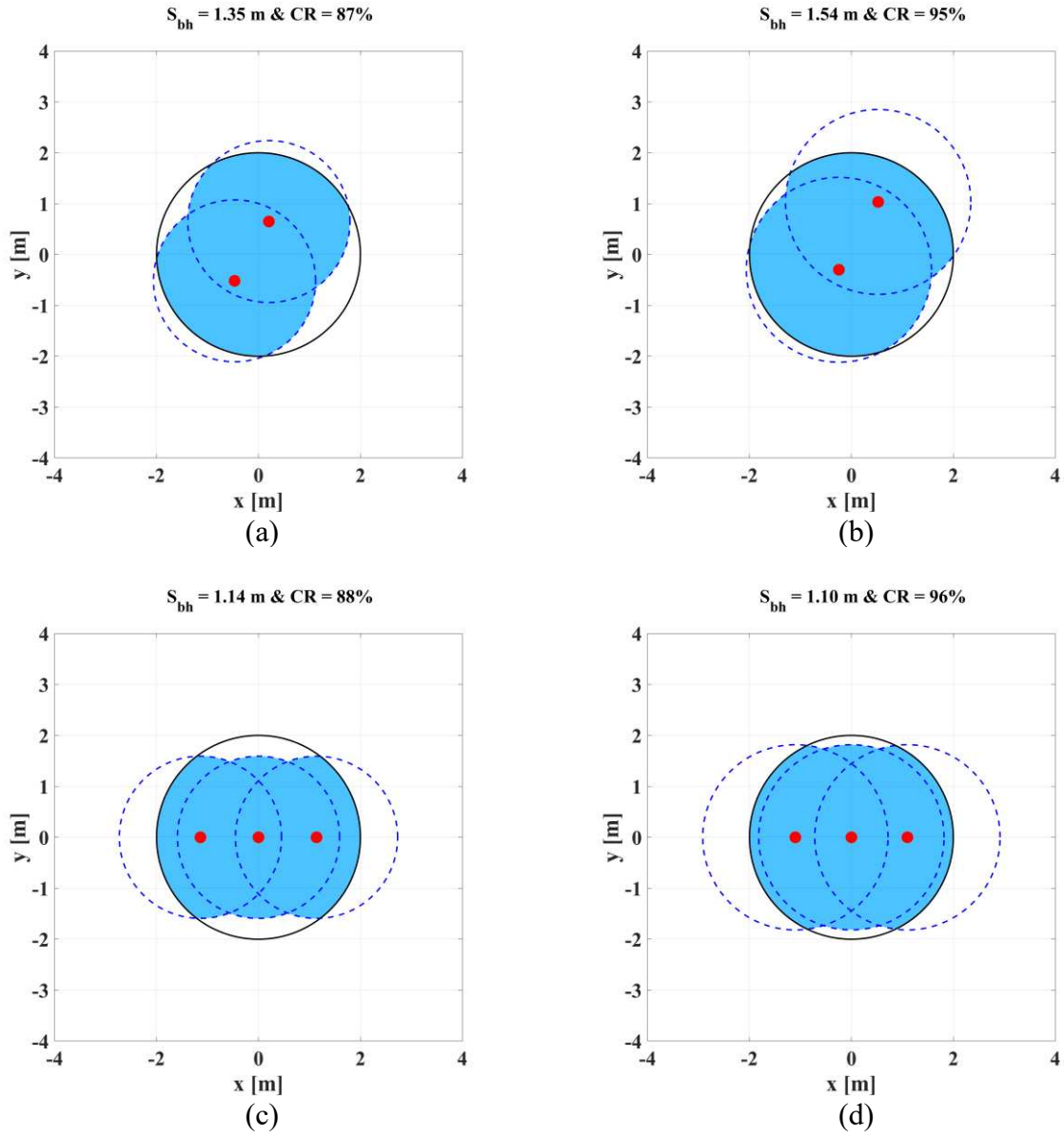


Fig. 4. 11. Estimated layout of bar holes and optimal spacing between bar holes (S_{bh}) with the average diameter of CH_4 plume (L_{CH_4}) of 2 m, aeration duration (T_c) of 10 minutes, and vacuum pressure of 0.3 atm (5 psi) for different numbers of bar holes (N_{bh}) and soil water saturations. Panels (a, b) and (c, d) present $N_{bh} = 2, 3, 4$, and 5. The left contours (a and c) represent dry soil with an average water saturation of 0.1, and the right contours (b and d) represent wet soil with an average water saturation of 0.80.

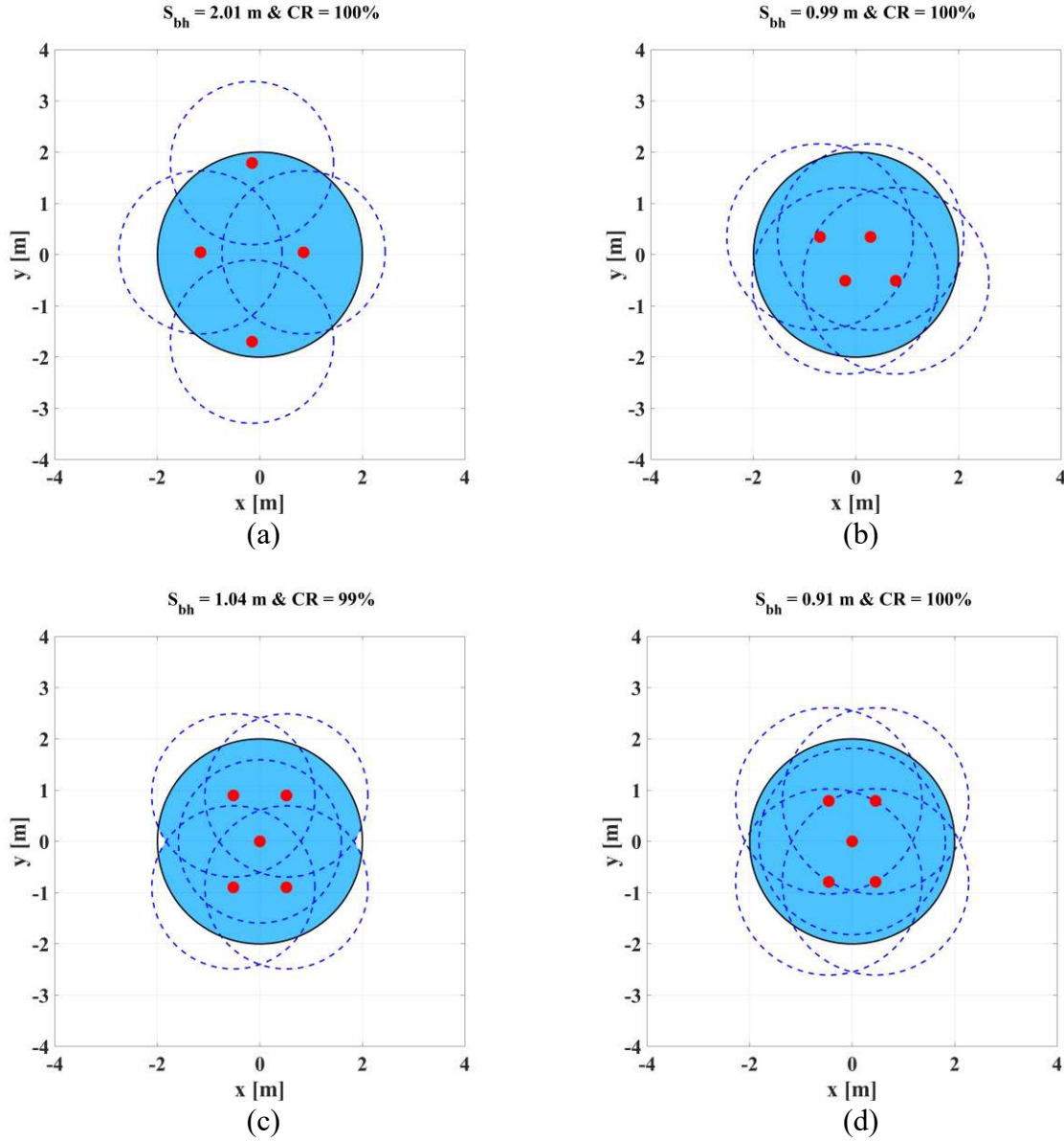


Fig. 4. 12. Estimated layout of bar holes and optimal spacing between bar holes (S_{bh}) with the average diameter of CH_4 plume (L_{CH_4}) of 2 m, aeration duration (T_c) of 10 minutes, and vacuum pressure of 0.3 atm (5 psi) for different numbers of bar holes (N_{bh}) and soil water saturations. Panels (a, b) and (c, d) present $N_{bh} = 2, 3, 4$, and 5. The left contours (a and c) represent dry soil with an average water saturation of 0.1, and the right contours (b and d) represent wet soil with an average water saturation of 0.80.

4.3.4.4 Practical Limitations and Future Research Directions

The reduced-order framework developed in this study provides a practical and operationally efficient method for preliminary design and performance evaluation of NG soil aeration using field-obtainable site information. Although the framework represents a substantial advancement toward screening-level NG soil aeration assessment, several assumptions and practical limitations should be recognized. The framework represents the subsurface CH₄ plume as an elliptical cylinder based on interpolated subsurface CH₄ concentration measurements. In field conditions, plume geometry may be irregular because of soil layering, spatially variable moisture conditions, surface cover effects, underground utilities, or preferential gas migration pathways. Because the framework is intended for screening-level application using limited field information, irregular plumes are approximated using equivalent elliptical geometries based on observed plume extents (Cho et al., 2020, 2022; Gao et al., 2021; Jayarathne et al., 2024; Ulrich et al., 2019). The base case further assumes idealized airflow contact with the target plume ($\eta = 1$). Under actual field conditions, airflow may bypass portions of the plume because of heterogeneity, preferential flow paths, poorly connected pore regions, surface sealing, or utility corridors. Reduced airflow contact may decrease actual removal efficiency and increase the aeration duration required to achieve target CH₄ concentrations. Therefore, field implementation should incorporate monitoring-based reassessment and, when warranted, more detailed numerical modeling to refine design assumptions under heterogeneous conditions or when rebound behavior is observed.

Near-surface water saturation is used as a screening-level representation of subsurface moisture conditions. However, soil moisture commonly varies with depth and time, influencing air permeability and airflow redistribution during aeration. When depth-resolved moisture measurements are available, representative plume-scale saturation estimates may improve

prediction accuracy. The framework also does not explicitly resolve transient back-diffusion or rebound processes following initial advective removal, particularly under dry-soil conditions. Instead, rebound behavior is addressed operationally through post-aeration monitoring and iterative reassessment of aeration design parameters. For multiple bar holes, the framework estimates total removal capacity using a first-order additive assumption based on individual bar-hole performance. This simplified representation does not explicitly account for airflow changes caused by overlapping aeration zones, manifold losses, or airflow interference between adjacent aeration zones. Consequently, predicted CH₄ removal efficiency and aeration duration should be interpreted as screening-level engineering estimates rather than fully coupled transient flow predictions. The controlled field experiments were conducted under representative scenarios rather than statistically replicated trials under identical conditions. Experimental measurements were obtained from a single cross-section using six subsurface CH₄ sensors and therefore do not fully resolve three-dimensional plume evolution or experimental variability. Therefore, the contour plots and error analysis presented in this study should be interpreted as an evaluation of reduced-order framework performance across the tested scenarios and within the monitored cross-section. A denser sensor network, three-dimensional monitoring, and repeated experiments under identical scenarios would be needed to quantify experimental variability more rigorously and characterize plume geometry and temporal evolution more completely.

Experimental evaluation of the framework was limited to sandy loam soil under contrasting near-surface moisture conditions. Framework performance varied with moisture conditions, with stronger agreement generally observed under wetter near-surface conditions within the tested range. Therefore, results for other soil conditions in this study should be interpreted as physics-based screening estimates rather than experimentally validated predictions. In addition, the target

residual CH₄ concentration used in this study represents a selected operational endpoint for framework evaluation rather than a universal regulatory threshold. In field applications, C_{target} should be selected based on utility procedures, site-specific risk conditions, land use, and applicable regulatory guidance.

Despite these limitations, this study establishes a field-evaluated reduced-order framework that quantitatively links measurable site conditions to subsurface CH₄ removal performance during NG soil aeration. The framework addresses an important operational gap in NG leak mitigation, where field-applicable quantitative design methods are currently limited. Future research should incorporate non-uniform plume geometries, spatially variable soil and moisture conditions, and back-diffusion processes, to improve predictive performance and extend the framework across a wider range of field conditions.

4.4 Conclusions

This study established a reduced-order, physics-based framework for evaluating and designing NG soil aeration using measurable field conditions and operational parameters. The framework links site characteristics (soil moisture, plume size, and soil properties), aeration design parameters (bar-hole number, spacing, and layout), and operating parameters (vacuum pressure and aeration duration) to quantitative estimates of subsurface CH₄ removal performance. By translating dominant subsurface gas transport behavior into a field-applicable engineering method, the framework provides a practical screening-level approach for NG soil aeration design and operational decision-making. The framework was experimentally evaluated using controlled field experiments conducted in sandy loam under contrasting dry ($S_w = 0.1$) and wet near-surface ($S_w = 0.8$) conditions. Comparison between measured and estimated CH₄ removal efficiencies showed reasonable agreement ($R^2 = 0.74$), demonstrating that the framework captures the dominant trends governing subsurface CH₄ removal across varying moisture conditions and bar-hole configurations. Agreement was generally stronger under wet near-surface conditions than under dry conditions, indicating that framework performance is influenced by near-surface moisture behavior and associated airflow redistribution.

Results demonstrate that effective NG soil aeration depends strongly on the interaction among plume geometry, soil moisture conditions, vacuum pressure, and bar-hole deployment. Aeration effectiveness increased when bar-hole spacing and placement enabled pressure-driven airflow to intersect the target plume while minimizing untreated regions and excessive overlap between adjacent aeration zones. Increasing the number of bar holes generally improved plume coverage and reduced local concentration rebound within the tested scenarios, provided that spacing remained compatible with the effective treatment area of individual bar holes.

Near-surface wet conditions enhanced aeration effectiveness by limiting upward CH₄ migration and promoting lateral gas transport toward the bar holes, reducing the aeration duration needed to achieve target removal objectives. In contrast, dry soil conditions exhibited stronger rebound behavior, indicating continued diffusion from less effectively aerated regions following initial advective removal. These findings further demonstrate the importance of post-aeration monitoring and operational reassessment during field implementation.

The framework additionally demonstrates that CH₄ removal efficiencies ($Re_{C_{CH_4}}$ and $Re_{M_{CH_4}}$) are governed primarily by vacuum pressure, aeration duration, and bar-hole number. When high vacuum pressures are unavailable, operators may partially compensate by extending aeration duration, although larger plumes require substantially greater treatment duration because of increased CH₄ mass and transport distances. Therefore, early characterization of plume geometry and site conditions is essential for determining whether NG soil aeration is feasible under operational constraints.

Future work should further test and refine the framework through additional field-scale experiments across broader soil types, moisture conditions, plume geometries, vacuum pressures, and bar-hole configurations representative of practical NG leak response operations. Future work should also extend the framework to represent non-uniform plume geometries, variable moisture distributions, transient rebound behavior, and airflow interactions among overlapping aeration zones to further improve predictive capability and operational applicability. Overall, this study establishes a new framework for quantitative NG soil aeration design and operation by demonstrating that reduced-order, physics-based models evaluated with controlled field measurements can support rapid and practical engineering decision-making during NG leak response. The framework addresses an important operational gap in subsurface NG mitigation by

providing utilities with a field-applicable method for improving aeration effectiveness, reducing operational uncertainty, and supporting safer pipeline response operations.

Chapter 5. Conclusions and Future Works

5.1 Conclusions

This dissertation advances both understanding and field-scale prediction of subsurface gas (i.e., CH₄) transport, quantification, and mitigation at NG leak sites by integrating observations and numerical models. This dissertation makes the following four main scientific contributions.

Contribution 1: Improving quantification of transient subsurface gas leak behavior by integrating surface and belowground near-surface (BNS) gas concentration measurements, soil properties, and atmospheric conditions with an inverse gas migration model

Observed BNS CH₄ concentrations showed the earlier and more consistent responses to controlled gas leak behavior than surface CH₄ concentration measurements, indicating that relying on surface measurements alone can bias the quantification of subsurface gas leak behavior. Furthermore, integrating surface and BNS observations, soil properties, and atmospheric conditions with an inverse transport model not only improves the quantification of subsurface transient gas leak behavior but also highlights the importance of considering the link between surface and subsurface conditions in the estimation of gas leak behavior below the ground surface.

Contribution 2: Establishing a controlled field-scale experimental foundation for natural gas soil aeration, enabling observation and evaluation of subsurface gas migration and removal during soil aeration under representative field conditions

This dissertation established and conducted controlled soil aeration experiments to understand subsurface CH₄ migration and to evaluate subsurface CH₄ removal under scenarios related to natural gas leak sites. The experimental design and operation provide a foundation for further

research on natural gas soil aeration, supporting the development and validation of soil aeration models.

Contribution 3: Demonstrating the impacts of soil characteristics and aeration designs on subsurface CH₄ migration and removal

By integrating field-scale controlled experiments with multiphase multicomponent transport modeling, this dissertation showed that soil characteristics and aeration designs control subsurface CH₄ migration and removal performance, which changes from an early advection-dominated stage to a late diffusion-limited stage. Furthermore, results indicate that the aeration design and operation parameters, including vacuum pressure, bar-hole number, spacing, and plume geometry, should be determined based on soil characteristics and subsurface gas plume geometry at site to avoid preferential airflow bypass and competition for removal, which can reduce removal efficiency. This contribution advances understanding of subsurface CH₄ removal during soil aeration and provides a foundation for more effective evaluation, design, and operation of natural gas soil aeration under site-specific conditions.

Contribution 4: Establishing a reduced-order, physics-based framework for quantitative prediction of subsurface gas removal efficiency, estimation of aeration duration, and determination of bar hole number and layout using observable site parameters

This dissertation developed and validated a reduced-order, physics-based framework that uses a limited set of observable site parameters to quantitatively predict subsurface CH₄ removal efficiency, estimate aeration duration to meet a target removal criterion, and determine bar-hole configuration. The framework shows good agreement with controlled experiments ($R^2 = 0.74$)

under wet near-surface conditions. The agreement between framework predictions and controlled experiments provides the support for interpreting overall removal trends and design-level responses under the tested conditions, while transient redistribution and rebound under dry-soil conditions remain more difficult to resolve. Under dry conditions, the performance decreases because the reduced-order framework does not fully capture diffusion-limited transport, rebound, and non-uniform subsurface CH₄ redistribution. These limitations motivate future work to incorporate back diffusion, variable soil moisture, non-uniform plume geometry, and airflow interference among overlapping aeration zones. Despite these limitations, the framework is grounded in the multiphase transport mechanisms and provides a rapid, efficient, and practical decision-support tool for the design and operation of soil aeration for subsurface CH₄ removal at gas leak sites. Overall, this dissertation advances scientific understanding of subsurface CH₄ migration and removal by improving the quantification of subsurface gas leak behavior, investigating mechanisms controlling subsurface CH₄ removal during soil aeration, and developing a practical framework for field-scale design and operation of soil aeration.

Limitations of Experimental and Modeling Approach

This work should be interpreted considering several important limitations. The experimental program was conducted using a single soil type and under relatively controlled field-scale conditions, which may not fully capture the heterogeneity and variability encountered in field settings. In addition, the numerical analyses relied on two-dimensional modeling assumptions that simplify inherently three-dimensional flow and transport processes. The modeling framework was developed under Darcy-based assumptions and should not be interpreted as a general representation of gas flow in clay-rich media, where nonlinear or non-Darcy flow behavior may

occur. Furthermore, the study was developed around conditions specific to the METEC site, including its subsurface characteristics and operational context, so the results may not be directly transferable to other locations without site-specific evaluation. Despite these limitations, the findings should be viewed as a strong basis for framework development and interpretation, while additional testing and validation across a broader range of soils, site conditions, and modeling approaches would further strengthen generality.

5.2 Future Work

This dissertation provides new insights into the quantification of subsurface gas leak behavior, understanding of subsurface gas transport and removal during soil aeration, and a reduced-order, physics-based framework for the design and operation of soil aeration in the field. Based on these contributions, there still remain a number of questions that are worth further study. Based on the research in this dissertation, some recommendations for future work are presented as follows.

1. Estimating transient subsurface gas leak rates by integrating surface and belowground near-surface (BNS) CH₄ measurements with an inverse gas migration model under variable surface, soil, and atmospheric conditions

The observed surface and BNS CH₄ concentrations in this dissertation were collected under dry soil and permeable surface (i.e., grass and soil) conditions to estimate transient subsurface gas leak rates. Future work should extend surface and BNS CH₄ measurements under variable environmental conditions, especially in the presence of impermeable surface covers (e.g., pavement and concrete), preferential flow paths (e.g., fractures or root networks), and precipitation that drives spatiotemporal changes in near-surface soil water saturation and air permeability. These extensions would improve understanding of surface and subsurface gas migration behavior and improve the ability of the inverse gas migration model to quantify transient subsurface gas leak behavior across a wider range of soil and atmospheric scenarios.

2. Evaluating subsurface gas migration and removal during soil aeration using controlled experiments and transport modeling under more realistic and complex field conditions

In this dissertation, controlled soil aeration experiments were conducted under constant vacuum pressure, symmetric bar-hole layouts, unfrozen soil conditions, and without impermeable surface covers or subsurface infrastructure. Future work should extend these experiments to more

realistic and complex field conditions, including variable vacuum pressures among bar holes, combined passive and active aeration strategies, and operation under conditions with impermeable surface covers, subsurface infrastructure, or frozen soils, all of which may significantly impact gas and water transport in the vadose zone during soil aeration. Furthermore, future modeling efforts should develop a three-dimensional transport model to investigate dimensional effects on simulated subsurface gas transport and removal, and to compare these results with the two-dimensional simulations used in this dissertation. Future work should also evaluate gas migration and aeration in clay-rich or very low-permeability soils using formulations that can represent nonlinear or non-Darcy gas flow behavior where Darcy-based assumptions may no longer be sufficient. These extensions would help clarify how field complexity influences subsurface gas transport, removal, and back-diffusion, improve transport model performance, and support more reliable, site-specific design and operation of soil aeration systems.

3. Expanding the applicability of a reduced-order, physics-based framework for more site-specific soil aeration decision-making supports

In this dissertation, a reduced-order, physics-based framework was developed and evaluated against results from controlled soil aeration experiments under known environmental conditions. However, the influences of impermeable surface covers, subsurface infrastructure, multiple leak sources, frozen soil, and irregular gas plume geometry on framework performance were not considered. Future work should extend the framework to a broader range of site and operational complexities, including impermeable surface covers, subsurface infrastructure, non-uniform vacuum distribution, irregular plume geometries associated with multiple leak sources, practical constraints on bar-hole number and layout, and frozen-soil conditions. Future work should also quantify predictive uncertainty in the reduced-order framework under more complex site

conditions by evaluating how uncertainty in site-measurable inputs, such as soil properties, vacuum pressure, and plume geometry, affect predictions of removal efficiency, aeration duration, and bar-hole configuration, and by defining confidence bounds for these predictions across variable site conditions. These efforts would strengthen the framework as a practical decision-support tool and improve confidence in its use for site-specific design and operation of soil aeration systems.

4. Real-Time and Adaptive Decision Support

The framework presented in this dissertation could be extended toward real-time or adaptive decision-support applications. Because the approach is physics-based, there is the potential to be coupled with real-time field measurements to provide near-real-time response on subsurface removal performance and support real-time operational adjustments. Such integration could support more responsive adaptation as site conditions evolve, improve decision-making during active operations, and enhance the practical value of the framework beyond retrospective analysis and scenario evaluation.

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Appendices

Appendix. A. Instrumentation, Calibration, and Data Acquisition (DAQ)

A. 1 Instruments in Controlled Experiments

All sensors, detectors, and aeration-related instruments used in the controlled experiments are summarized in Table A. 1, together with their manufacturers, primary measurement purposes, and data acquisition (DAQ) configurations. Surface and below-near-surface (BNS) CH₄ concentrations were monitored using a low-cost detector package built around the Figaro TGS 2611-E (MOS) sensor, with environmental compensation provided by an integrated BME280 (air temperature, relative humidity, and pressure) and signal digitization handled by an ADS-1115 analog-to-digital converter. The low-cost detector system was logged using a Raspberry Pi with microSD storage at 1 Hz. Detector calibration was performed using a Picarro G4302 GasScouter (CRDS) as a reference CH₄ analyzer, operated at approximately 1 s measurement intervals during calibration.

Meteorological conditions and soil moisture/temperature were recorded to support interpretation of CH₄ behavior and subsequent derivation of resistance and flux metrics. Site meteorology (precipitation, solar radiation, relative humidity, air temperature, pressure, and wind velocity) was measured using an ATMOS 41 weather station connected to a ZL6 logger. Soil moisture and soil temperature were measured using 5TM sensors, and additional soil moisture/temperature tracking during aeration experiments was conducted using TEROs 10/11 sensors; these soil and meteorological measurements were logged using a ZL6 logger with a 5 s recording interval. Subsurface CH₄ concentrations during soil aeration experiments were monitored using INIR-ME100 (NDIR) sensors recorded at 5 s intervals.

For mitigation testing, soil aeration was implemented using venturi purgers coupled to an air compressor to generate negative pressure and induce soil gas aeration. Operational monitoring for

the aeration system included target vacuum drawdown (e.g., 5 psi) and aeration flow rate (e.g., 14 scfm), as summarized in Table A. 1. Overall, these instruments provided synchronized measurements of CH₄ concentrations, meteorological forcing, soil hydrothermal conditions, and aeration operating conditions required to execute and interpret the controlled experiments reported in Chapters 2–4.

Table A. 1. Sensors, detectors, and aeration instruments used in the controlled gas release and soil aeration experiments at METEC, including manufacturer, measurement purpose, and data acquisition (DAQ) configuration.

Instrument	Manufacturer	Measurement/Purpose	DAQ
TGS 2611-E (MOS)	Figaro USA Inc.	Surface and BNS CH ₄ monitoring	Raspberry Pi + microSD; 1 Hz (system logging)
BME280	Bosch Sensortec	Air temperature, relative humidity, pressure for detector compensation	Integrated within low-cost detector; logged with detector system
ADS-1115	Texas Instruments	Analog-to-digital conversion for MOS sensor output	Integrated within low-cost detector; logged with detector system
G4302 GasScouter	Picarro, Inc.	CH ₄ analyzer for calibrating TGS 2611-E (MOS)	Analyzer ~1 s interval during calibration
ATMOS 41	METER Group	Precipitation, solar radiation, relative humidity, air temperature, pressure, wind velocity	ZL6 logger. Time interval = 5 s
5TM	METER Group	Soil moisture and soil temperature monitoring	ZL6 logger. Time interval = 5 s
INIR-ME100	SGX Sensortech	Subsurface CH ₄ monitoring	5 s intervals
TEROS 10/11	METER Group	Soil moisture/temperature tracking during aeration experiments	ZL6 logger; Time interval = 5 s
Venturi purgers	Millibar Robotics (BHP-375)	Apply vacuum-driven soil aeration and monitor drawdown	Maximum vacuum pressure = 19 psi. Maximum flow rate = 28 scfm

Air compressor	Facility Rental	Deliver high-pressure compressed airflow to purger to generate vacuum	Vacuum pressure = 90 psi; Flow rate = 185 scfm
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A. 2 Calibration of the CH₄ Detector

Nineteen low-cost CH₄ detectors were calibrated in a laboratory at the Methane Emission Technology Evaluation Center (METEC) at Colorado State University in Fort Collins, Colorado, USA. Prior to calibration, all detectors were preheated for two days in ambient air to stabilize the sensors. The environmental sensor in each detector was factory-calibrated.

During the calibration, CH₄ concentrations were measured using low-cost CH₄ detectors and a cavity ring-down spectrometry analyzer (G4302 GasScouter, Picarro, Inc.). Each low-cost CH₄ detector was mounted on top of a stainless-steel bracing frame measuring 60.96 cm in length and 24.77 cm in height. The inlet tube of the analyzer was placed at the same height as the bottom of the detector's tube to ensure consistent CH₄ measurements. The calibration was conducted at an average ambient temperature of 19°C and 37% averaged relative humidity. CH₄ gas with a purity of 86% was released at a pressure of 1-1.5 psig for 20 minutes. The gas supply was then turned off, and measurements continued for an additional 15 minutes until the measured methane concentration from the gas analyzer decreased to the background CH₄ concentration of 2 ppmv.

During the calibration process, the resistance values from the CH₄ sensors were recorded at a frequency of 5 seconds, while the gas analyzer provided CH₄ concentration measurements every second under identical environmental conditions. The resistance values were normalized by dividing them by the resistance of the background methane concentration in the air to calculate the corresponding methane concentrations. This was achieved by using the normalized resistance values from each CH₄ sensor in conjunction with the corresponding relative humidity and air temperature readings. The calculated CH₄ concentrations from the CH₄ sensors were then compared with the CH₄ concentration measurements obtained from the gas analyzer. Fig. A. 1 shows that the correlation of measurement between two CH₄ sensors and the gas analyzer was

generally greater than 0.7 ($R^2 > 0.7$). Fig. A. 2 shows that the correlation of measurement between two CH_4 sensors and the gas analyzer was generally greater than 0.7 ($R^2 > 0.7$).

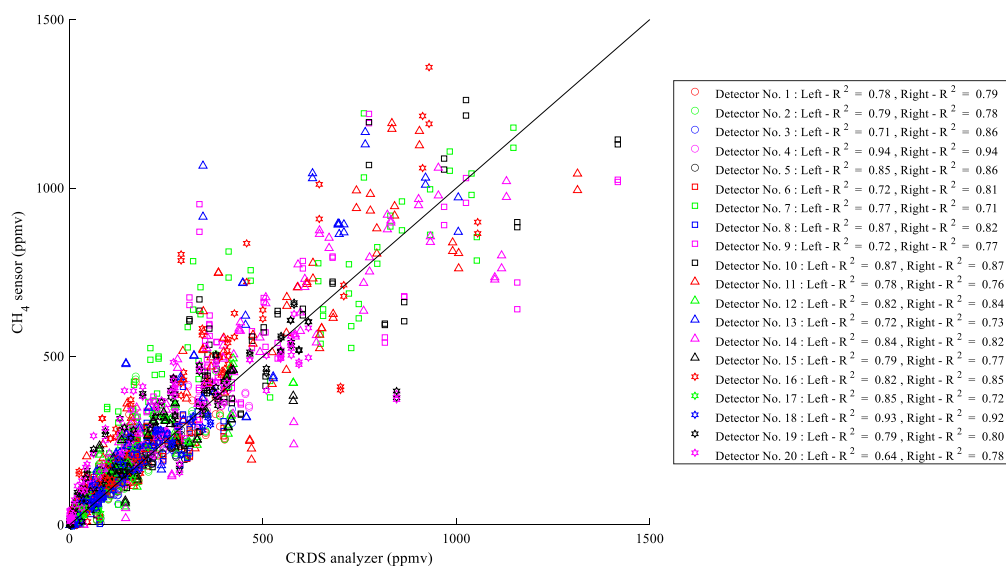
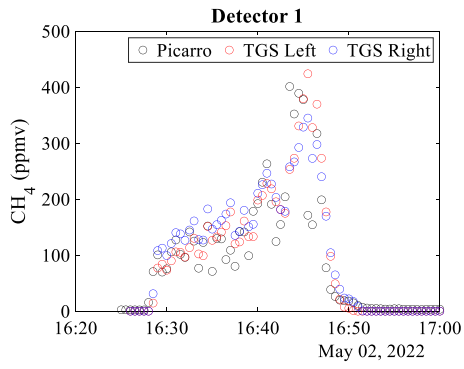
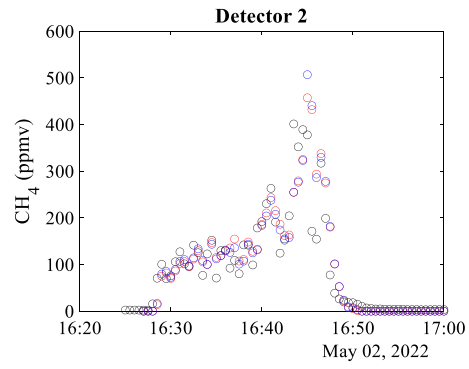


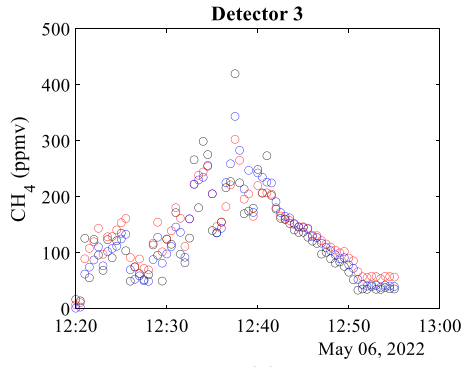
Fig. A. 1. Comparison of 30-second averaged CH_4 concentrations from methane sensors (TGS2611-E00) and the trace gas detector analyzer (Picarro G4302). The correlation coefficient of the left methane sensor (Left- R^2) and right sensor (Right- R^2) were estimated from linear regression for each LCS unit and were listed in the right table. The black line represents the identity line (1:1 line).



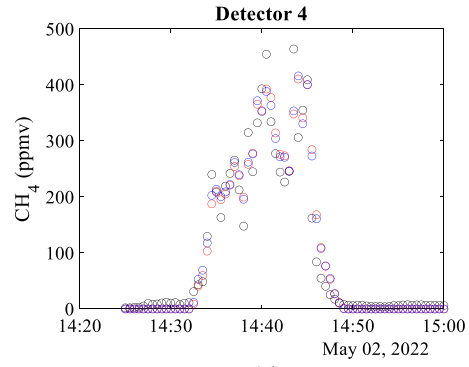
(a)



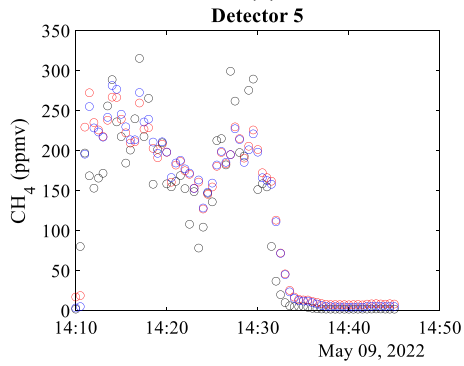
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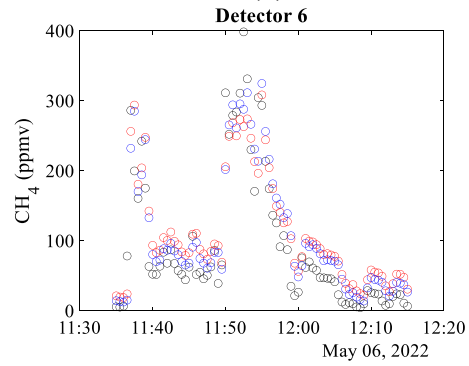
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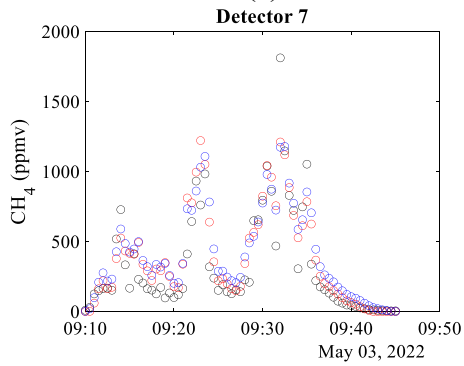
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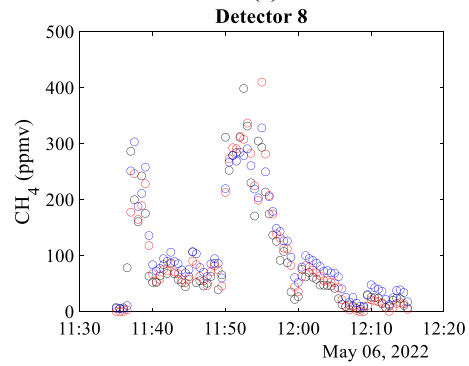
(e)



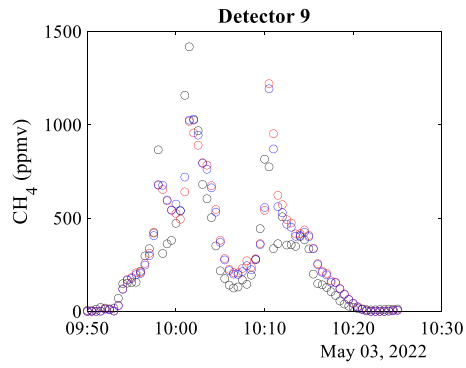
(f)



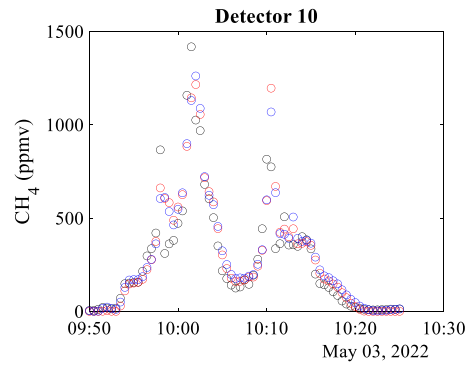
(g)



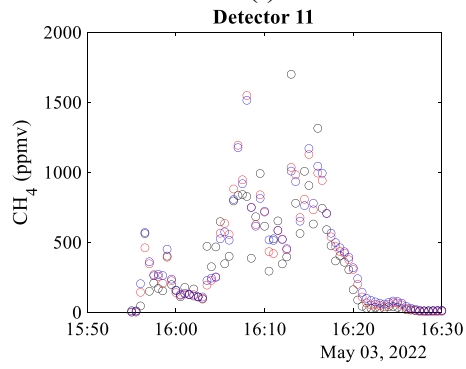
(h)



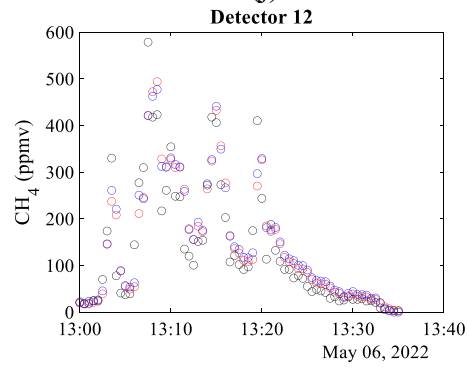
(i)



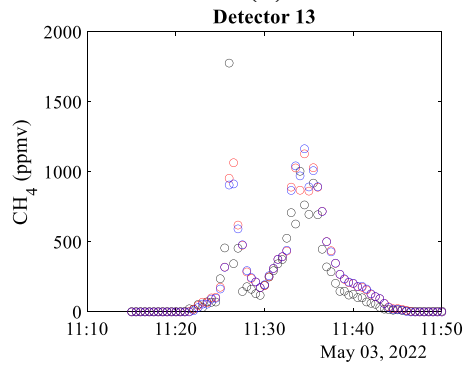
(j)



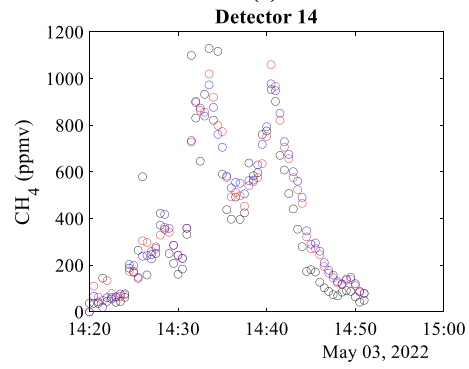
(k)



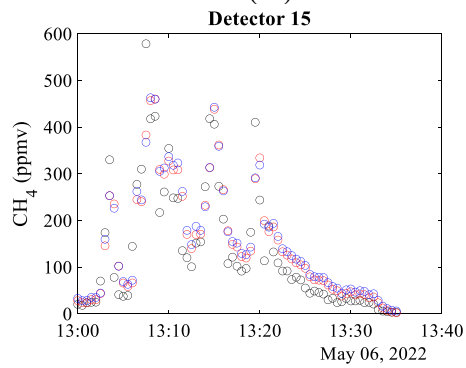
(l)



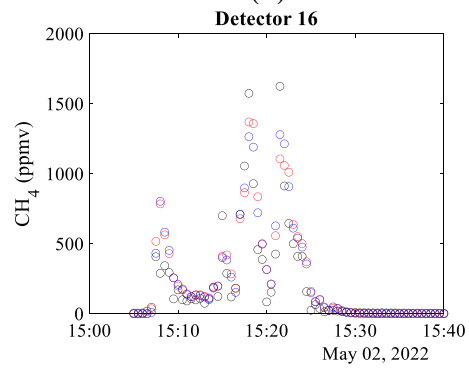
(m)



(n)



(o)



(p)

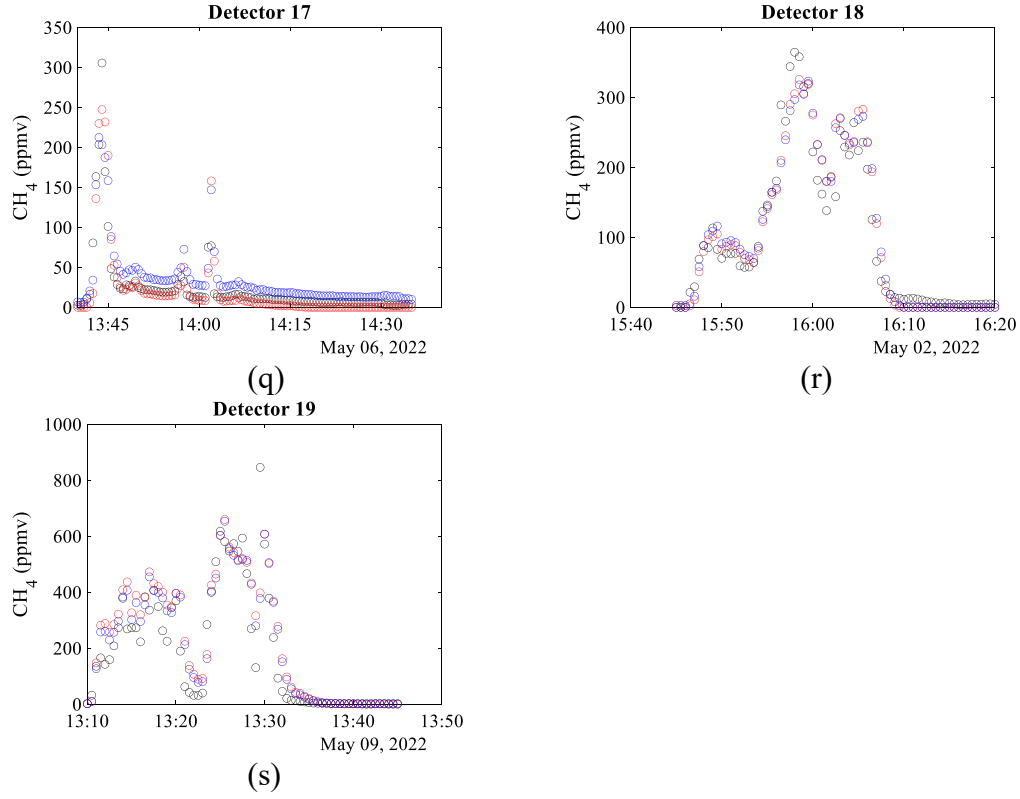


Fig. A. 2. Measured CH₄ concentrations from two CH₄ sensors in 19 low-cost CH₄ detectors and the trace gas detectors analyzer (Picarro G4302). The red circles present measurements from the CH₄ sensor which is used to monitor the surface CH₄ concentrations, while blue circles show measurements from the CH₄ sensor, which is used to measure the belowground near-surface CH₄ concentrations. The black circles indicate the measured CH₄ concentrations by the trace gas detector analyzer (Picarro G4302).

A. 3 Calibration of the INIR sensors

Sensor description

Subsurface CH₄ concentrations were measured using integrated infrared (INIR) sensors (SGX Europe, Katowice, Poland; model INIR-ME100%). The INIR-ME100% is designed to measure CH₄ in air from 100 ppm to 100 vol.%, operates over −40 to 75 °C and 0–99% RH, and provides either digital or analog output. The sensor is housed in stainless steel (approximately 20 mm diameter and 17 mm height) and uses a 5-pin interface (TXD, VCC, GND, RXD, OUT).

Calibration setup

Calibration was performed using the SGX Smart IR evaluation board and the SMIR/INIR evaluation software. The sensor was connected to the evaluation board, the evaluation board was connected to a computer, and the correct COM port was selected before initiating device detection (“Search for Devices”). Once detected, the existing sensor configuration was read before any edits by selecting “Read Parameters from Single Device,” which displays current coefficients, the date of last calibration, and stored zero/span/offset values.

Communication settings and coefficient verification

Before calibration, the sensor coefficients were verified against the manufacturer-recommended values for the INIR-ME100%. Communication and processing settings were standardized by keeping the baud rate at 38400 and setting the internal averaging to 20, followed by writing the updated configuration to the device (including updating sensor date/time). The software mode was then switched from Configuration Mode to Engineering Mode to perform zeroing and span/offset calibration.

Three-point calibration procedure (zero, high-span, target)

Calibration gases were delivered to the sensing element using a calibration cap that directs gas flow over the sensor. Gas flow was maintained at a low rate (approximately 500 mL/min; if a flow meter was unavailable, flow was adjusted such that a faint breeze was felt at the outlet tubing).

(1) Zero (0 vol.%)

The sensor was conditioned with 100% N₂ and allowed to warm up until the internal diagnostics (e.g., “Temp” and “Ratio”) stabilized (typically ~15 min). For full standardization across field deployments, N₂ flow was maintained for an extended stabilization period (up to 45 min) prior to recording the zero value. After stabilization, “Calibrate Zero” was executed to store the zero point. Firmware note: For sensors running firmware v2.31, the mode was toggled Engineering → Configuration → Engineering after clicking “Calibrate Zero” to ensure the zero value was saved (and “START (Sensor Readings)” was restarted after returning to Engineering Mode).

(2) High span (20 vol.% CH₄)

After zeroing, 20% CH₄ was flowed through the cap until readings stabilized (approximately 5 min), and “Set High Span” was executed to store the span value (20%). A 100% N₂ flush was then applied for ~5 min (or until the reading returned to approximately 0.00 vol.%) to remove residual CH₄.

(3) Offset / target (2 vol.% CH₄)

Next, 2% CH₄ was flowed until readings stabilized (~5 min), and “Calculate Offset” was executed to store the target-point correction. A final N₂ flush (~5 min) was applied prior to disconnecting the sensor for deployment. Firmware note: For firmware v2.31, the Engineering → Configuration → Engineering toggle was repeated after each calibration action (zero/span/offset) to ensure values were written to the sensor.

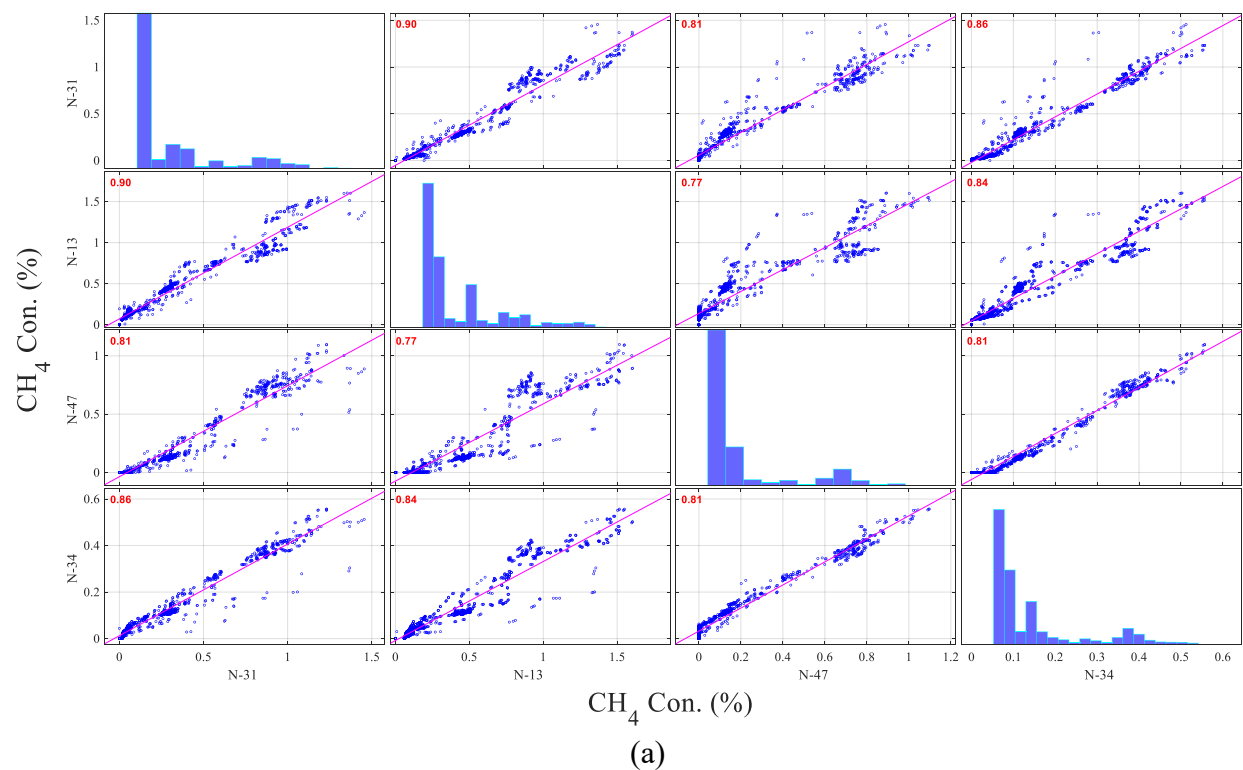
Post-calibration performance characterization (air vs. dry soil)

After three-point calibration, sensor performance was characterized using calibration gases spanning low-to-high concentrations (400 ppm, 5,000 ppm, 5%, 50%, and 100 vol.% CH₄). In air, gases were passed over the sensor via the calibration cap and N₂ was applied between steps to flush residual CH₄. The INIR response was linear from 5,000 ppm to 100%, but the sensor tended to underestimate lower concentrations. To evaluate response in porous media, dry soil was prepared by oven-drying for 24 h, packing into a sealed 2-inch PVC tube with gas-flow fixtures, and sealing the open end using a sensor holder. Similar to the air test, the response was linear between 5% and 100%, while low concentrations in soil (500–5,000 ppm) were underestimated.

Response time

Sensor response time was quantified using a step exposure to 500 ppm CH₄ and defining T₉₀ as the time for the output to reach 90% of the maximum change from background. The INIR-ME100% exhibited T₉₀ ≈ 10 s.

The calibration of nine SGX INIR-ME100 sensors were shown in Fig. A. 3 using Kenall Rank method. All Kendall's rank correlation coefficient for each sensor pair were higher than 0.7, indicating strong agreement across sensors.



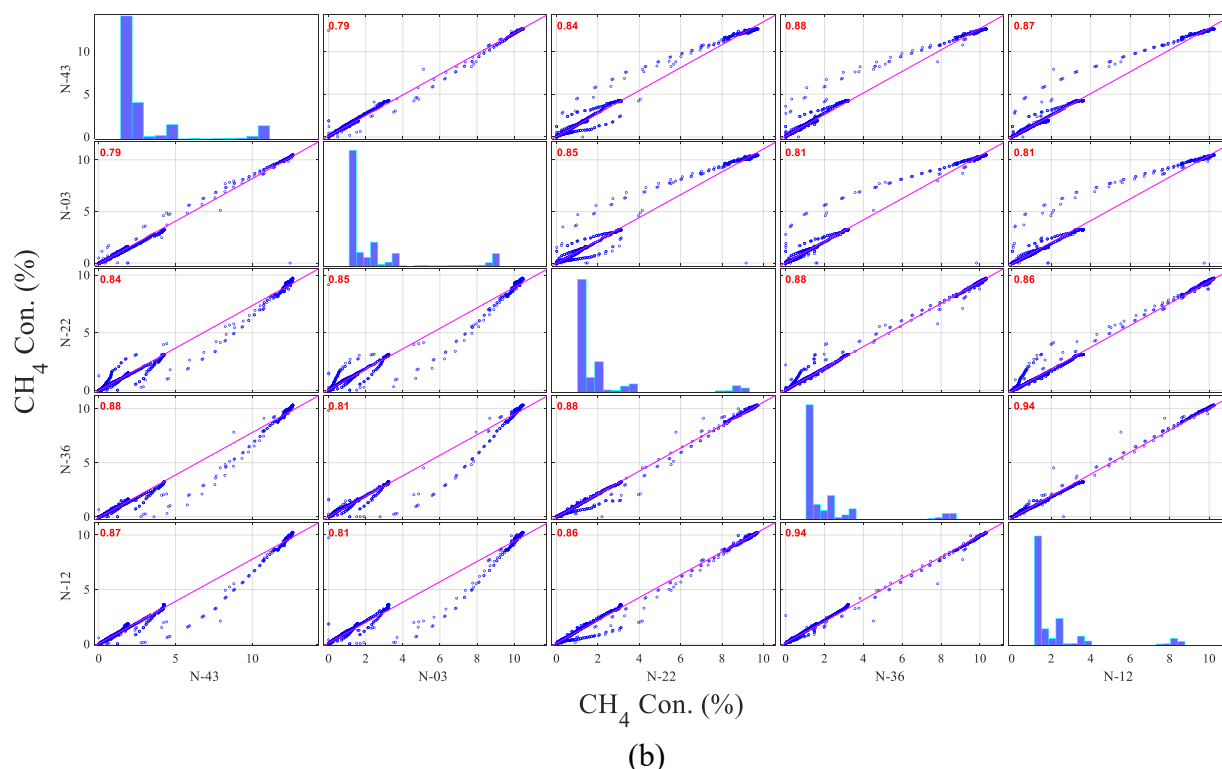


Fig. A. 3. Calibration results of nine SGX INIR-ME100 sensors. (a) N-31, N-13, N-47, and N-34. (b) N-43, N-03, N-22, N-36, N-12. Diagonal panels show the distribution (histogram) of each readings of sensor. Off-diagonal panels show paired observations between sensor pairs. The magenta line denotes the 1:1 agreement line, and red values report Kendall's rank correlation coefficient for each sensor pair, indicating strong agreement across sensors.

Appendix. B. Controlled Experiments at METEC

B. 1 Experimental Site – METEC

We conducted a series of controlled field-scale experiments at the Methane Emissions Technology Evaluation Center (METEC) operated by Colorado State University (CSU). METEC is a 7-acre field test facility with dedicated aboveground and underground infrastructure designed to support controlled methane (CH_4) releases and quantitative evaluation of emission detection and subsurface transport. The facility includes realistic well-pad and compressor-station layouts and an underground pipeline testbed that enables CH_4 releases at known locations and controlled leakage rates. Detailed descriptions of the METEC experimental infrastructure and pipeline testbeds are provided in Ulrich et al. (2019) and Gao et al. (2021). The underground pipeline testbed provides a unique platform to investigate subsurface CH_4 migration and mitigation under variable boundary conditions, including subsurface heterogeneity (e.g., soil texture and moisture) and surface conditions (e.g., precipitation, vegetation, and pavement). Continuous monitoring of subsurface and near-surface conditions, together with spatially distributed soil-gas measurements, enables characterization of the spatiotemporal evolution of CH_4 concentrations and migration pathways. This controlled capability makes METEC well suited for evaluating sensitivities in subsurface CH_4 transport and testing soil-aeration mitigation configurations under repeatable field-scale conditions.

B. 2 Low-cost, Near-real-time, Wire/Wireless Natural Gas Detector Network

Developing a network of low-cost, near real-time, wireless CH₄ detectors linking monitoring of surface/belowground gas concentrations, weather conditions, and soil moisture/temperature to an inverse gas migration model to establish a comprehensive system for effectively tracking and quantifying belowground NG leak rates.

Framework of the CH₄ detector network

The conceptual framework of the low-cost, near real-time, wireless CH₄ detector network is shown in Fig. B. 1. The detector network consists of low-cost near real-time CH₄ detectors, soil moisture and temperature sensors (5TM, METER Group, Inc.), and a weather sensor (ATMOS 41, METER Group, Inc.). Controlling software in the CH₄ detector was used to transfer collected measurements of CH₄ concentrations via wire and wireless connection.

The CH₄ detector is used to monitor surface and belowground near-surface CH₄ concentrations and the surrounding air temperature, air pressure, and relative humidity. The variations in the environmental CH₄ concentration induce the change in the voltage in the detector. This change in voltage and measured relative humidity and air temperature are used to calculate CH₄ concentration (Cho et al., 2022). Meteorological and soil conditions are collected using data loggers and then transferred wirelessly to the network database. Furthermore, the background CH₄ concentration in the atmosphere, the depth of the pipeline, and the location of potential leak determined by the handheld detector (e.g., DP-IR+) are investigated and then transferred wirelessly to the network database. These data are used to calculate the required parameters in the modified ESCAPE model (Lo et al., 2024). The required parameters include atmospheric and soil resistances and spatial-temporal distribution of CH₄ concentration. Parameters are then input into the modified

ESCAPE model to estimate the non-steady belowground NG leak rate. The collected data and simulated results from the modified ESCAPE model are uploaded to a user website that can be used to (1) visualize the gas concentration spatially over time or (2) understand the model estimates of leak rate over time. Details about used detectors and sensors in the network are described in the following sections.

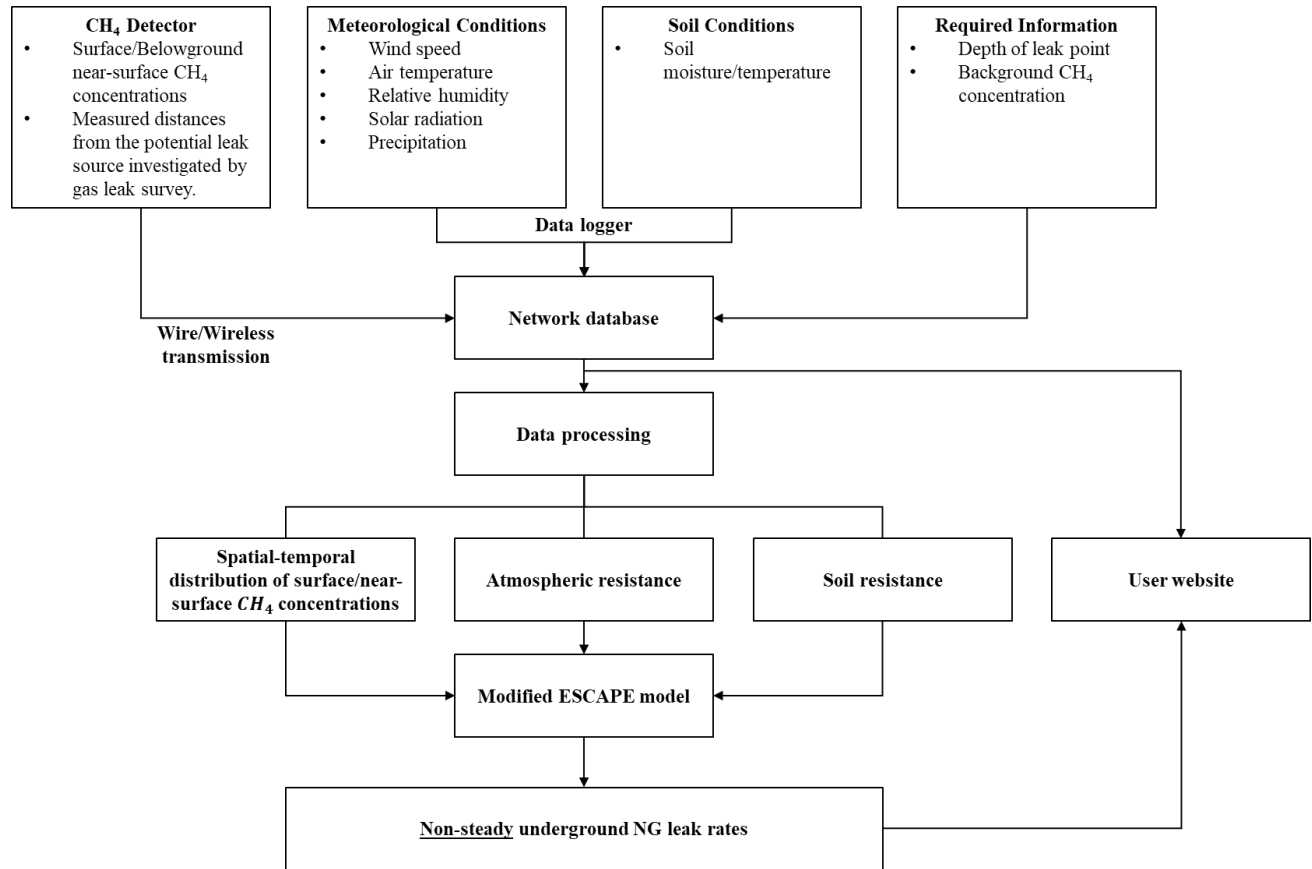


Fig. B. 1. Conceptual framework of low-cost, near real-time CH₄ detector network. Required measurements include surface/near-surface CH₄ concentrations, meteorological conditions, soil conditions, depth of leak point, and the background CH₄ concentration. The measurements from CH₄ detectors could be transmitted wire and wirelessly through WiFi to the network database. Measured CH₄ concentrations were used to estimate the spatial-temporal distribution of surface and belowground near-surface CH₄ concentrations. Meteorological data and soil conditions were used to calculate the atmospheric resistance and the soil resistance. Estimated parameters are used

in the modified ESCAPE model to estimate the non-steady belowground NG leak rates. The collected data and simulated results from the modified ESCAPE model are uploaded to the user website.

Low-cost Near Real-time CH₄ Detector

The low-cost, near real-time CH₄ detector, has been modified based on a previous low-cost CH₄ sensor design to incorporate several enhancements (Cho et al., 2022). These enhancements include the capability to measure both surface and subsurface CH₄ concentrations, the integration of built-in connectivity options for wireless data transmission, and an expanded memory capacity for data storage.

The low-cost, near real-time CH₄ detector, consists of two metal oxide semiconductor (MOS) sensors (TGS2611-E, Figaro Engineering Inc.), an environmental condition sensor (BME280, Bosch Sensortec Inc.), and a 16-bit analog-to-digital converter (ADS-1115) in a plastic case. The height, width, and length of the plastic case are 83.61 mm, 158.75 mm, and 177.7 mm, respectively (Fig. B. 2). The MOS sensor is used to detect CH₄ concentrations due to its low cost, relatively high accuracy, and suitability for measuring CH₄ concentration levels in the atmosphere. The MOS has an optimal detection range of 500 to 12500 ppmv. The environmental condition sensor (BME280, Bosch Sensortec Inc.) was used to monitor relative humidity with an accuracy of $\pm 3\%$ and atmospheric temperature with a range from -40 to 85 °C. Cho et al., 2020 suggested an approach to incorporate signals from the MOS sensor, atmospheric temperature, and relative humidity to estimate the CH₄ concentrations. Measured data is collected by a microcontroller, Raspberry Pi, with a microSD card in the detector at the frequency of 1 Hz. Two open tubes at the bottom of detectors (long and short) allow the surface and belowground near-surface CH₄ to meet MOS sensors. The depth of belowground near-surface CH₄ measurement is 1.2 cm (0.47 inches). The tube length on the CH₄ detector can be changed to measure at different depths as needed. In

the soil and grass area, the shorter tube is placed flush on the soil surface while the longer tube penetrates 1.2 cm (0.47 in) below the ground surface. In the area with the impermeable surface cover (e.g., the asphalt), the two short tubes are used to monitor surface CH₄ concentration on the asphalt surface because we cannot dig a hole in the asphalt to bury the long tube (Fig. B. 3).

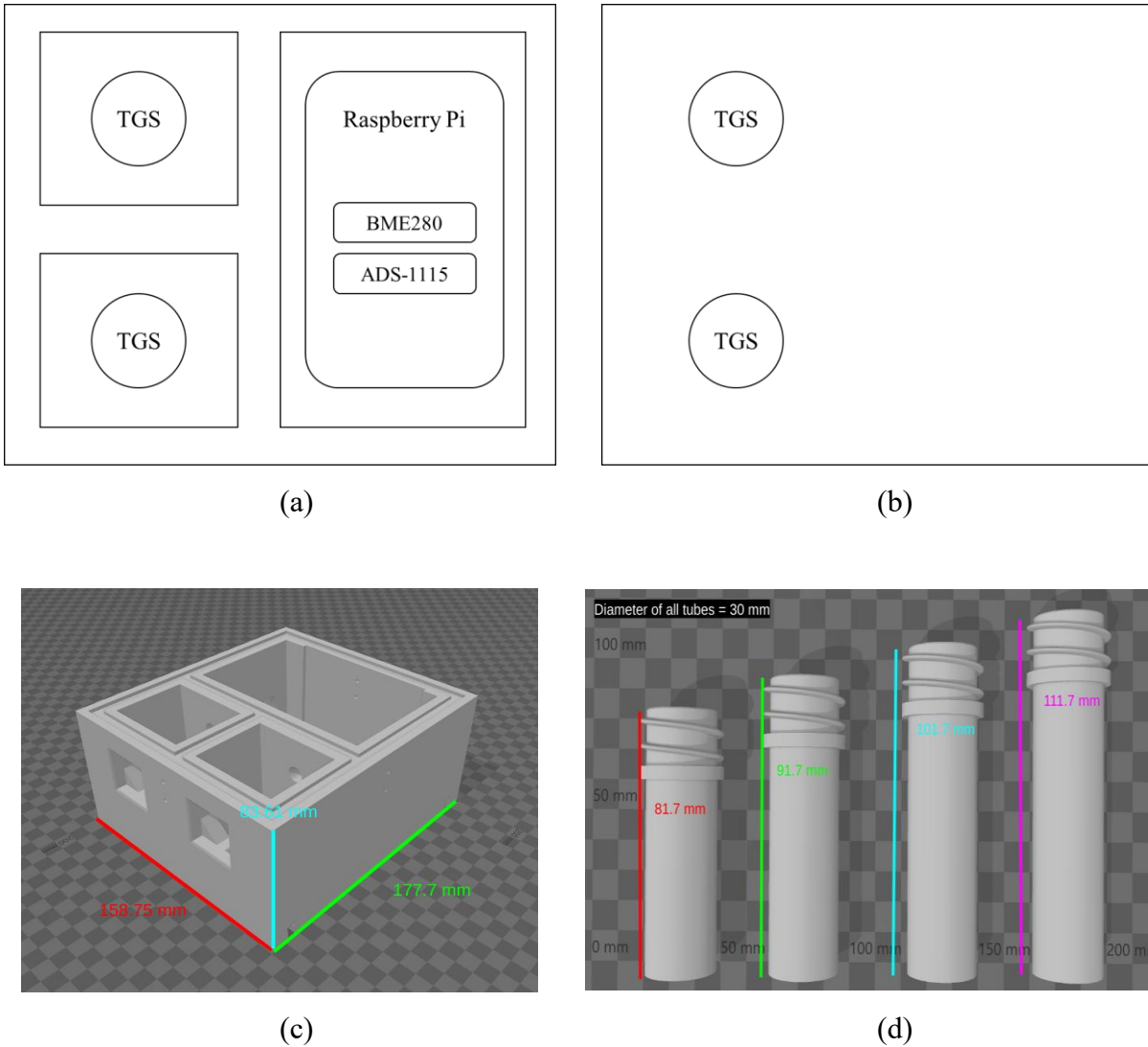


Fig. B. 2. (a) Top view and (b) bottom view of the CH₄ detector. In the top view, the upper left CH₄ concentration sensor (TGS 2611-E, Figaro Engineering Inc.) is used to measure the surface CH₄ concentration, while the bottom left is used to measure belowground near-surface (BNS) CH₄ concentration (1.2 cm below the ground surface). The BME280 sensor is utilized to monitor air temperature, relative humidity, and atmospheric pressure. The ADS-1115 is used to convert the measured signal from CH₄ concentration sensors. In the bottom view, the two holes at the bottom

of the detector are connected to the opened tubes. (c) The size of the plastic case of the detector. (d) The lengths of opened tubes, which are used to measure CH_4 concentrations in different scenarios.



Fig. B. 3. Side views of the natural gas detector on (a) the asphalt area and (b) the soil and grass area. The detector on the asphalt area has two short open tubes of the same lengths. Both tubes connect to natural gas sensor (TGS) to measure surface methane concentrations. (b) The detector on the soil and grass area with one long and one short open tube. The short tube is responsible for measuring the surface methane concentration, while the long tube is responsible for monitoring the near-surface methane concentration at the depth of 1.2 cm below the ground surface.

Meteorological conditions

To measure the weather parameters needed for the model, a weather station (ATMOS 41, METER Group, Inc.) was utilized to monitor the changes in precipitation, solar radiation, relative humidity, atmospheric temperature, atmospheric pressure, and wind velocity. Measured meteorological data were used to estimate the atmospheric resistance in the modified ESCAPE model. The atmospheric resistance describes the influence of the quasi-laminar sub-layer of vegetation and the atmospheric stability on the gas migration between the surface and the atmosphere. Details of the estimation of atmospheric resistance can be found in Section C.1. Measurements from ATMOS 41 were recorded by ZL6 data loggers (METER Group, Inc.) at 30-second intervals.

Soil moisture and temperature

The soil moisture and temperature sensor (5TM, METER Group, Inc.) was used to monitor soil moisture and temperature at a depth of 10 cm below the ground surface at the leak site. Measured soil moisture and temperature were used to estimate the average soil resistance at a depth of 10 cm below the ground surface in the modified ESCAPE model. Soil resistance describes the influence of soil moisture on the belowground gas migration. Details of the estimation of soil resistance can be found in Section C.1. Measurements from 5TM were recorded by ZL6 data loggers (METER Group, Inc.) at 30-second intervals.

B. 3 Soil Aeration Experiments : Experimental Procedure

Overview and experimental phases

The soil aeration experimental method consisted of three phases: (1) system setup, (2) aeration operation, and (3) aeration completion and rebound assessment. The experiments were conducted at the METEC rural testbed, where a controlled subsurface CH₄ release and spatially distributed monitoring enable repeatable field-scale evaluation of aeration performance.

System setup

To evaluate removal of residual CH₄ via soil aeration, a field-scale aeration system was constructed within a 5 m × 5 m and approximately 2 m depth at the testbed. Site preparation prior to each experiment included: (a) drilling aeration bar holes using handheld augers, (b) assembling hoses and the manifold system, and (c) installing bar-hole purgers (BHP-375) in selected bar holes (Fig. B. 4).

A total of five bar holes were pre-drilled due to hard subsurface conditions to ensure consistent geometry across scenarios. For each scenario, only a subset of bar holes was activated; unused bar holes were sealed with plastic caps to isolate experimental variables. Each bar hole had a 2-inch diameter and was drilled to approximately 3 ft (0.9 m) depth (average installed depth approximately 2.5 ft when refusal occurred). Bar holes were spaced at approximately 5 ft (1.5 m) to enable systematic evaluation of spatial aeration effects.

Five BHP-375 units were available, each connected to a ½-inch hose (≈ 16 ft / 5 m) leading to a central manifold. The manifold was supplied by a ¾-inch main hose (≈ 50 ft / 15 m) connected to an air compressor. In addition to the METEC site-wide monitoring network, the aeration zone was instrumented with 13 sensors/detectors to monitor subsurface CH₄ concentrations, soil

moisture and temperature, and meteorological conditions. Meteorological variables (wind speed, ambient temperature, and barometric pressure) were measured at the METEC weather station during the test period.



(a)



(b)



(c)



(d)

Fig. B. 4. Site preparation for the soil aeration experiments. (a) Drilling the aeration bar holes using handheld augers. (b) Setting up the manifold and hose system. (c) Installing bar hole purgers into pre-drilled bar holes. (d) Wetting the near-surface soil to simulate a partial saturation layer (water cap) for selected tests. All bar holes were pre-drilled prior to the experiments due to hard subsurface conditions and were capped to ensure consistent configuration and allow controlled activation of specific bar holes during each test.

Aeration operation

(a) Preconditioning: controlled CH₄ release prior to aeration

To ensure sufficient subsurface gas accumulation prior to aeration, compressed natural gas containing approximately 86% CH₄ (v/v) was released through stainless-steel tubing at a controlled rate of 8 to 10 SLPM for at least 6 h before each aeration test. Subsurface CH₄ concentrations and soil moisture/temperature were monitored continuously during the release period to track gas distribution and soil conditions. Once the subsurface concentration at the central location approached 100 vol.% (or after approximately 8 to 9 h of release), the gas release was manually shut off and the aeration phase was initiated.

(b) Near-surface “water-cap” condition (wet-surface scenarios)

For scenarios requiring a near-surface water cap, surface watering was performed immediately prior to aeration to increase near-surface moisture and reduce gas permeability in the upper soil layer. Water was applied using fire hoses (Poudre Fire Authority), producing a partially saturated surface layer (“water-cap” condition). This condition was used to evaluate how surface sealing influences subsurface CH₄ retention and aeration performance under more restrictive gas-migration conditions.

(c) Aeration operation and rounds

Aeration was conducted in one to three rounds depending on the observed CH₄ rebound after each operation. Total aeration duration and the number of active bar holes varied by scenario, with individual aeration periods typically ranging from 1 to 5 h (up to 6 h depending on scenario definitions).

During aeration, compressed air from the compressor (185 SCFM, 80 psi) was delivered to the BHP-375 units. The venturi mechanism generated suction at the bar holes, producing an average vacuum of approximately 5 psi at each active bar hole. The induced vacuum aerated subsurface CH₄ through the perforated BHP assemblies. Subsurface CH₄ concentration at the central aeration location was monitored continuously to guide operational decisions, including when to stop the compressor.

Aeration completion and rebound assessment

Aeration was considered complete when the CH₄ concentration measured at the bottom of the central aeration bar hole decreased to or below the operational threshold of 50 ppm (0.005 vol.%). After shutdown, subsurface CH₄ concentrations were monitored continuously for 15 min to assess rebound. If CH₄ exceeded 50 ppm during the rebound window, an additional aeration round was conducted using the same configuration. This rebound-based operational logic ensured that residual gas remaining in the soil was adequately removed or stabilized before concluding each test.

Experimental design

We conducted two, one-week controlled soil aeration experiments with 9 different aeration scenarios (Table B. 1). The experiments were performed with an average methane leakage rate of 10 SLPM (369.5 g CH₄ h⁻¹) and involved varying soil moisture conditions from 0.04 (dry) to 0.48 (wet). While each experiment will be described in detail in the following sections, a summary of the experimental scenarios is provided in Table B. 1. In addition to soil moisture, the main difference between experiments were the number of aeration bar holes, ranging from 1 to 5, the amount and time of aeration (1 to 6 hrs) and the average gas release rate (8 to 20 slpm (0.3 to 0.7 kg/hr)).

Table B. 1. Overview of experimental scenarios and operation conditions of soil aeration experiments

Scenario #	Experimental Scenarios	Number of aeration bar holes	Averaged gas release rate (SLPM)	1st aeration (hours)	2nd aeration (hours)	3rd aeration (hours)	Total aeration duration (hours)	Watering ^a (hours)
S1	Dry soil	1	20 ^b	1	-	-	1	-
S2	Near-surface water cap	1	10	2	2	-	4	0.5
S3	Surface impermeable cover	1	10	1	-	-	1	-
S4	Dry soil	3	8	5			5	-
S5	Near-surface water cap	3	10	1.3	1.3	1	3.6	0.5
S6	Surface impermeable cover	3	10	1	-	-	1	-
S7	Dry soil	5	10	1.8	4.1	-	5.9	-
S8	Near-surface water cap	5	10	1	-	-	1	0.5
S9	Surface impermeable cover	5	10	1	-	-	1	-

Appendix. C. Experimental Data Processing

This appendix documents the observation data-processing methods used to quantify CH₄ transport and soil aeration performance across the controlled release and mitigation experiments described in Appendix B. The objective is to provide transparent, reproducible procedures for converting raw measurements (meteorological, surface, and subsurface observations) into the derived quantities used throughout the analysis, including interfacial resistances, CH₄ fluxes, response times, and removal efficiency.

Section C.1 summarizes the calculation of aerodynamic and boundary-layer resistances, which govern gas transfer between the near-surface soil and the atmosphere and provide the link between meteorological forcing and surface exchange. Section C.2 describes how surface and subsurface CH₄ fluxes were estimated from the detector network. Section C.3 defines and computes the response time from the pipeline leak source to the surface and to the belowground monitoring system (BNS), providing a consistent basis for comparing plume development and timing across scenarios. Finally, Section C.4 compiles the observation-based CH₄ removal efficiency across all soil-aeration scenarios and outlines the processing steps used to ensure comparability among tests with different leak rates, soil moisture conditions, and operational settings.

All processing steps reported here were applied consistently across scenarios to minimize subjective interpretation and to isolate differences attributable to experimental controls rather than data handling.

C. 1 Aerodynamic and Boundary Layer Resistances

Aerodynamic resistance (R_a)

The aerodynamic resistance (R_a), as shown in Eq. C.1, can be estimated using several parameters, including the roughness length (z_0), the displacement length (z_d), the Monin-Obukhov length (L), the von Karman constant ($k = 0.41$), the wind speed at a height of z meters above the ground surface (u_z), and a stability correction function (ψ_m). In this study, the roughness length (z_0) was determined to be 0.05 m, while the displacement length (z_d) was 0.01 m based on the environmental conditions of the test site. The stability correction function was defined using Eq. C.2 for stable conditions and Eq. C.3 for unstable conditions. The aerodynamic resistance (R_a) increases during stable conditions, which occur under low wind and low solar radiation conditions. Conversely, high wind and high solar radiation induce unstable conditions, leading to a decrease in R_a . The measurement of wind speed from a weather sensor (ATMOS 41, METER Group, Inc.) is shown in Fig. C. 1. The wind speed varied from 0.5 m/s to 4 m/s. The increase in the wind speed could create turbulence on the surface, decreasing the atmospheric resistance and enhancing vertical gas transportation from the surface to the atmosphere. The wind speed was assumed as a homogeneous distribution at the experimental site.

$$R_a = \frac{\left[\ln \left(\frac{z - z_d}{z_0} \right) - \psi_m \left(\frac{z - z_d}{L} \right) \right]^2}{k^2 u_z} \quad (C.1)$$

Stable Condition ($L > 0$):

$$\psi_m \left(\frac{z - z_d}{L} \right) = -\frac{5z}{L} \quad (C.2)$$

Unstable Condition ($L < 0$):

$$(C.3)$$

$$\psi_m\left(\frac{z - z_d}{L}\right) = 2 \ln\left(\frac{1 + X}{2}\right) + \ln\left(\frac{1 + X^2}{2}\right) - 2 \tan^{-1}(X), \quad X = \left(1 - 16 \frac{z}{L}\right)^{\frac{1}{4}}$$

where z is the height of measurement of weather conditions (m), z_0 is the roughness length (m), z_d the displacement length (m), L is the Monin-Obukhov length (m), k is the von Karman constant ($k = 0.41$), u_z is the wind speed at the height z m (m/s), and ψ_m is a stability correction function.

Boundary layer resistance (R_b)

The boundary layer resistance (R_b) can be calculated using Eq. C.4. The Schmidt number for mass transfer (Sc) is determined by the ratio of the kinematic viscosity to the molecular diffusivity of water vapor in the air. For this study, Sc was approximately 0.7. The kinematic viscosity of air (ν) is temperature dependent. The upper height of the logarithmic wind profile above the ground surface (z_l) was assumed to be the height of the local weather station at the test site.

$$R_b = \frac{Sc - \ln\left(\frac{\nu}{ku_*}/z_l\right)}{ku_*} \quad (C.4)$$

where R_b is the boundary layer resistance (s/m), Sc is the Schmidt number for mass transfer (-), ν is the kinematic viscosity of air (m^2/s), z_l is the height of the measurement of weather conditions (m), and u_* is the wind friction velocity (m).

The atmospheric resistance (R_{at} , s/m) can be described as the summation of the aerodynamic resistance (R_a , s/m) and the boundary layer resistance (R_b , s/m) (Eq. A.5). The estimated atmospheric (R_{at}) and soil resistance (R_s) during the experiment are shown in Fig. C. 2.

$$R_{at} = R_a + R_b \quad (C.5)$$

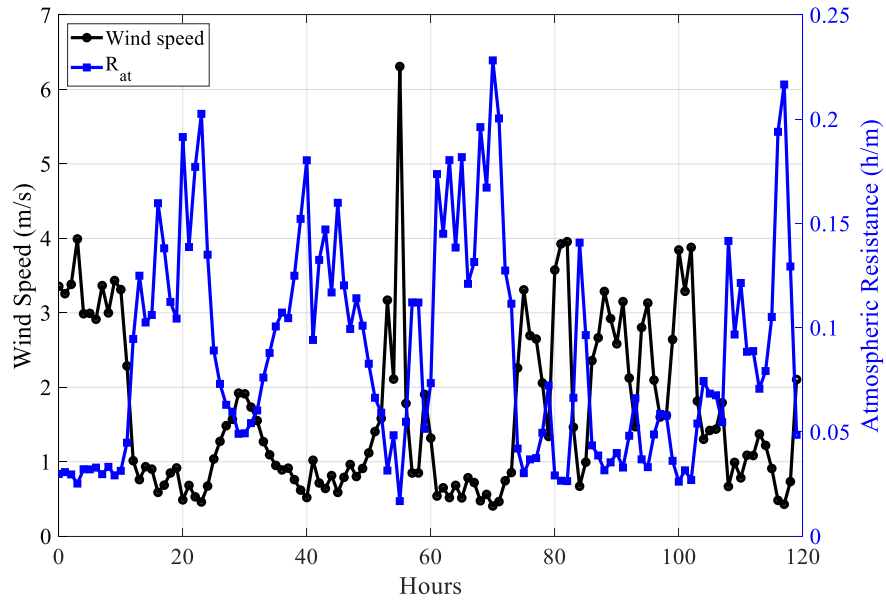


Fig. C. 1. The variations of wind speed measured by a weather station (ATMOS 41, METER Group, Inc.) and the estimated atmospheric resistance (R_{at}) during the experiment.

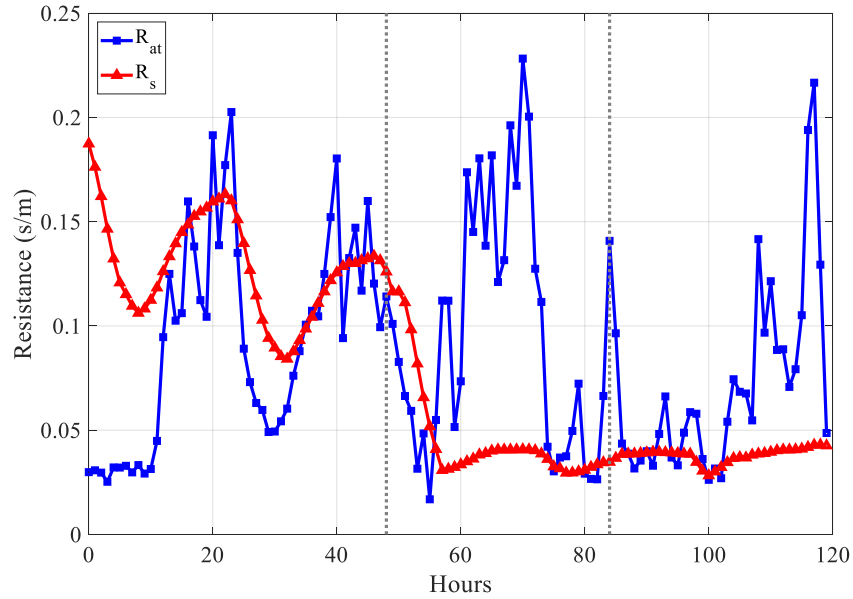


Fig. C. 2. The variations of atmospheric resistances (R_{at}) and soil resistance (R_s) were determined during the experiment. The gray dotted lines indicate the time when controlled NG release rates (g/h) were increased from 37.08 (g/h) to 88.76 (g/h) at hour 48 and from 88.76 (g/h) to 120.96 (g/h) at hour 84.

C. 2 Surface and Subsurface CH₄ Fluxes

Variations of Surface CH₄ Flux with Atmospheric Resistance

The varied range of surface CH₄ flux in Fig. C. 3 was from 0 to 120 (g/m²/h). Comparison between surface CH₄ flux and the atmospheric resistance (R_{at}) indicates that the high atmospheric resistance could reduce the transportation of CH₄ flux from the surface to the atmosphere.

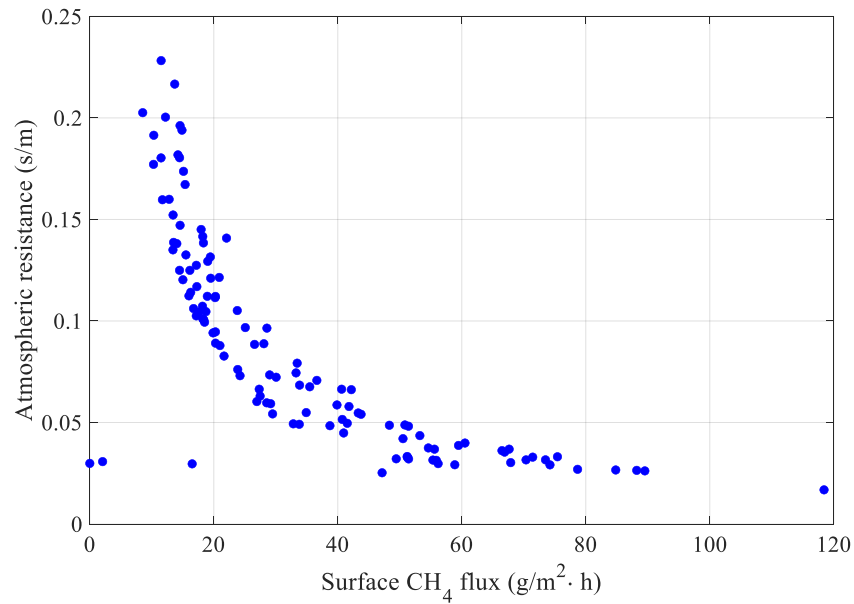


Fig. C. 3. Comparison of surface CH₄ fluxes (g/m²/h) and atmospheric resistances (s/m) throughout the experiment.

Variations of BNS CH₄ Flux with Soil Moisture and Soil Resistance

Fig. C. 4 shows the variation of BNS CH₄ with estimated soil resistances and soil moisture during the experiment. The soil resistances were calculated by Eq. 8.

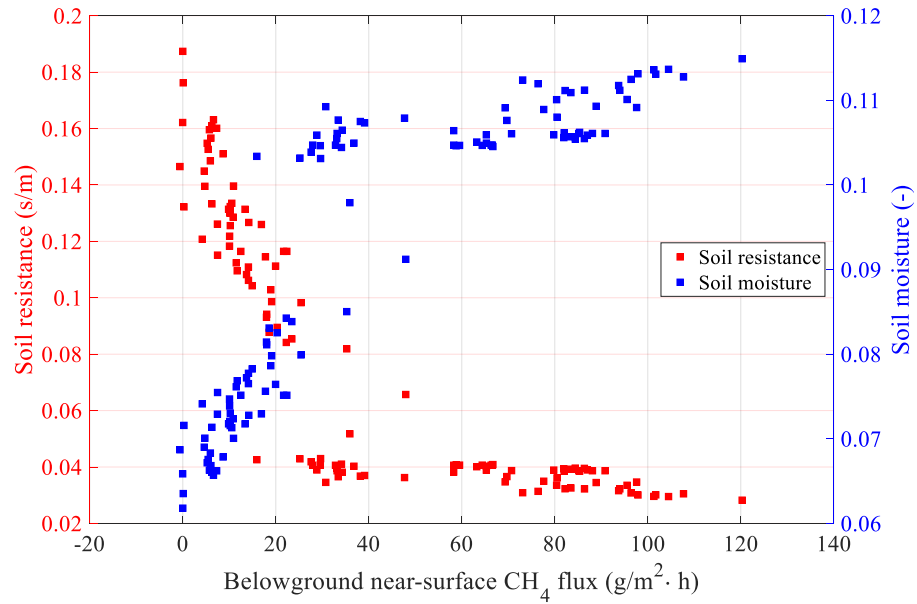


Fig. C. 4. The variations of BNS CH₄ flux with the changes in soil resistance (red) and soil moisture (blue) during the experiment.

Measurements of precipitation and soil moisture and the estimation of soil resistance

Fig. C. 5 depicts the measured soil moisture and precipitation data obtained during the experiment. Precipitation occurred at hour 45, with a value of 0.0014 (mm/hr), and between hour 81 and hour 93, with an average value of 0.0057 (mm/hr). Analysis of the variations in soil moisture and soil resistance indicates that precipitation significantly increased soil moisture at hour 45. Nevertheless, the precipitation that occurred between hour 81 and hour 93 did not induce significant changes in soil moisture.

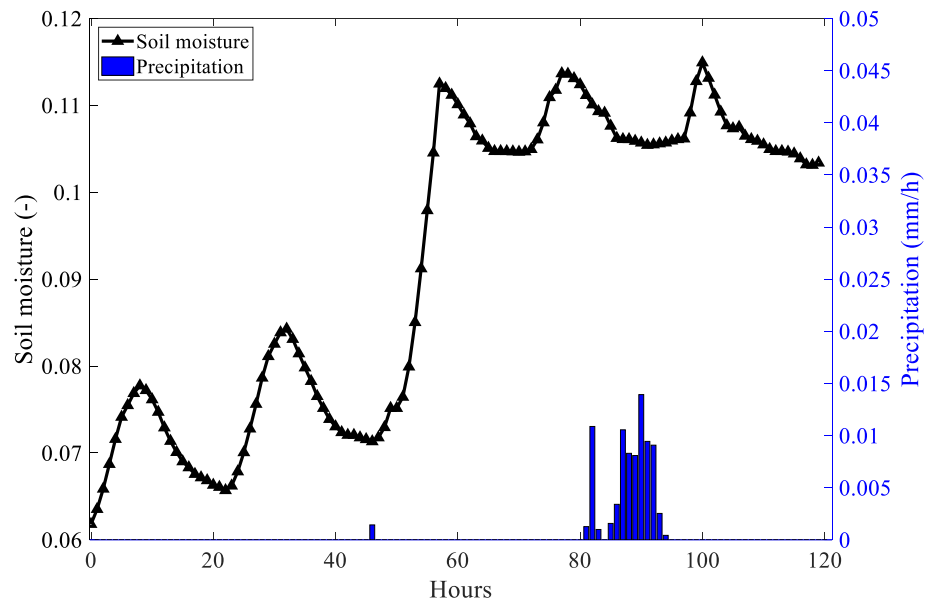


Fig. C. 5. Measurements of soil moisture from 5TM sensors (black line) and precipitation (blue bar) by ATMOS 41 during the experiment.

C. 3 Response Time of NG from the Pipeline to Surface and BNS

In this study, the surface and BNS CH₄ fluxes were used to determine the time when the underground NG leak rates changed. Fig. C. 6 shows determined response times in surface and BNS CH₄ fluxes with the experimental NG leak rate. The surface CH₄ flux only showed two increased trends at hours 51 and 71 as the experimental NG leak rate increased from Level 1 to Level 2. However, after the experimental NG leak rate increased from Level 2 to Level 3 at hour 84, the increased trends were difficult to determine. However, the BNS CH₄ flux presented two increased trends at hours 51 and 62 as the experimental NG leak rate increased from Level 1 to Level 2, and two increased trends at hours 85 and 97 as the experimental NG leak rate increased from Level 2 to Level 3. These results not only indicate the response time presenting the time for leaked gas from pipeline to surface and BNS (Table C. 1) but also suggested that the BNS CH₄ flux was more useful to determine the time when the underground NG leak rate changed than the surface CH₄ flux.

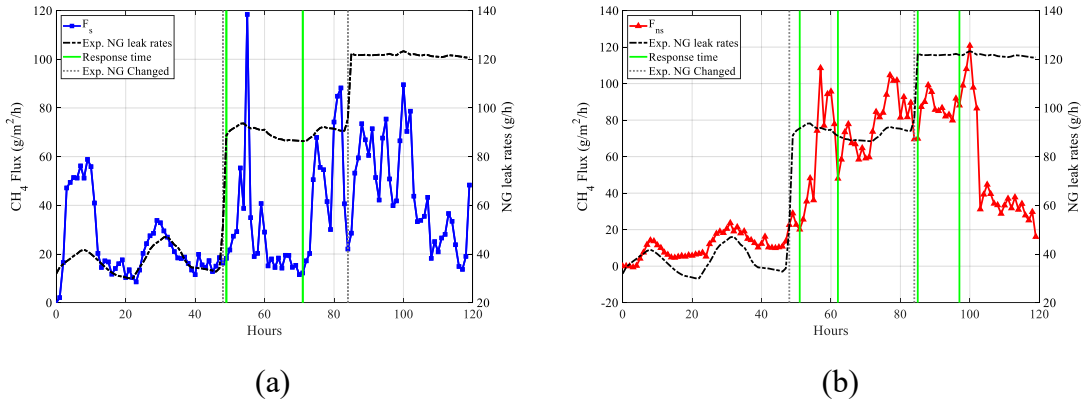


Fig. C. 6. Comparison between the experimental NG leak rates and the response times when the increase trends occurred in (a) surface and (b) BNS CH₄ fluxes. The green lines represent the estimated response times of surface and BNS CH₄ flux. The grey dotted line shows the time of the increase in the experimental NG leak rate.

Table C. 1. The response times in surface and BNS CH₄ fluxes when the experimental NG leak rate increased from Level 1 to Level 2 and from Level 2 to Level 3.

NG Release Level	Time of the increase in NG leak rate	Time of the increase in CH ₄ flux		Response Time (Hours)
Lv. 1 to Lv. 2	Hour 48	BNS CH ₄ flux	Hour 51	3
			Hour 62	14
Lv. 2 to Lv. 3	Hour 84		Hour 85	1
			Hour 97	13
Lv. 1 to Lv. 2	Hour 48	Surface CH ₄ flux	Hour 51	3
			Hour 71	23
Lv. 2 to Lv. 3	Hour 84		-	-
			-	-

C. 4 Observed CH₄ removal efficiency across all scenarios

Fig. C. 7 shows the observed CH₄ removal efficiency from the controlled experiments (Re_{CH_4}). In the wet near-surface scenarios (S2, S4, and S6), Re_{CH_4} increases rapidly and consistently reaches 100 percent. This behavior indicates that high near-surface water saturation restricts vertical gas migration, forcing CH₄ to migrate laterally toward the bar hole, which substantially enhances removal effectiveness during the early stage of aeration. In contrast, the dry-soil scenarios (S1, S3, and S5) show lower and more variable Re_{CH_4} , ranging from 10 to 90 percent. In S1, Re_{CH_4} reaches approximately 60 % at $t/t_0 \approx 0.2$ and remains near this value for most of the aeration period before decreasing to 53 % at the end. This decline reflects CH₄ rebound at D2, caused by diffusion from regions outside the main aeration zone. Scenario S3 shows oscillations in Re_{CH_4} after reaching 80 % within the first 5 % of the aeration period, indicating rebound driven by diffusion from poorly aerated zones and interference caused by overlapping aeration areas. In S5, Re_{CH_4} increases monotonically and approaches 80% by the end of aeration. The comparison among S1, S3, and S5 shows that increasing the number of bar holes improves local removal efficiency and mitigates rebound when spacing provides adequate coverage of the plume. Negative values observed at the beginning of the dry-soil experiments reflect a brief increase in CH₄ concentration at D2, resulting from the advective displacement of a high-concentration plume toward the sensor during aeration.

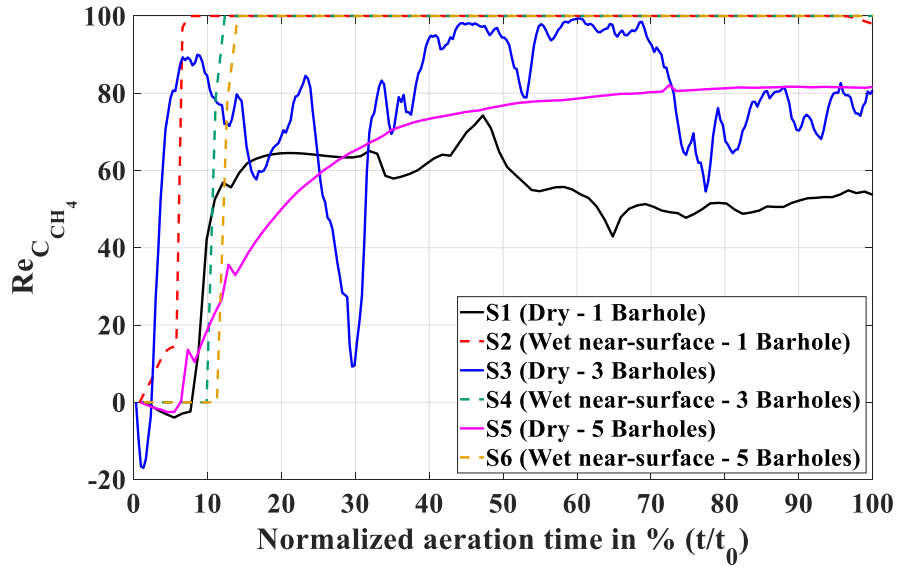


Fig. C. 7. Removal efficiency of residual CH₄ ($Re_{C_{CH_4}}$) at the measured location D2 (1.1 m, -0.9 m) via normalized aeration duration in percentage (t/t_0) for six controlled experimental scenarios (S1 to S6). t_0 is the length of aeration duration. The solid line presents the aeration in dry soil conditions (S1, S3, and S5). The dashed line describes the aeration in wet near-surface soil layer conditions. The D2 is located closest to the isolated leak (Fig. 1). Removal efficiency is calculated from measured concentration based on Eq. 5. Normalization enables direct comparison across scenarios with different operating durations. The negative value in $Re_{C_{CH_4}}$ indicates the increases in the residual CH₄ concentration.

Appendix. D. Numerical Transport Model Setup and Supplementary

This appendix presents supplementary results from the numerical transport model to support interpretation of the main modeling analyses. The materials compiled here document model initialization choices and provide additional diagnostic outputs that are not shown in the main text but are essential for understanding the simulated CH₄ migration mechanisms and the response of the system under different cases.

Section D.1 summarizes the model initialization procedure and initial/boundary conditions used to establish consistent starting states across simulations. Section D.2 shows the variations of radius of influence (R_I) of a single bar hole in sand and silt loam with the vacuum pressure ranging from 0 to 0.9 atm and soil water saturations (S_w) at 0.2, 0.4, and 0.6. Section D.3 provides additional results characterizing belowground CH₄ migration behavior in sand, highlighting storage and transport patterns that influence subsequent system response. Section D.4 decomposes modeled CH₄ transport into advective and diffusive flux components for Cases #2 and #3, enabling direct comparison of transport regimes and their controlling factors. Section D.5 reports spatial and temporal evolution of pressure gradients for Cases #1 to #3, which quantify the driving force for airflow-induced advection and help explain differences in plume capture and removal performance among cases. Section D.6 describes the Reynolds number of gas flow in the vadose zone during soil aeration in sand for Case #1.

D. 1. Model initialization

The model initialization was conducted to obtain the appropriate initial distribution of pore water pressure and residual CH_4 in the vadose zone due to a belowground natural gas (NG) leak event before soil aeration. The conceptual configuration of the initialization represented a two-dimensional homogeneous porous medium with dimensions of 40 m in length and 5 m in depth. The NG pipeline was located at a depth of 0.91 m, as indicated by the black dashed line in Fig. D. 1. An active NG leak was located at the center of the domain along the pipeline (red circle), releasing NG at a constant rate of 369 g/hr (10 SLPM) over a 12-hour period. All domain boundaries were assigned no-flux conditions, except for the top boundary, which represented the ground surface. The top boundary was defined by a flux condition to describe the gas flux (J_g) from the vadose zone to the atmosphere. This flux boundary condition incorporated the effects of meteorological conditions (i.e., wind speed (u_w) and net radiation (R_n)) on CH_4 transport from the near-surface to the atmosphere (Brutsaert, 1982; Gao et al., 2021; Lo et al., 2024; Vanderborght et al., 2017). The pore water in the vadose zone was assumed to be immobilized. Therefore, the water flux (J_w) at the ground surface was assumed as 0.

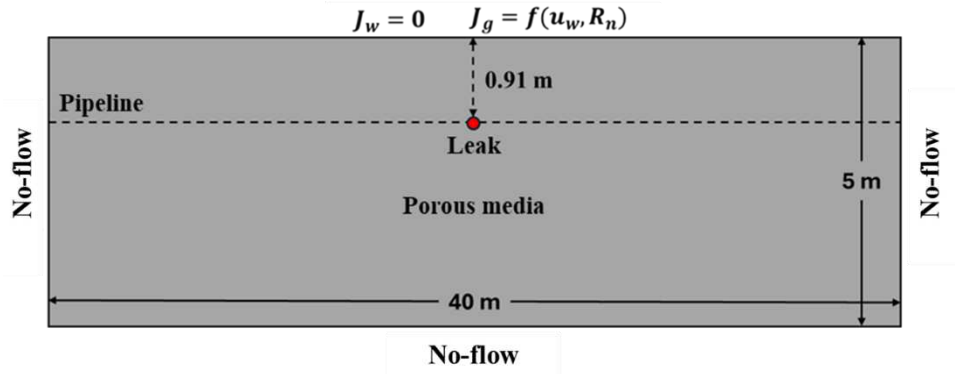


Fig. D. 1. Two-dimensional conceptual configuration of model initialization. A natural gas (NG) leak (red circle) is located at a depth of 0.91 m along a buried NG pipeline (black dashed line), releasing NG at a constant rate of 369 g/hr (10 SLPM) for 12 hours. J_w and J_g indicate water and gas flux, respectively. u_w denotes the average wind speed. R_n is the net radiation. No aeration is conducted during the gas release period.

D. 2. Radius of Influence (R_I)

The radius of influence (R_I) defines the effective aeration zone as the maximum lateral distance from the bar hole to the point where advection can reach. In SVE, the R_I is defined as the distance at steady state from the extraction well to the point where pressure equals 10% of the applied vacuum, or where pressure drawdown is below 1% at the well (Johnson et al., 1990; Kuo, 2014; Sun et al., 2023; Suthersan et al., 1999). However, NG soil aeration is typically conducted over a short duration (15 to 60 minutes), during which pressure conditions remain transient. Therefore, in this study, R_I represents the maximum lateral distance (at $z = 0.9$ m) over which advective transport remains non-negligible during transient aeration. R_I is estimated as the farthest distance where the simulated advective CH_4 flux exceeds a small threshold (Eq. (B1)). Because the controlled experiments did not include independent pressure-drawdown measurements to quantify R_I , R_I is estimated from the simulated advective CH_4 flux for Case #1 (single bar hole) during a 60-min aeration.

$$R_I = \max\{r \mid J_{adv_{\text{CH}_4}}(r, z, t) > \varepsilon\} \quad (\text{D1})$$

where R_I is the radius of influence (m), $J_{adv_{\text{CH}_4}}$ is the advective flux of CH_4 ($\text{kg m}^{-2} \text{min}^{-1}$) at horizontal distance r from the bar hole and depth z (0.9 m in this study), t is the aeration duration (min), and ε is a small threshold value ($10^{-8} \text{ kg m}^{-2} \text{min}^{-1}$ in this study) below which the advective flux is considered negligible.

The variation of R_I for Case #1 (single bar hole) in sand and silt loam with P_b ranging from 0.1 to 0.9 atm (1.47 to 13.23 psi) and at $S_w = 0.2, 0.4$, and 0.6 are shown in Fig. S2. Overall, the increase in P_b enhances the removal capacity and extends the R_I . In sand, as P_b increases from 0.1 to 0.9 atm at $S_w = 0.2$ (low saturation), the overall R_I approximately increases from 3.15 to 3.45

m (approximately 10 % increase). When S_w increases from 0.2 to 0.4 (medium saturation), the R_I at $T = 60$ min only decreases by 0.6 %, while it decreases by 2.2 % when S_w increases from 0.2 to 0.6 (high saturation). These results indicate that low S_w in sand causes the large air-filled porosity, inducing large R_I and effective aeration zone. In contrast, R_I increases only from 3.1 to 3.2 m (changes only 3%) in fine-grained, lower-permeability soil at all S_w scenarios, highlighting that tight packing and small pores significantly constrain advection. Thus, increasing vacuum pressure or decreasing S_w increases R_I only slightly in fine-grained, lower-permeability soil, indicating that diffusion dominates CH_4 transport in low-permeability soil. These findings also emphasize that R_I is more controllable in high-permeability soil (e.g., sand), while in fine-grained, lower-permeability soil, increasing bar hole density is more effective than enhancing P_b to reach the target removal performance.

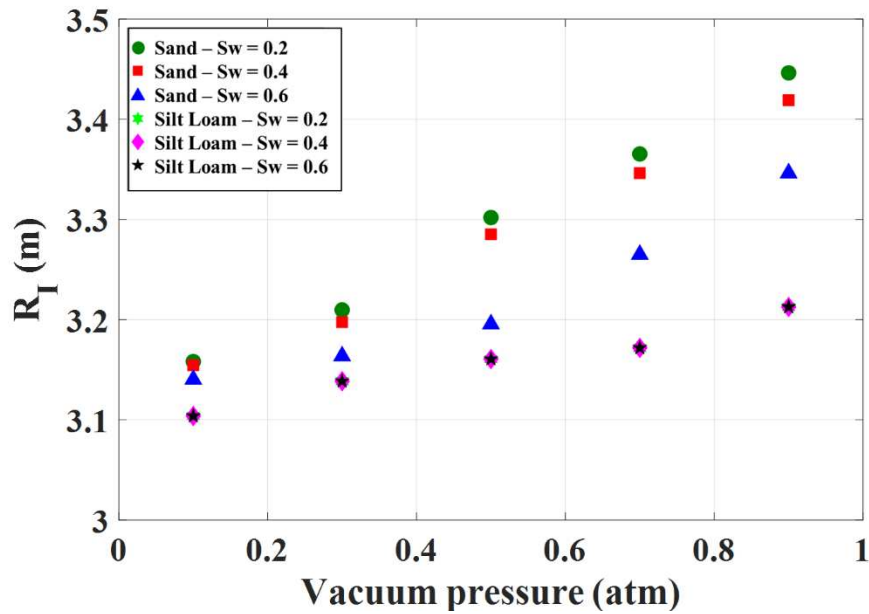


Fig. D. 2. The radius of influence (R_I) for a single aeration bar hole (Case #1) evaluated at $T = 60$ min in sand and silt loam for vacuum pressures 0.1–0.9 atm and soil water saturations (S_w) of 0.2, 0.4, and 0.6.

D. 3. Belowground CH₄ migration behavior in the fine-grained, lower-permeability soil

Fig. D. 3 shows the temporal distribution of CH₄ concentration in the vadose zone over a 60-minute aeration period for Cases #1 to #3 in the fine-grained, lower-permeability soil with a soil water saturation of 0.2 and vacuum pressure of 0.9 atm (13 psi). After 30 minutes of soil aeration, the residual CH₄ mass decreased to 13 % in Case #1 (a single bar hole) (Fig. D. 3a-c). In Case #2 (Fig. D. 3d-f), the residual CH₄ mass decreased by 81 % during the same aeration period. In Case #3, where three bar holes were installed with a spacing of 5 m and two of them were located outside the initial plume, the large residual CH₄ plume was observed concentrated below the central aeration bar hole, with approximately 50 % of the CH₄ mass remaining.

After 60 minutes of aeration in the fine-grained, lower-permeability soil, Case #1 achieved near-complete removal of residual CH₄, demonstrating the most effective aeration with 96% of the CH₄ mass removed from the vadose zone. Case #2 also shows substantial removal, decreasing residual CH₄ mass from 100 % to 6 %. In contrast, Case #3 only removed CH₄ from the vadose zone with 67 % of the CH₄ mass. Overall, the mass removal efficiency in the fine-grained, lower-permeability soil is lower than that in sand. The low permeability in fine-grained, lower-permeability soil restricted the airflow through the vadose zone and limited the removal of residual CH₄, reducing the removal performance of soil aeration.

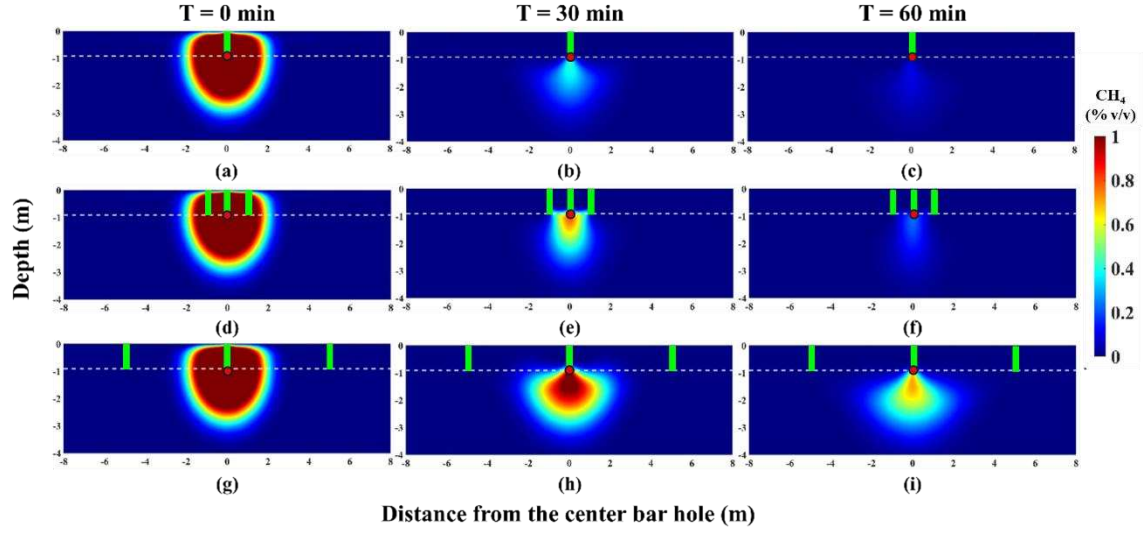


Fig. D. 3. Cross-section plots of the belowground residual CH_4 concentrations in fine-grained, lower-permeability soil ($S_w = 0.2$ and $P_b = 0.9$ atm) for Cases #1 to #3 before ($T = 0$ min) and during ($T = 30$ and 60 min) soil aeration. The remaining CH_4 at $T = 0$ min (a, d, and g) indicates the initial distribution of belowground CH_4 directly prior to aeration. The green squares represent the bar holes for scenarios with a single bar hole (a to c), three bar holes spaced 1.5 m from the center bar hole (d to f), and three bar holes spaced 5 m from the center bar hole (g to h). The vacuum pressure (P_b) at each aeration bar hole is 0.9 atm. The white dashed line indicates the pipeline at 0.91 m below the ground surface. The red circle represents the isolated leak point. The colorbar shows the CH_4 concentration by volume (vol.%).

D. 4. Advective and diffusive fluxes for Cases #2 and #3

This section shows the simulated advective and diffusive fluxes in sand and silt loam for Cases #2 and #3 to discuss the impacts of the number of bar holes and spacing on gas migration during soil aeration.

In Cases #2 and #3, the horizontal and vertical advective CH_4 fluxes (F_{Adv}) in both sand (Fig. D. 4a, 3c, 5a, and 5c) and silt loam (Fig. D. 5a, 4c, 6a, and 6c) demonstrate peaks near the bar hole locations (at $x = 0$ and 1 m). The peak vertical F_{Adv} is typically higher than the horizontal F_{Adv} , reflecting a more significant vertical pressure differential between the applied vacuum and atmospheric pressure. In comparison to Case #1 (a single bar hole), the peak F_{Adv} observed in Case #2 and #3 are lower. This result is induced by the interference between the closely spaced bar holes. This interaction leads to reduced local pressure gradients and diminished advective migration.

With increasing distance from the bar holes, the advective flux (F_{Adv}) decreases rapidly, and the diffusive flux (F_{Dif}) gradually dominates transport. From $x = 2$ m, the overall migration is primarily diffusion-controlled. Compared with Case #1 (single bar hole), the peak F_{Dif} in Cases #2 and #3 is higher. This occurs because adding bar holes causes pressure interference, reducing local pressure gradients and thus weakening advective fluxes. The reduced advection induces a higher residual CH_4 concentration, elevating F_{Dif} .

From a practical perspective, increasing the number of bar holes does not effectively improve advective transport. When bar holes are placed too closely together (Case #2) or out of the gas plume (Case #3), it can result in pressure interference and an overlapped aeration zone to diminish local pressure gradients and advective gas migration. Consequently, the spacing of bar holes is a critical parameter in the design and operation of soil aeration systems. Proper spacing must be

decided to ensure an adequate advective zone at each hole while ensuring sufficient areal coverage. Failing to do so may lead to a transition towards diffusion-limited removal, resulting in reduced effectiveness from adding more holes.

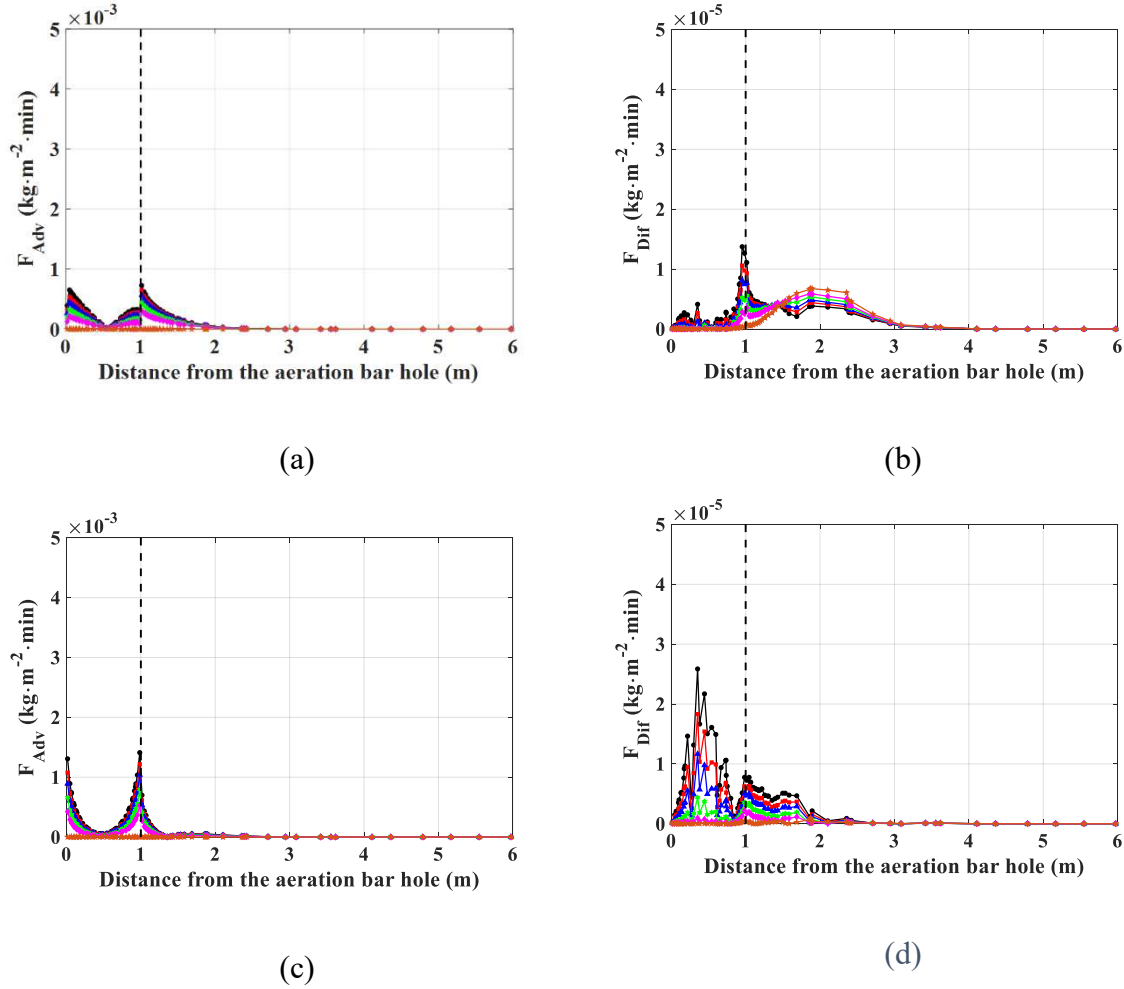
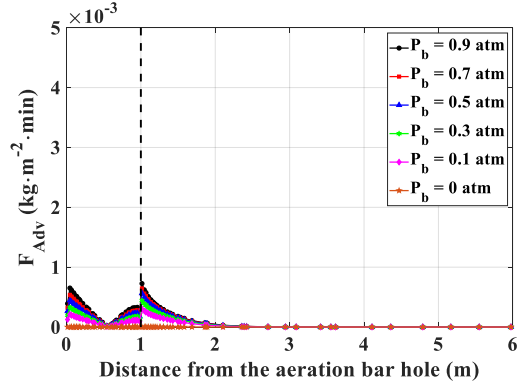
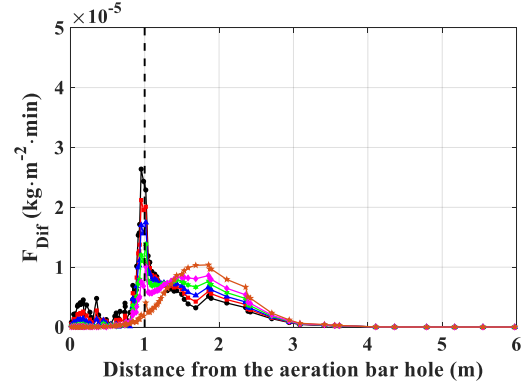


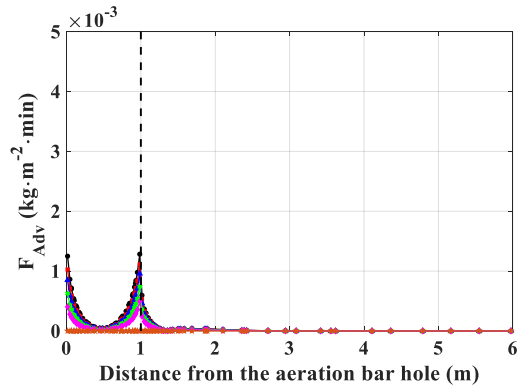
Fig. D. 4. Simulated (a and b) horizontal and (c and d) vertical advective (F_{Adv}) and diffusive (F_{Dif}) fluxes for Case #2 in sand condition with a soil water saturation of 0.2 and vacuum pressures from 0 to 0.9 atm along a horizontal transect 0.9 m below the ground surface during aeration at 30 minutes.



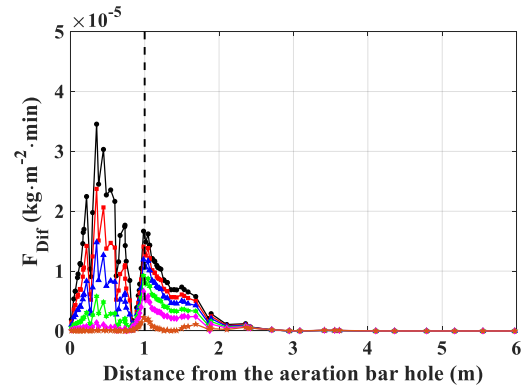
(a)



(b)

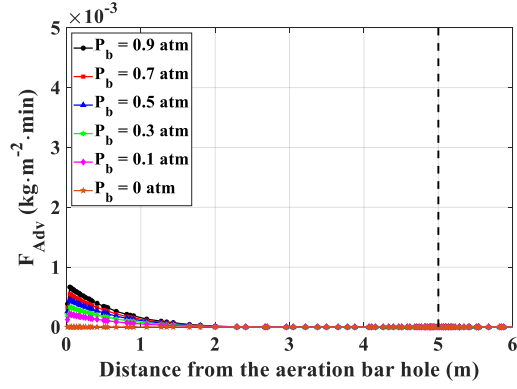


(c)

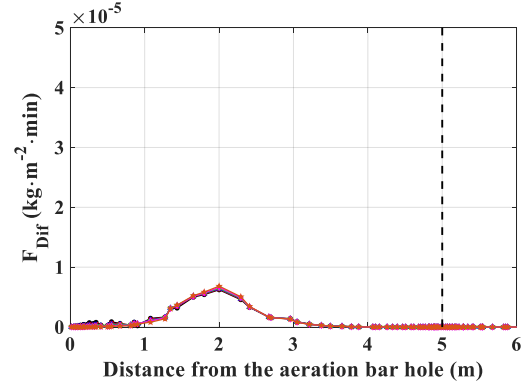


(d)

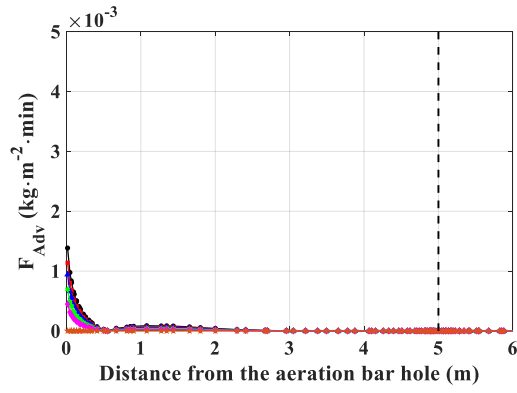
Fig. D. 5. Simulated (a and b) horizontal and (c and d) vertical advective (F_{Adv}) and diffusive (F_{Dif}) fluxes for Case #2 in fine-grained, lower-permeability soil with a S_w of 0.2 and vacuum pressures from 0 to 0.9 atm along a horizontal transect 0.9 m below the ground surface during aeration at 30 minutes.



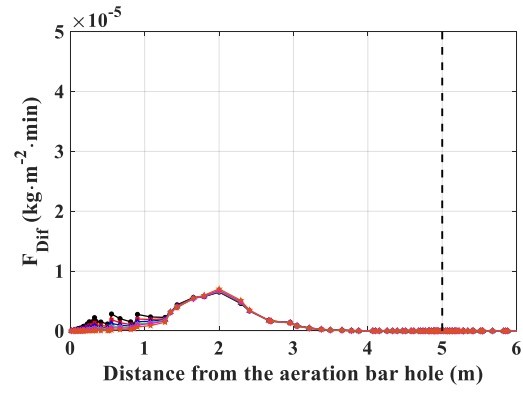
(a)



(b)

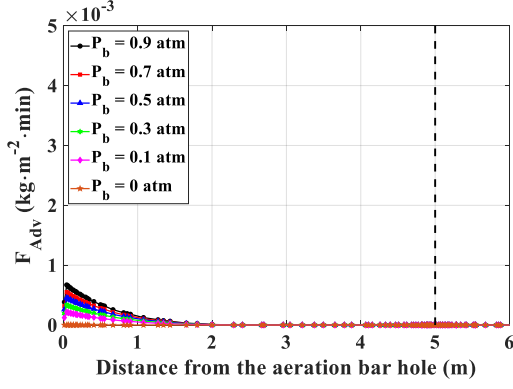


(c)

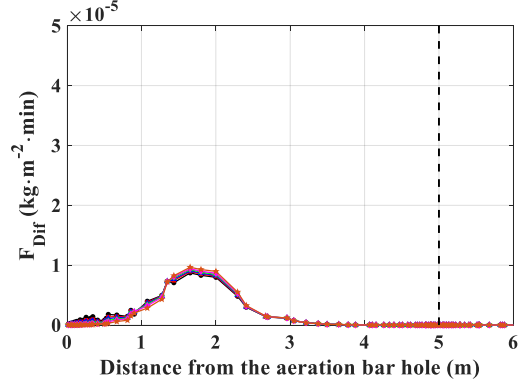


(d)

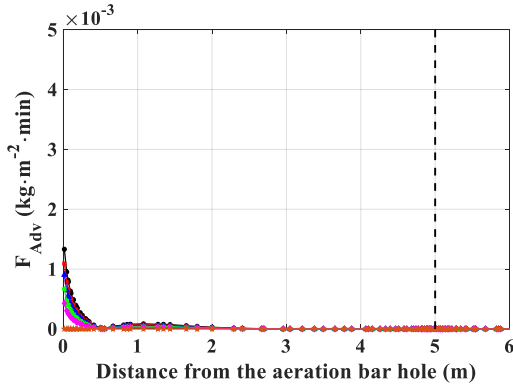
Fig. D. 6. Simulated (a and b) horizontal and (c and d) vertical advective (F_{Adv}) and diffusive (F_{Dif}) fluxes for Case #3 in sand condition with a soil water saturation of 0.2 and vacuum pressures from 0 to 0.9 atm along a horizontal transect 0.9 m below the ground surface during aeration at 30 minutes.



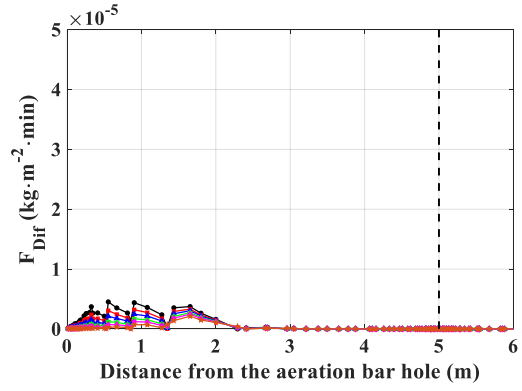
(a)



(b)



(c)

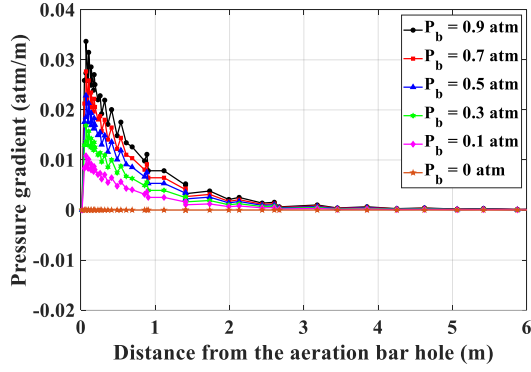


(d)

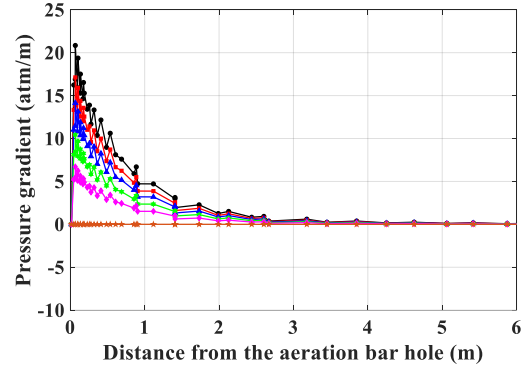
Fig. D. 7. Simulated (a and b) horizontal and (c and d) vertical advective (F_{Adv}) and diffusive (F_{Dif}) fluxes for Case #3 in fine-grained, lower-permeability soil with S_w of 0.2 and vacuum pressures from 0 to 0.9 atm along a horizontal transect 0.9 m below the ground surface during aeration at 30 minutes.

D. 5. Pressure gradients for Cases #1 to #3

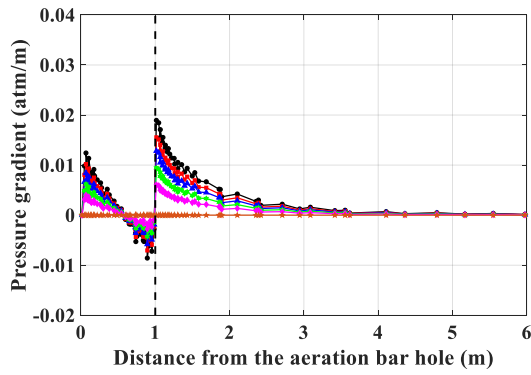
Fig. D. 8 shows horizontal pressure gradient from the center aeration bar hole ($x = 0$) in sand and silt loam for Cases #1 to #3 with vacuum pressures ranging from 0 to 0.9 atm. In Cases #1 to #3, all pressure gradients near the bar hole are higher in silt loam than in sand by four orders of magnitude. These results indicate that aeration with low soil permeability requires a large pressure gradient to maintain the required aeration flow rate. The overall pressure gradient in Case #1 (a single bar hole) is higher than in Cases #2 and #3. This difference indicates that the overlapping vacuum zones between the two bar holes cause the airflow interference and the divergence of gas migration between bar holes. As the spacing increases (from Case #2 to #3), the pressure gradients between bar holes become smooth (Fig. D. 8 e and f). The spacing larger than the gas plume reduces overlap of the vacuum pressure zone between bar holes, inducing the slow change and small pressure gradients between bar holes ($x = 2.5$ m in Fig. D. 8 e and f). The variations in pressure gradients for Cases #1, #2, and #3 support insights into the behavior of gas migration in Section 3.1. The localized advective fluxes near bar holes in both sand and silt loam display similarities, as the elevated pressure gradients in fine-grained, lower-permeability soil compensate for its lower permeability. As the pressure gradient declines, the impact of advection diminishes, enhancing the diffusion to control the gas migration. For example, in Case #3 in fine-grained, lower-permeability soil (Fig. D. 7), the peak of horizontal diffusive flux occurs at the location with the lowest pressure gradient between bar holes (Fig. D. 8f).



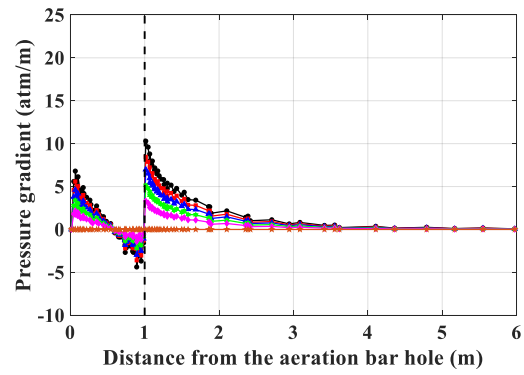
(a)



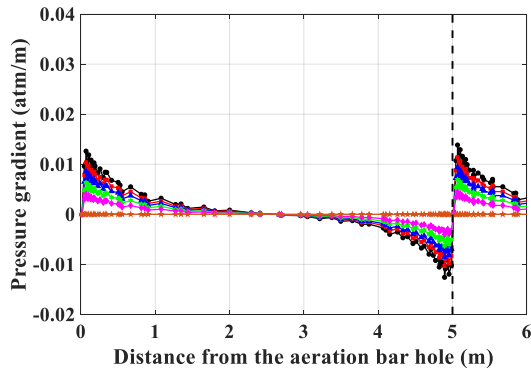
(b)



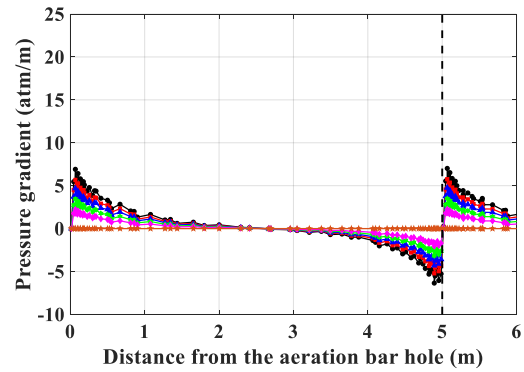
(c)



(d)



(e)



(f)

Fig. D. 8. Simulated pressure gradient with distance from the center aeration bar hole ($x = 0$) for Cases #1, #2, and #3 in (a, c, and e) sand and (b, d, and f) silt loam with a soil water saturation of 0.2 and vacuum pressures from 0 to 0.9 atm along a horizontal transect 0.9 m below the ground surface during aeration at 30 minutes. Since the deployment of aeration bar holes is symmetric, the figure only shows the right side of the pressure. $x = 0$ represents the central bar hole. The vertical dashed lines indicate the positions of additional bar holes in Cases #2 and #3.

D. 6. Reynolds number in the vadose zone (Re_{gCH_4}) during soil aeration

Reynolds number in the vadose zone (Re_{gCH_4}) is estimated by:

$$Re_{gCH_4} = \frac{\rho_{gCH_4} u_{pgCH_4} d_{50}}{\mu_{gCH_4}} \quad \text{Eq. D. 1}$$

$$u_{pgCH_4} = \frac{u_{DgCH_4}}{\phi S_{gCH_4}} \quad \text{Eq. D. 2}$$

where ρ_{gCH_4} is the density of CH₄ (kg/m³), u_{pgCH_4} is the pore CH₄ velocity (m/s), d_{50} is the representative grain diameter (m), μ_{gCH_4} is the CH₄ dynamic viscosity (Pa·s), u_{DgCH_4} is the Darcy velocity of CH₄ (m/s), ϕ is porosity (-), and S_{gCH_4} is the gas saturation of CH₄.

Fig. D. 9 shows the distribution of Re_{gCH_4} in the vadose zone induced by active airflow during soil aeration. Before aeration (T=0 min), Re_{gCH_4} is negligible in the vadose zone. During aeration (T = 30 and 60 min), Re_{gCH_4} elevated and developed only in the near-bar-hole region, where pressure gradients and pore-gas velocities are highest, while Re_{gCH_4} decrease rapidly away from the aeration bar hole. The region of Re_{gCH_4} is slightly broader in sand than in silt loam, consistent with stronger induced gas flow in the higher-permeability soil. These results support the use of a Darcy flow representation for gas flow in the vadose zone under the simulated soil aeration conditions.

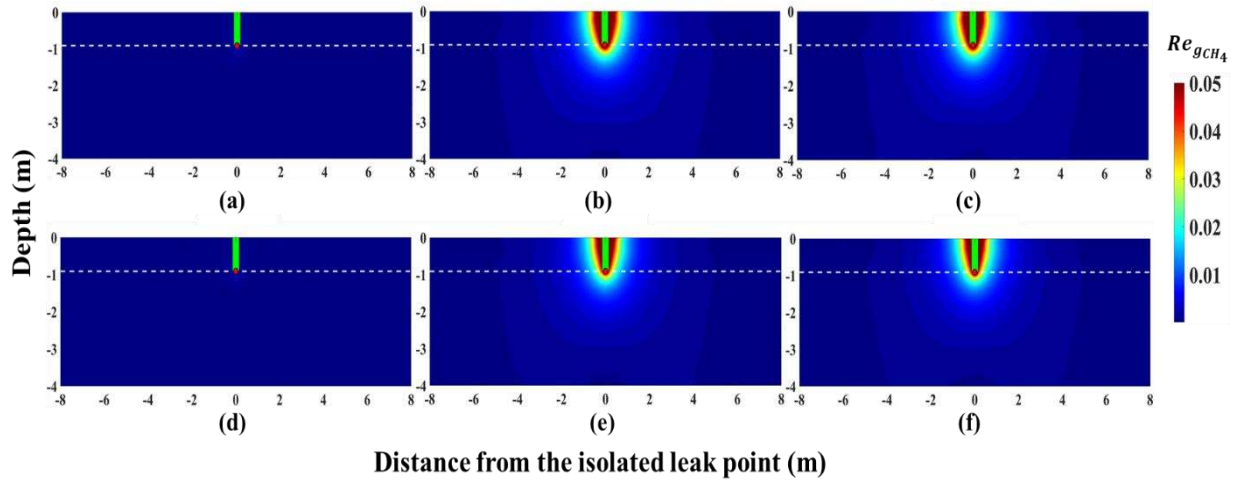


Fig. D. 9. Cross-section plots of Reynolds number of subsurface CH_4 ($Re_{g\text{CH}_4}$) in sand (a–c) and silt loam (d–f) for Cases #1 before ($T = 0$ min) and during ($T = 30$ and 60 min) soil aeration. Before aeration ($T = 0$ min), $Re_{g\text{CH}_4}$ are negligible throughout the vadose zone. The green squares represent the bar holes for scenarios with a single bar hole. The vacuum pressure (P_b) at each aeration bar hole is 0.9 atm. The S_w is 0.2 . The white dashed line indicates the pipeline at 0.91 m below the ground surface. The red circle represents the isolated leak point. The colorbar shows the range of $Re_{g\text{CH}_4}$.

Fig. D. 10 shows that the maximum $Re_{g\text{CH}_4}$ for the single-bar-hole in both sand and silt loam increases rapidly after aeration and reaches a near-steady level. Only minor changes are observed over the aeration period, indicating that the induced pore-gas flow field is established quickly after vacuum application and that the overall flow regime remains stable thereafter. For both soils, the maximum $Re_{g\text{CH}_4}$ increases with vacuum pressure. This trend indicates that stronger pressure gradients induced by vacuum pressure cause higher pore-gas velocities near the aeration bar hole, which increase the local maximum $Re_{g\text{CH}_4}$. The maximum $Re_{g\text{CH}_4}$ in sand is slightly higher than that in silt loam, suggesting that sand with higher permeability and better gas connectivity allows stronger localized induced gas flow, producing larger local $Re_{g\text{CH}_4}$. In contrast, the silt loam with lower permeability restricts pore gas movement and therefore maintains lower maximum $Re_{g\text{CH}_4}$.

values. The $Re_{g_{CH_4}}$ in sand shows a slight decline after the initial peak, whereas $Re_{g_{CH_4}}$ in silt loam case remains nearly constant after the initial rise. Furthermore, the maximum $Re_{g_{CH_4}}$ for both soils remain well below 1 for all vacuum pressures and throughout the full aeration period. Therefore, these results also support that the flow condition of gas flow in the vadose zone can be described by Darcy's law.

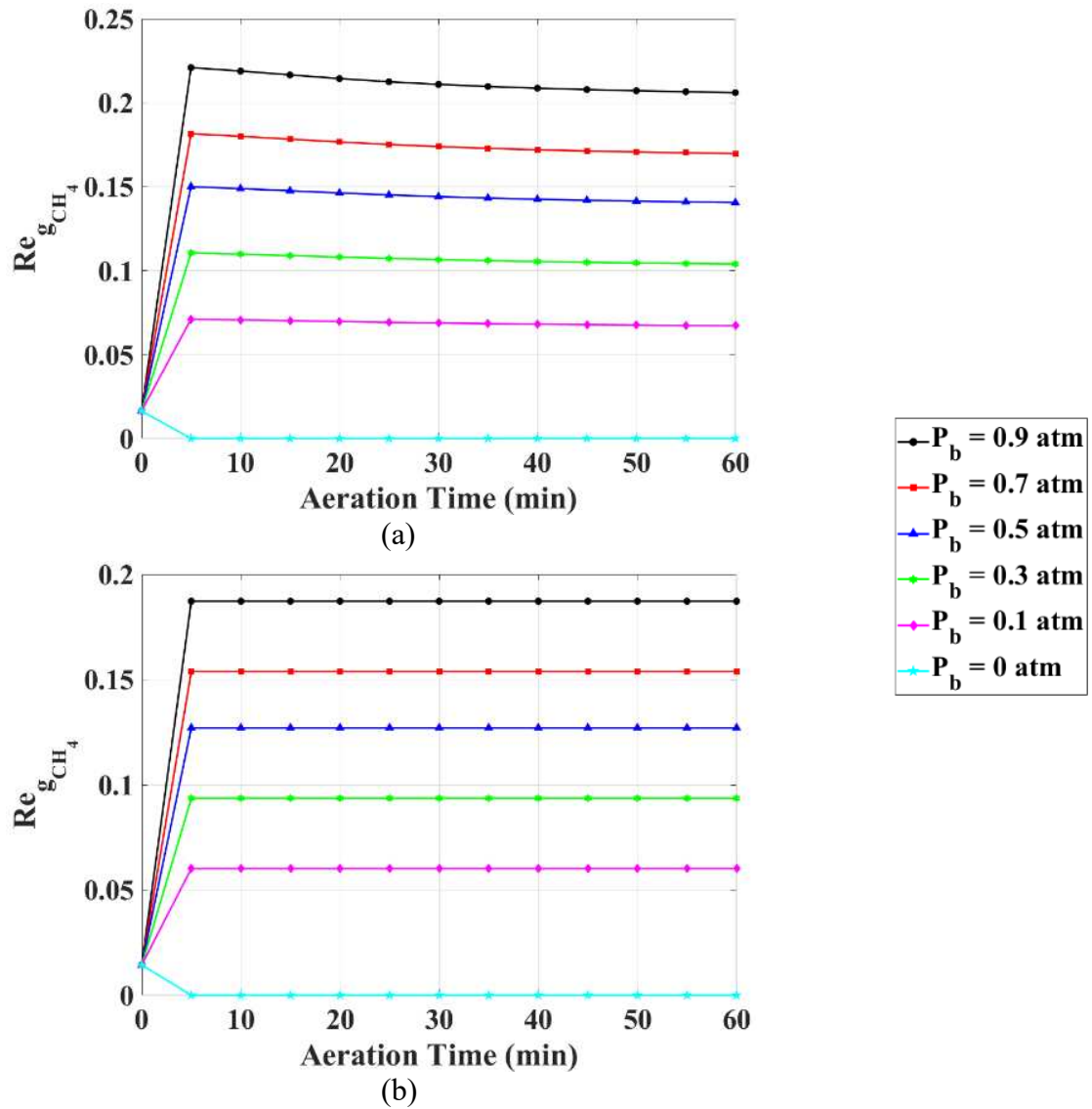


Fig. D. 10. Maximum Reynolds number of subsurface CH_4 ($Re_{g_{CH_4}}$) for Case #1 (a single bar hole) with vacuum pressures (P_b), ranging from 0 to 0.9 atm, in (a) sand and (b) silt loam.

Appendix. E. Reduced-order Physics-Based Framework Supplementary

This appendix compiles the engineering calculations used to translate the modeling and experimental insights into practical soil-aeration design. The purpose is to provide transparent, reproducible derivations for estimating airflow, CH₄ removal capacity, and system layout requirements as functions of plume size, aeration duration, and soil conditions. These calculations serve as a bridge between mechanistic transport behavior (e.g., pressure-driven flow and advection–diffusion competition) and field-operational decisions such as compressor selection, achievable removal rates, expected aeration duration, and bar-hole placement.

Section E.1 describes van Genuchten model to illustrate the relationship between soil water saturation and permeability in the vadose zone. Section E.2 derives the radial Darcy velocity field and the corresponding aeration flow rate under specified pressure conditions. Section E.3 defines the maximum removal flow rate (i.e., the upper bound on aeration capacity under assumed constraints) and the assumptions used to compute it. Section E.4 presents the framework for estimating CH₄ removal efficiency across a range of plume sizes and aeration durations, enabling direct comparison among design scenarios. Section E.5 uses the same framework to estimate the aeration duration required to meet a specified concentration or mass-removal criterion. Finally, Section E.6 provides calculations for recommended bar-hole spacing as plume dimensions and soil properties vary, offering a consistent method for scaling aeration layouts to site-specific conditions.

E. 1. Van Genuchten Model

The soil water retention curve (SWRC) is a fundamental soil hydraulic property that relates soil water matric potential (or capillary pressure) to volumetric water content (or water saturation). In this study, the SWRC is represented using the van Genuchten (1980) formulation, which has been widely adopted to describe saturation-dependent capillary behavior in variably saturated porous media. The normalized (effective) water saturation, S_e , is expressed as

$$S_e = \begin{cases} \left[1 + \left(\alpha \frac{p_c}{\rho_w g} \right)^n \right]^{-m}, & p_c > 0 \\ 1, & p_c \leq 0 \end{cases} \quad (\text{E.1})$$

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{gr}} \quad (\text{E.2})$$

where S_e (–) is the effective water saturation, S_w (–) is water saturation, S_{wr} (–) and S_{gr} (–) are the residual saturations of water and gas, respectively. p_c (Pa) is capillary pressure (defined as $p_g - p_w$), ρ_w (kg/m³) is water density, and g (m/s²) is gravitational acceleration. The parameters α (m⁻¹) and n (–) are van Genuchten fitting parameters, and m is commonly defined as

$$m = 1 - \frac{1}{n} \quad (\text{E.3})$$

Saturation-dependent relative permeabilities for water and gas are described using the Mualem–van Genuchten relationships:

$$k_{rw} = S_e^l \left[1 - (1 - S_e^{1/m})^m \right]^2 \quad (\text{E.4})$$

$$k_{rg} = (1 - S_e)^l (1 - S_e^{1/m})^{2m} \quad (\text{E.5})$$

where k_{ri} ($i = w, g$) denotes the relative permeability of phase i (water or gas), and l (–) is the pore-connectivity (tortuosity) parameter (often treated as an empirical constant = 0.5).

E. 2. Radial Darcy velocity and aeration flow rate calculation

This appendix provides the governing equations used to estimate the radial Darcy velocity and the volumetric aeration flow rate at each bar hole. The derivation is based on Darcy's law under radial flow conditions and incorporates soil hydraulic properties through the van Genuchten model. These relationships allow the estimation of aeration flow rate under field conditions or during pilot pressure testing.

Radial Darcy Velocity

The airflow induced by a bar hole is assumed to be homogeneous and isotropic within the radial aeration zone. Under this assumption, the radial Darcy velocity at the bar-hole interface, u_w , is calculated using:

$$u_w = \frac{k}{2\mu} \left(\frac{P_w}{R_w \ln \left(\frac{R_w}{R_I} \right)} \right) \left[1 - \left(\frac{P_{RI}}{P_w} \right)^2 \right] \quad (\text{E.6})$$

where k (m^2) is the intrinsic soil permeability, μ is the dynamic viscosity of air ($= 1.8 \times 10^{-4} \text{ g m}^{-2} \text{ s}^{-2}$), P_w (atm) is the applied vacuum pressure at the bar hole, R_w (m) is the radius of the bar hole, R_I (m) is the radius of influence, P_{RI} (atm) is the vacuum pressure at the radius of influence (assumed to be 1 atm)

Volumetric Aeration Flow Rate

The total aeration flow rate (Q_w) delivered by a bar hole is computed using:

$$Q_w = H \left(\frac{\pi k}{\mu} \right) \left(\frac{P_w}{\ln \left(\frac{R_w}{R_I} \right)} \right) \left[1 - \left(\frac{P_{RI}}{P_w} \right)^2 \right] \quad (\text{E.7})$$

where H (m) is the bar-hole depth

E. 3. Maximum removal flow rate

Fig. E. 1 illustrates how the number of bar-holes (N_{bh}) and vacuum pressures impact maximum removal flow rate ($RF_{CH_4_{max}}$) for dry and wet near-surface conditions. Color variation for $RF_{CH_4_{max}}$ shows that increasing the vacuum pressure under both dry and wet soil conditions with a constant number of bar holes increases $RF_{CH_4_{max}}$. In contrast, at constant vacuum pressure, additional bar holes are required to achieve higher removal capacities. Compared between dry and wet near-surface conditions, a combined effect of soil water saturation and bar-hole configuration is observed when evaluating the removal flow rates. For example, to reach a removal flow rate of 100 g/min, aeration under dry soil conditions requires approximately two bar holes at a vacuum pressure of 0.3 atm. However, under wet near-surface conditions, achieving the same removal capacity requires over five bar holes at the same vacuum pressure. This difference suggests that high near-surface water saturation impedes gas migration and reduces the effective pore space for CH_4 transport, lowering the achievable removal rate.

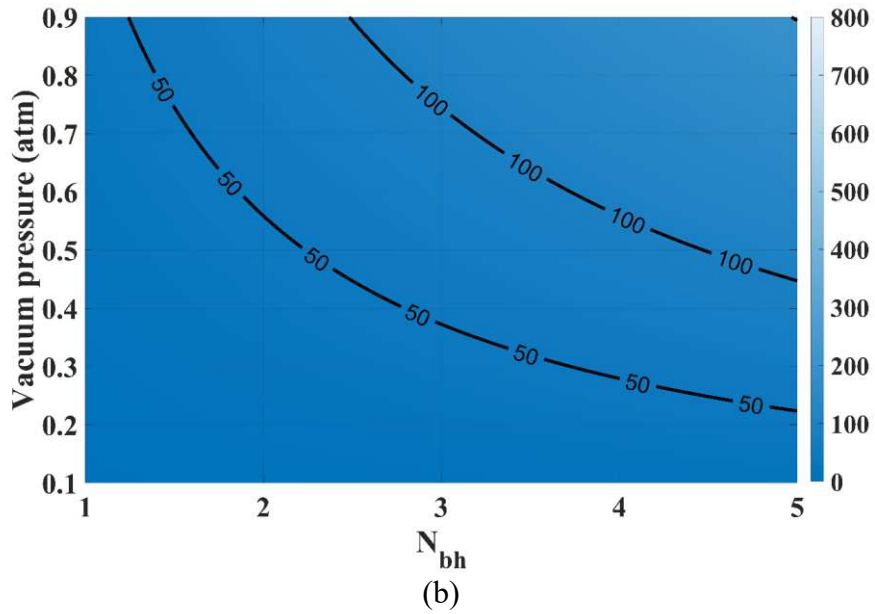
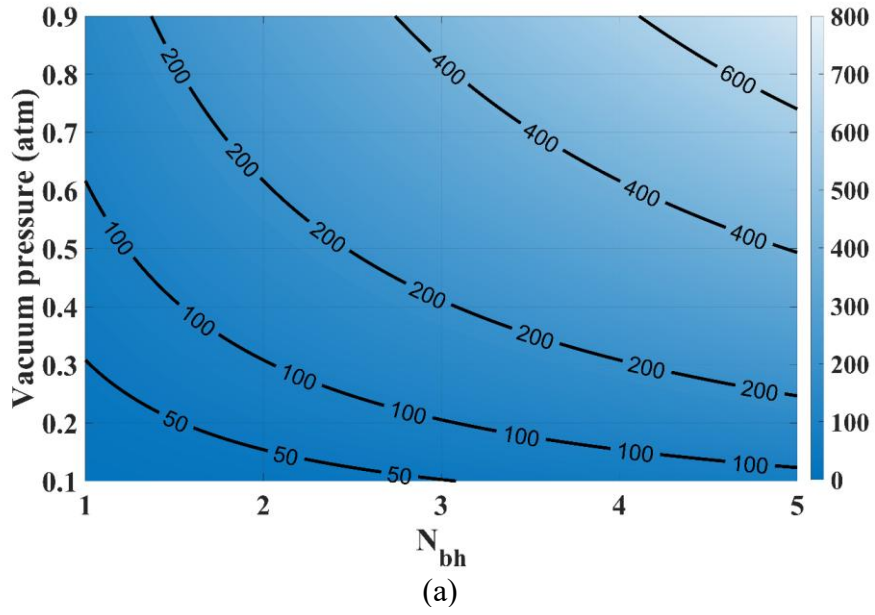


Fig. E. 1. Estimated maximum removal flow rate ($RF_{CH_4_{max}}$) with vacuum pressures from 0.1 to 0.9 atm and number of bar holes from 1 to 5 for (a) dry soil with average water saturation of 0.1 and (b) wet near-surface with average water saturation of 0.80. The estimations were represented with the initial CH_4 concentration of 100 vol.%.

Fig. E. 2 presents the estimated maximum removal flow rate across CH_4 concentrations ranging from 0 to 100% by volume for all scenarios in controlled experiments with a vacuum pressure of 0.3 atm. The results reflect the plume geometry observed in the controlled experiments, which had an average diameter of 2.6 m. The values were calculated using Eq. 6 in the reduced-order approach, which relates the volumetric aeration flow rate to the CH_4 mass transported from the subsurface. The results show that the maximum removal flow rate increases with increasing CH_4 concentration because higher gas concentrations produce a stronger advective mass flux toward the bar hole. These estimations provide an upper bound on achievable aeration rates for given subsurface CH_4 concentrations and serve as practical inputs for determining appropriate bar-hole numbers, aeration duration, and expected removal performance in field applications.

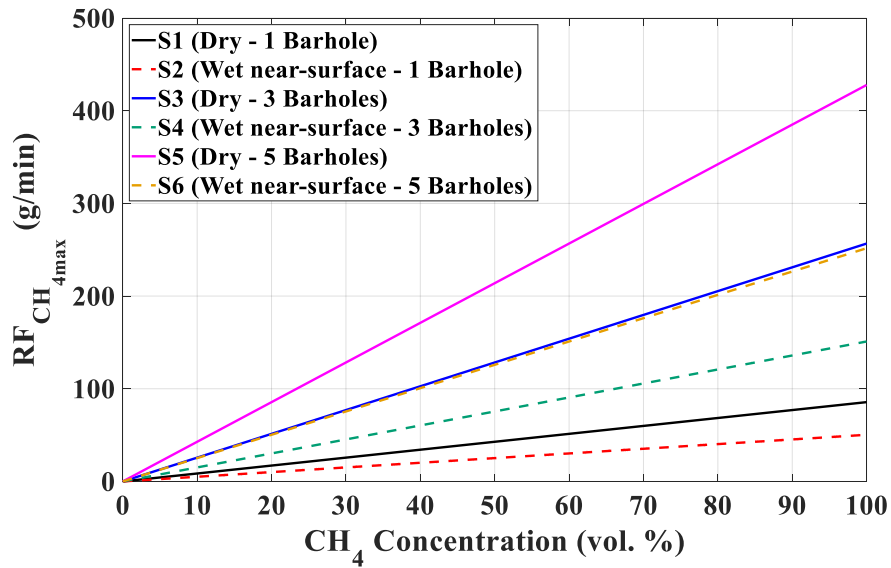


Fig. E. 2. Estimated maximum removal flow rate ($RF_{\text{CH}_4_{\text{max}}}$) with residual CH_4 concentration (vol.%) ranging from 0 to 100 vol.% in six aeration scenarios. The vacuum pressure is given as 0.3 atm (5 psi). The estimations were represented with the subsurface gas plume in the controlled experiments with an average diameter of 2.6 m.

E. 4. Estimated CH₄ removal efficiency across plume sizes and aeration durations

Fig. E. 3 and Fig. E. 4 presents the estimated Re_{MCH_4} for a fixed plume size of $L_{CH_4} = 2$ m across a range of bar-hole numbers (1-5), soil water saturations (dry = 0.1 and wet = 0.8), and vacuum pressures between 0.1 and 0.9 atm as a variation in aeration duration T_c (1-120 minutes). The results show that increasing vacuum pressure enhances the aeration capacity of each bar hole and leads to faster and higher subsurface CH₄ removal. For example, in dry soil with one bar hole, Re_{MCH_4} reaches 80% at $T_c = 23$ minutes when the vacuum pressure is 0.3 atm, whereas the same removal level is achieved at 12 minutes when the vacuum pressure increases to 0.8 atm. The increase in Re_{MCH_4} is also impacted by the number of bar holes. Higher N_{bh} expands the high-efficiency region represented by the dark red color in Fig. E. 3 and Fig. E. 4, indicating that the required aeration duration to achieve a target Re_{MCH_4} decreases as more bar holes are installed. However, at $T_c = 10$ minutes, increasing N_{bh} from one to two increases removal efficiency by 25%, whereas increasing from four to five advances only a 2% improvement. This diminishing increase also reflects overlapping aeration zones, which reduce the effective removal using additional bar holes. Soil water saturation is another factor impacting Re_{MCH_4} . Wet near-surface conditions create a barrier that suppresses upward gas migration and forces CH₄ to move laterally toward the bar holes. As a result, removal efficiency in wet near-surface soils is consistently higher and reaches target values more quickly. For the same plume size and bar-hole configuration, the time required to reach 95 % efficiency is approximately 80 minutes in dry soil, compared to only 25 minutes in wet near-surface conditions.

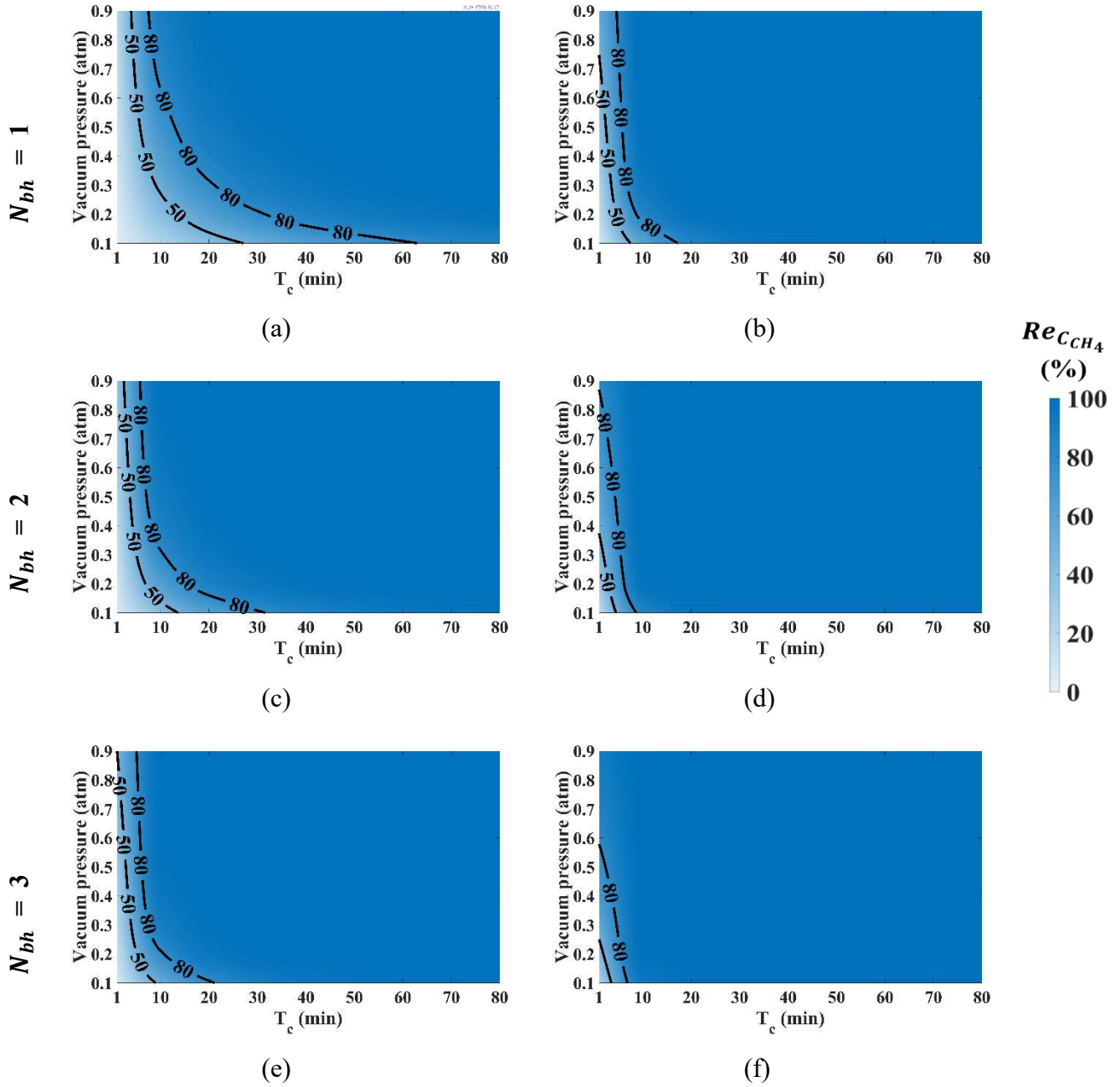


Fig. E. 3. Estimated removal efficiency (Re_{CH_4}) with vacuum pressures ranging from 0.1 to 0.9 atm and aeration duration (T_c) from 1 to 120 minutes for different numbers of bar holes (N_{bh}) and soil conditions. Panels (a, b), (c, d), and (e, f) present $N_{bh} = 1, 2$, and 3. The left panels (a, c, and e) represent dry soil with an average water saturation of 0.1, and the right panels (b, d, and f) represent wet soil with an average water saturation of 0.80. Color variations and contour lines

denote the estimated removal efficiency (%) calculated using Eq. 4.4 in the reduced-order approach. All estimations were represented with the CH₄ plume with an average diameter of 2 m.

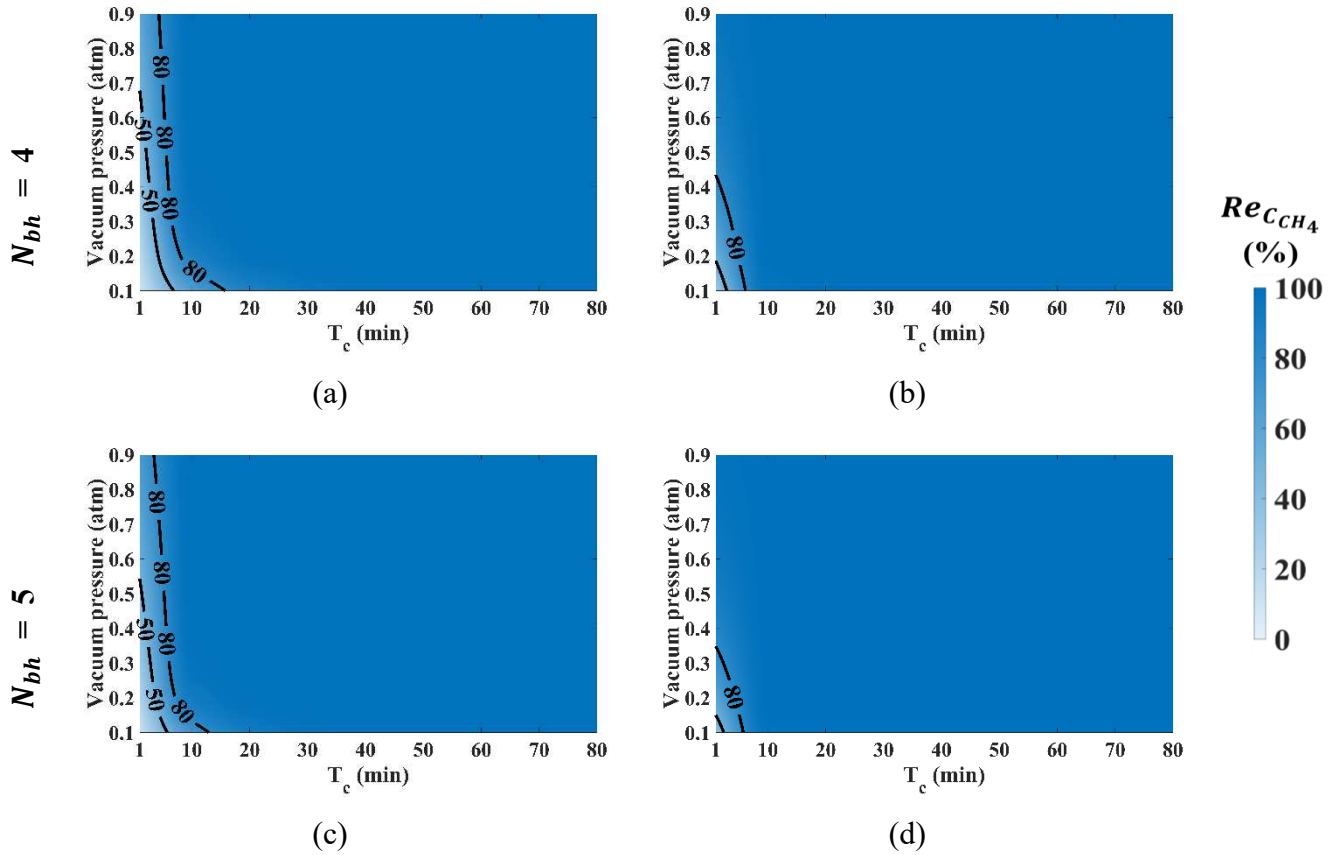


Fig. E. 4. Estimated removal efficiency (Re_{CH_4}) with vacuum pressures ranging from 0.1 to 0.9 atm and aeration duration (T_c) from 1 to 120 minutes for different numbers of bar holes (N_{bh}) and soil conditions. Panels (a, b) and (c, d) present $N_{bh} = 4$, and 5. The left panels (a and c) represent dry soil with an average water saturation of 0.1, and the right panels (b and d) represent wet soil with an average water saturation of 0.80. Color variations and contour lines denote the estimated removal efficiency (%) calculated using Eq. 4.4 in the reduced-order approach. All estimations were represented with the CH₄ plume with an average diameter of 2 m.

Fig. E. 5 and Fig. E. 6 presents the estimated CH₄ removal efficiency (Re_{MCH_4}) with plume diameters from 0.5 to 20 m and aeration durations from 1 to 120 minutes under dry and wet near-surface conditions at a constant vacuum pressure of 0.3 atm. Re_{MCH_4} increases with aeration duration due to cumulative advective gas transport, while larger plume sizes reduce the achievable efficiency within a given duration. A rapid increase in efficiency is observed during the first 30 minutes, after which the rate of improvement slows because most accessible CH₄ has already been removed. Increasing the number of bar holes (N_{bh}) enhances removal performance and expands the high-efficiency region ($Re_{MCH_4} > 80\%$). For example, the area exceeding 80% efficiency increases by more than 120% when the number of bar holes increases from one to five. The improvement is non-linear because overlapping aeration zones limit the additional airflow gained from adding more bar holes. Re_{MCH_4} is consistently higher under the tested plume geometries, saturation contrasts, and aeration configurations, which restrict upward migration and redirect gas laterally toward the bar holes. For instance, at a 4 m plume and two bar holes, Re_{MCH_4} is 68% in dry soil and nearly 99% under wet conditions at 30 minutes. Wet near-surface soils also accelerate removal, reaching 95% efficiency in about 25 minutes compared with 80 minutes in dry soil. These results highlight the combined influence of plume size, aeration duration, soil saturation, and bar-hole configuration on subsurface CH₄ removal performance.

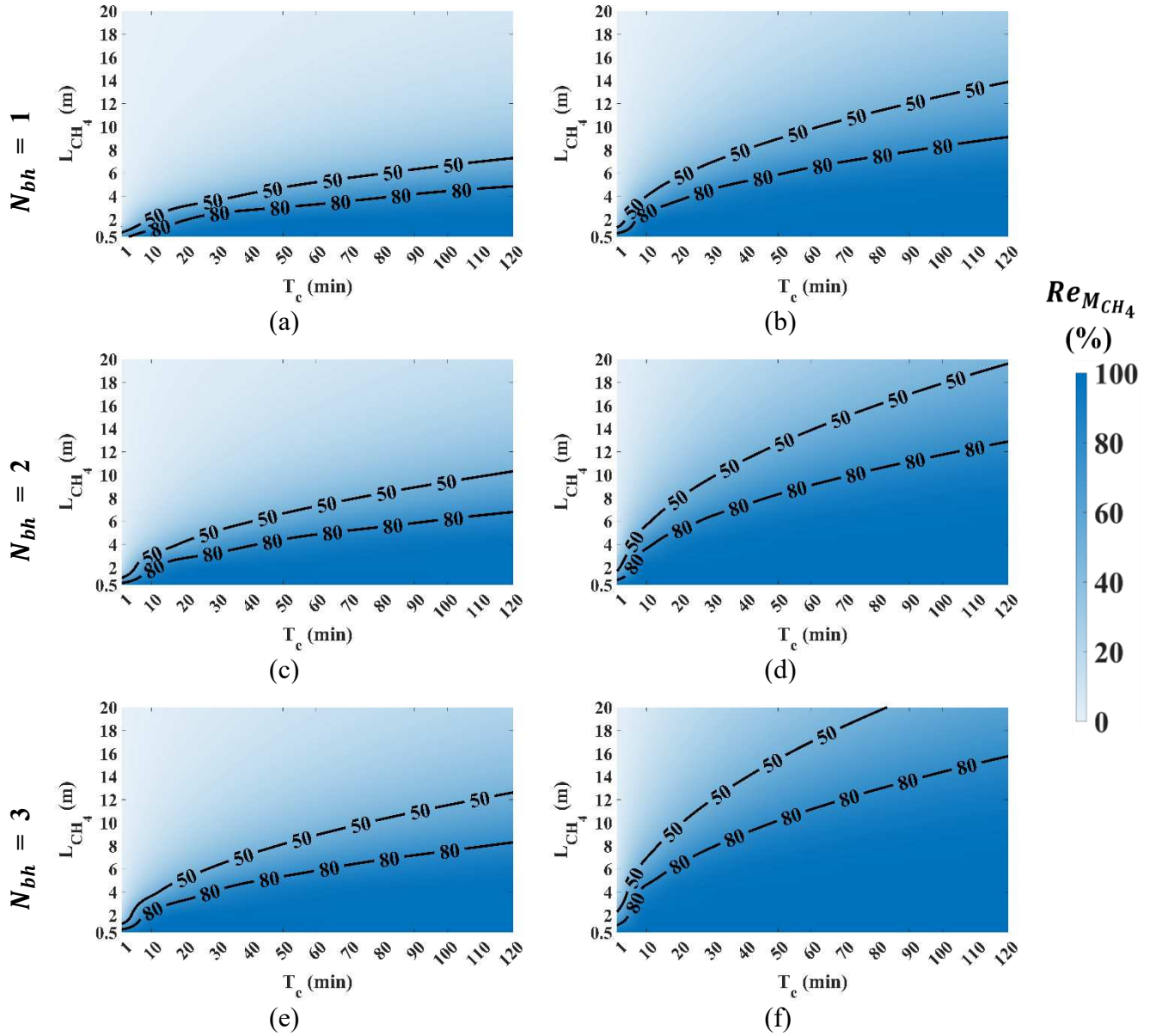


Fig. E. 5. Estimated overall removal efficiency (Re_{MCH_4}) with the average diameter of CH_4 plume (L_{CH_4}) ranging from 0.5 to 20 m and aeration duration (T_c) from 1 to 120 minutes for different numbers of bar holes (N_{bh}) and soil conditions. Panels (a, b), (c, d), and (e, f) present $N_{bh} = 1, 2$, and 3. The left contours (a, c, and e) represent dry soil with an average water saturation of 0.1, and the right contours (b, d, and f) represent wet soil with an average water saturation of 0.80. Color variations and contour lines denote the estimated removal efficiency (%) calculated using Eq. 4.4 in the reduced-order approach. All estimations were performed under a vacuum pressure of 0.3 atm (5 psi).

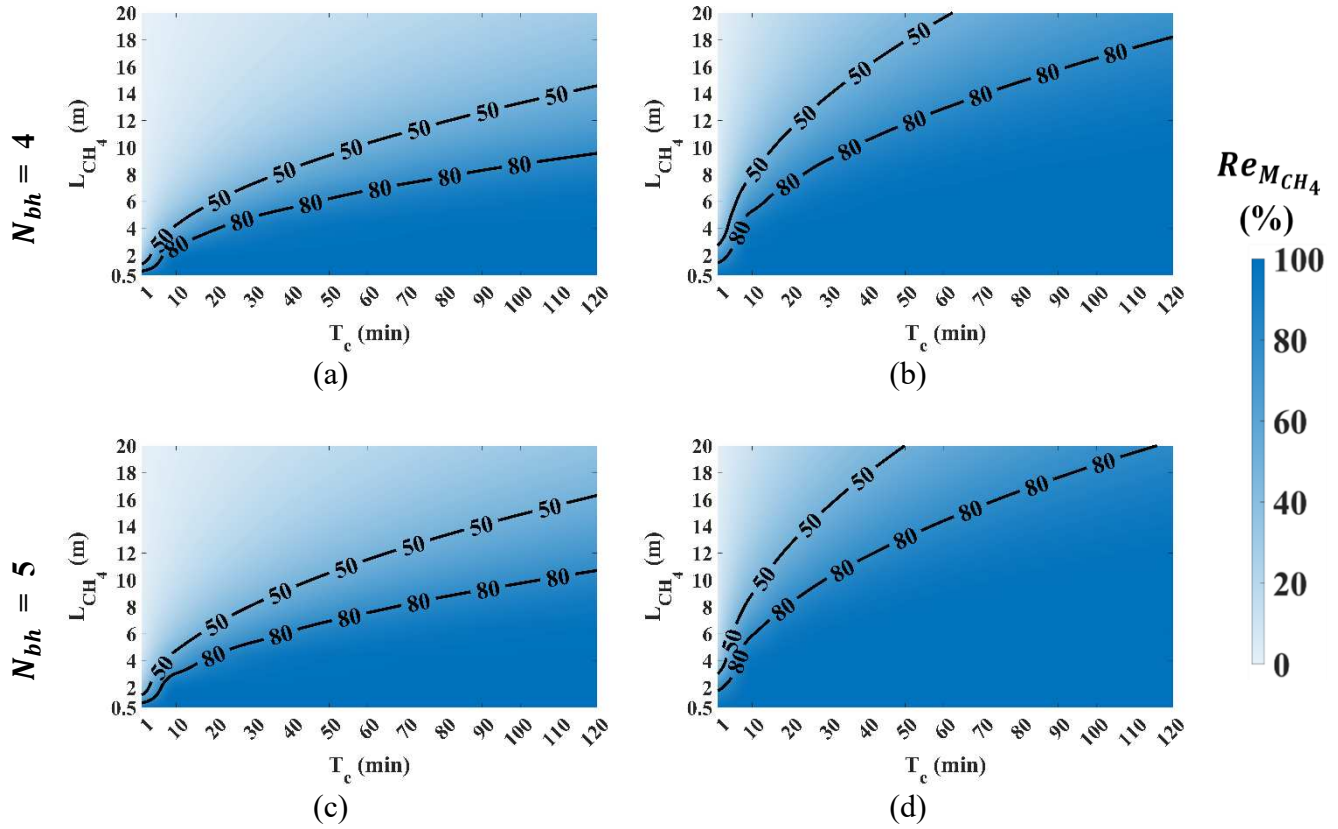


Fig. E. 6. Estimated overall removal efficiency (Re_{MCH_4}) with the average diameter of CH_4 plume (L_{CH_4}) ranging from 0.5 to 20 m and aeration duration (T_c) from 1 to 120 minutes for different numbers of bar holes (N_{bh}) and soil conditions. Panels (a, b) and (c, d) present $N_{bh} = 4$ and 5. The left contours (a and c) represent dry soil with an average water saturation of 0.1, and the right contours (b and d) represent wet soil with an average water saturation of 0.80. Color variations and contour lines denote the estimated removal efficiency (%) calculated using Eq. 4.4 in the reduced-order approach. All estimations were performed under a vacuum pressure of 0.3 atm (5 psi).

E. 5. Estimated aeration duration

Aeration duration (T_c) is a key operational parameter for field implementation because it determines how long a NG soil aeration must be operated to reach the target CH_4 concentration. Fig. E. 7 and Fig. E. 8 present the estimated T_c for various combinations of soil water saturation, vacuum pressure, bar-hole number (N_{bh}), and plume diameter (L_{CH_4}). The threshold criterion of 50 ppm was used to determine T_c based on the operator guidance of field-scale NG soil aeration.

Overall, T_c decreases with increasing vacuum pressure and bar-hole number because higher vacuum pressure and larger bar hole number enhance advective airflow toward the bar holes and removal capacity. For example, under dry soil conditions with $L_{\text{CH}_4} = 2$ m Fig. E. 7a), T_c decreases from 10 minutes to 2 minutes when N_{bh} increases from one to five at a vacuum pressure of 0.4 atm. At the same plume size and $N_{bh} = 1$, increasing the vacuum pressure from 0.1 to 0.9 atm reduces T_c from 20 minutes to 2 minutes.

In addition, the subsurface CH_4 plume size affects T_c . Larger gas plumes require significantly longer durations to reach the same removal target because the CH_4 mass and transport distance increase with plume diameter. For instance, with $N_{bh} = 2$ and a vacuum pressure of 0.3 atm, a plume with $L_{\text{CH}_4} = 2$ m requires only 7 minutes to reach the threshold concentration, whereas a plume with $L_{\text{CH}_4} = 18$ m requires approximately 528 minutes. Furthermore, high near-surface water saturation at a depth of 10 cm restricts vertical CH_4 migration and directs gas laterally, resulting in faster removal. Therefore, fewer bar holes are needed under wet near-surface conditions to achieve the same removal target at the same vacuum pressure and plume size. For example, at a vacuum pressure of 0.6 atm, aeration in dry soil requires approximately two bar holes to reach the target concentration (Fig. E. 7a), whereas wet near-surface conditions achieve the same performance with one bar hole (Fig. E. 7b).

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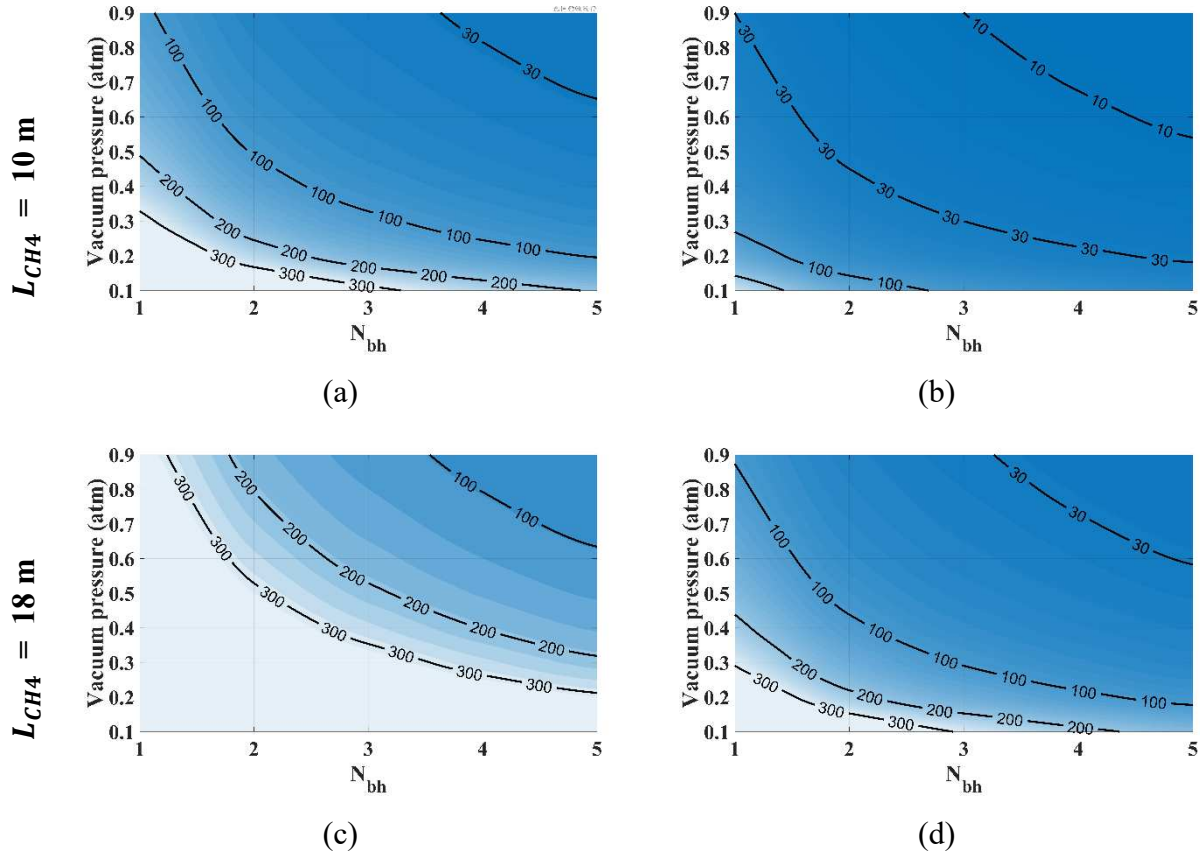


Fig. E. 8. Estimated aeration duration (T_c) with vacuum pressure ranging from 0.1 to 0.9 atm and the number of bar holes (N_{bh}) from 1 to 5 for different average diameters of CH_4 plume (L_{CH_4}). Panels (a, b) and (c, d) present $L_{CH_4} = 10$ and 18 m. The left contours (a and c) represent dry soil with an average water saturation of 0.1, and the right contours (b and d) represent wet soil with an average water saturation of 0.80. T_c (min) is estimated using Eq. 4. 9 with the target concentration of 50 ppm.

E. 6. Estimated bar-hole spacing under varying plume sizes and soil conditions

Fig. E. 9 and Fig. E. 10 present the estimated spacing between bar holes for two to five bar holes under dry soil ($S_w = 0.1$) and wet near-surface conditions ($S_w = 0.80$). The spacing calculations were conducted for plume diameters ranging from 0.5 to 20 m and aeration durations from 1 to 120 minutes at a constant vacuum pressure of 0.3 atm. The spacing values shown in the contours represent the minimum distance required to achieve a coverage rate greater than 95%, ensuring that the bar holes fully encompass the gas plume.

Across all configurations, optimal spacing decreases as the number of bar holes increases because the gas plume must be subdivided into smaller aeration regions. This geometric constraint requires bar holes to be placed closer together to maintain adequate overlap and avoid uncovered zones. The results also show that wet near-surface soils allow for slightly larger spacing than dry soils. Reduced air-filled porosity in the wet soil layer increases the effective aeration area of each bar hole, which permits greater spacing while still meeting the target coverage. In contrast, the higher air-filled porosity in dry soil reduces the lateral extent of each aeration zone, necessitating shorter spacing to achieve the same level of coverage. The contours further indicate that layouts with an odd number of bar holes contain a central bar hole, which improves symmetry and reduces the likelihood of an uncovered region near the plume center. This effect is most evident in the three and five bar-hole configurations, where the central bar hole enhances the consistency and robustness of the spacing requirement across different plume sizes.

The spacing maps provided in this section serve as a practical reference for determining bar-hole layouts under varying plume sizes, soil water saturations, and aeration durations. These results describe the spacing ranges that maintain sufficient plume coverage while minimizing unnecessary

overlap, enabling operators to select configurations that are both efficient and suitable for field constraints.

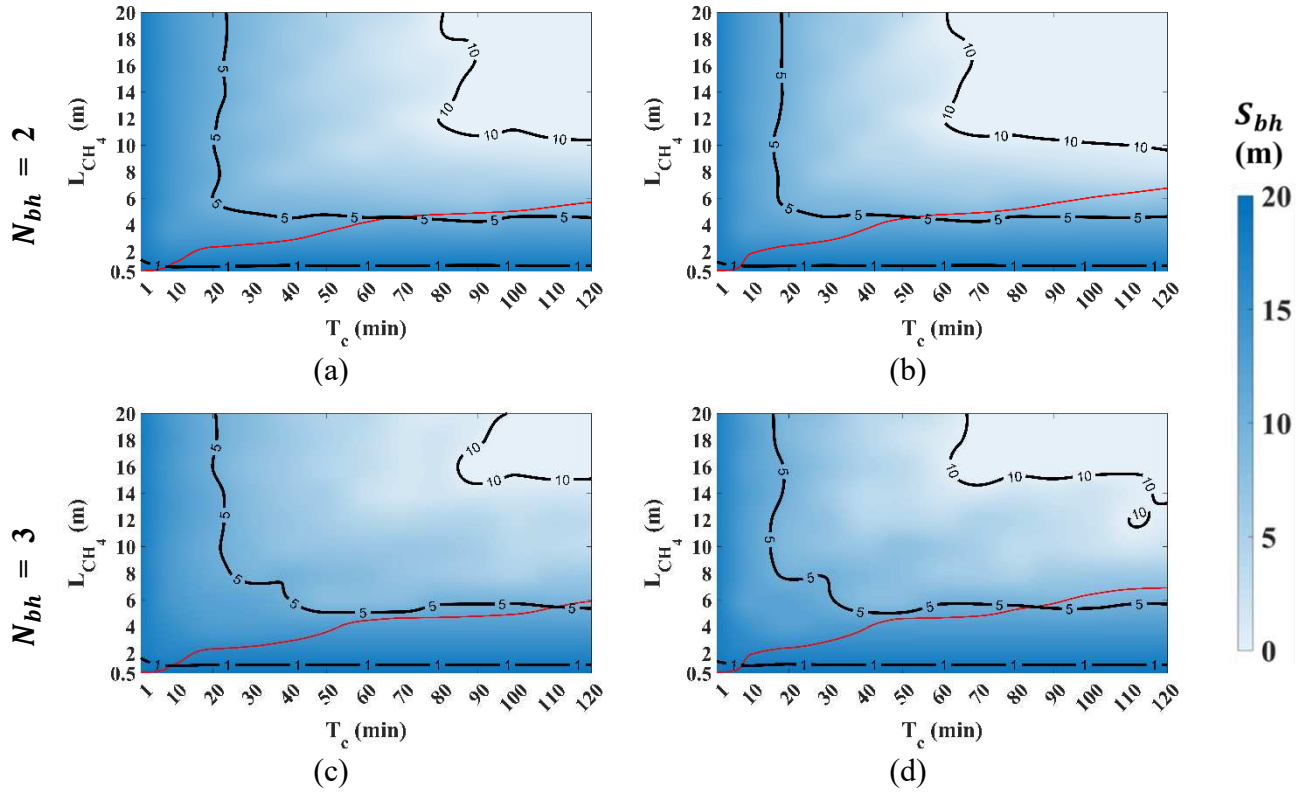


Fig. E. 9. Estimated spacing between bar holes (S_{bh}) for different numbers of bar holes (N_{bh}) and soil water saturations with the average diameter of the CH_4 plume (L_{CH_4}) ranging from 0.5 to 20 m and aeration duration (T_c) from 1 to 120 minutes. Panels (a, b) and (c, d) present $N_{bh} = 2$ and 3. The left contours (a and c) represent dry soil with an average water saturation of 0.1, and the right contours (b and d) represent wet soil with an average water saturation of 0.80. All estimations were performed under a vacuum pressure of 0.3 atm (5 psi).

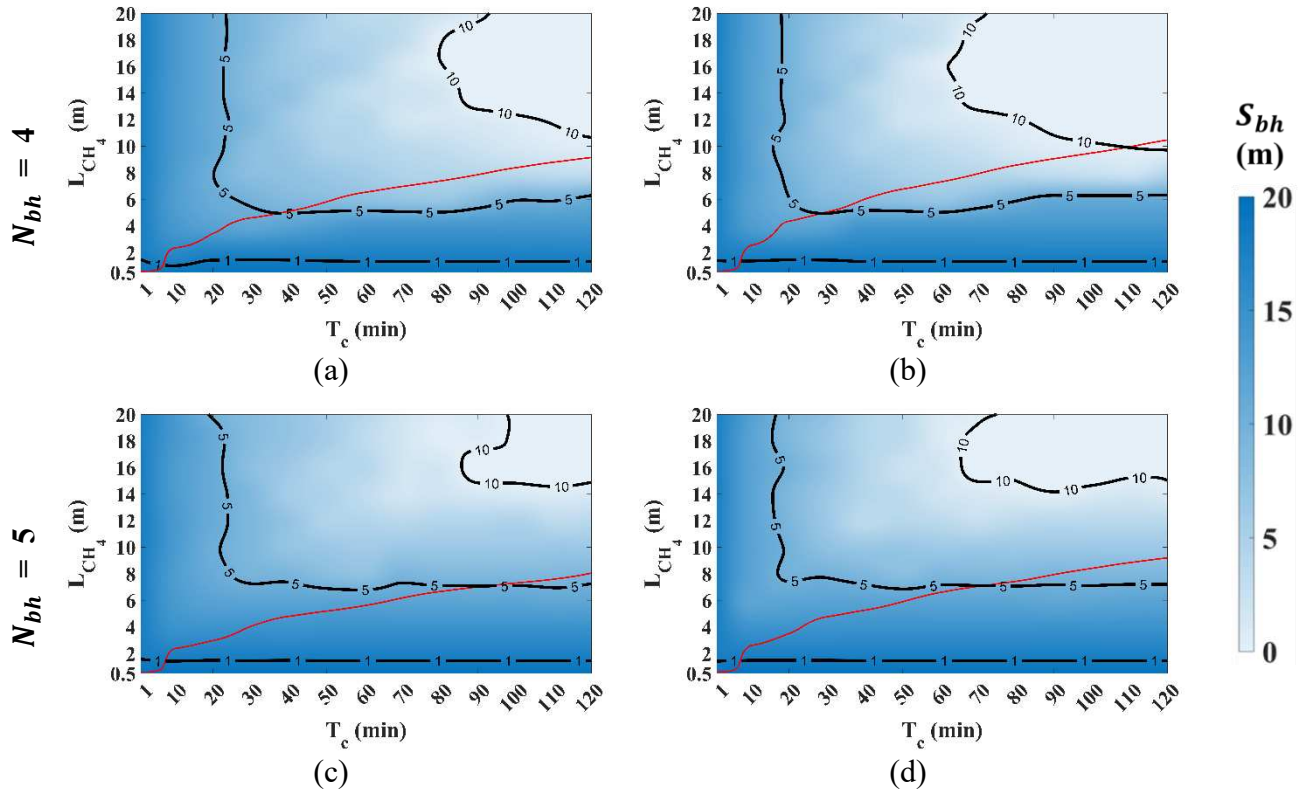


Fig. E. 10. Estimated spacing between bar holes (S_{bh}) for different numbers of bar holes (N_{bh}) and soil water saturations with the average diameter of the CH_4 plume (L_{CH_4}) ranging from 0.5 to 20 m and aeration duration (T_c) from 1 to 120 minutes. Panels (a, b) and (c, d) present $N_{bh} = 4$ and 5. The left contours (a and c) represent dry soil with an average water saturation of 0.1, and the right contours (b and d) represent wet soil with an average water saturation of 0.80. All estimations were performed under a vacuum pressure of 0.3 atm (5 psi).

E. 7. Sensitivity analysis of coverage rate (CR)

The 95% plume coverage rate threshold used to determine bar hole spacing was evaluated through a sensitivity analysis. The purpose of this analysis was to determine whether the selected threshold provides a practical balance between minimizing uncovered area and avoiding excessive overlap area among adjacent aeration zones. The threshold was not intended to represent a universal physical cutoff. Instead, it was used as an engineering design criterion to define near-complete plume coverage for field-scale NG soil aeration.

The uncovered area rate (UAR) was then calculated as:

$$UAR = 100\% - CR \quad \text{E. 8}$$

To evaluate redundant coverage, the overlap area rate (OAR) was calculated as:

$$OAR = \frac{A_{overlap}}{A_{plume}} \times 100\% \quad \text{E. 9}$$

where $A_{overlap}$ is the portion of the plume area covered by two or more aeration zones. A high OAR indicates greater overlap among adjacent bar hole aeration zones, which may reduce the efficiency of bar hole deployment because multiple bar holes are aerating the same plume region.

In the sensitivity analysis, the bar-hole spacing, UAR, and OAR were calculated using CR thresholds of 85%, 90%, 95%, and 99%. For each threshold scenario, aeration is conducted in sand using three bar holes, with a vacuum pressure of 0.4 atm and a water saturation of 0.1. The radius of the plume is 2 m. The aeration duration is 10 minutes. The results show that the 85% and 90% thresholds create the same bar-hole spacing under the tested scenario, leaving approximately 8.09% of the plume area uncovered. Although these lower thresholds reduced overlap, the remaining uncovered area may be less suitable for NG soil aeration because portions of the residual CH_4 plume could remain outside the effective aeration zones.

Increasing the threshold to 95% reduced the uncovered plume area to approximately 4.99%. This substantially decreased the non-aerated area compared with the 85% and 90% thresholds. The corresponding OCR increased to 67.16%, indicating greater overlap among aeration zones, but the overlap remained lower than that required by the 99% threshold. The 99% threshold further reduced the uncovered plume area to 2.89%. However, this improvement was accompanied by an increase in OCR to 84.07%, indicating substantially greater redundant overlap among adjacent aeration zones. This result suggests that a near-complete geometric coverage requirement can lead to a dense bar-hole layout and reduce removal efficiency, particularly when plume boundaries and bar-hole placement are subject to field uncertainty. Therefore, the 95% *CR* threshold is used as the design criterion to determine bar hole spacing. This threshold reduced the uncovered plume area to approximately 5%, while avoiding the substantial overlap ($OAR > 80\%$) associated with the 99% threshold. The results indicate that 95% provides a practical balance between adequate plume coverage and efficient bar hole deployment. The 95% threshold is interpreted as a field-applicable engineering criterion rather than a physically unique or universally optimal cut off.

Table E. 1. Estimated bar-hole spacing, uncovered area rate (UAR), and overlap area rate (OAR) for sand using three bar holes at water saturation of 0.2. The vacuum pressure is 0.4 atm. The aeration is conducted for 10 minutes. The radius of the plume is 2 m.

<i>CR</i> threshold (%)	Estimated bar-hole spacing (m)	UAR (%)	OAR (%)
85	1.97	8.09	46.12
90	1.97	8.09	46.12
95	1.58	4.99	67.16
99	0.54	2.89	84.07

Appendix. F. Supplemental Electronic Files

- The link to the experimental and simulated dataset in Chapter 2.zip can be found in <https://doi.org/10.18738/T8/SPE8QJ> .
- The link to the experimental and simulated dataset in Chapter 3.zip can be found in <https://doi.org/10.18738/T8/6NQJPI>.

Files	Contents	Description / Purpose
Chapter 2. zip	Input Parameters & Simulation Results.csv	Estimated transient belwoground NG leak rates, surface/BNS CH ₄ fluxes, atmospheric/soil resistances, response time, and optimal number of monitoring locations
	Experimental Data.xlsx	Surface/BNS CH ₄ concentrations, soil moisture/temperature, atmospheric conditions, and relative humidity
	Calibration Data.csv	Calibration results of 20 TGS 2611-E sensors
Chapter 3. zip	Simulation data.csv	Simulated advective/diffusive fluxes and CH ₄ concentration across soil types, vacuum pressure, soil moisture, and number of bar holes.
	Experimental data.csv	Measured subsurface CH ₄ concentration from INIR sensors, soil moisture/temperature, and atmospheric conditions
	Data processing code package (.mat)	Matlab script (.mat) for data processing, data visualization, and INIR calibration
Chapter 4. zip	Equations and framework concept.docx	A Word file includes the equations and concept of a reduced-order, physics-based framework.