Two-dimensional vapour intrusion model involving advective transport of vapours with a highly permeable granular layer in the vadose zone serving as the preferential pathway

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Response to reviews - Ms. Ref. No.: STOTEN-D-22-17016

We are highly indebted to the reviewers for the constructive comments on our manuscript entitled "Two-dimensional chlorinated vapour intrusion model involving advective transport of vapours with a highly permeable granular layer in the vadose zone serving as the preferential pathway". We have undertaken revision of our manuscript based on the comments and all changes are highlighted in the manuscript. Listed below are actions that we have taken in response to the comments by the reviewers on a point-by-point basis.

Reviewer #1: The authours only partially addressed my comments to the first version of the paper. In general, rewriting of the paper was quite limited, the minimum work required to address the issues raised in my review. Instead, the following points still need to be addressed:

Table 3: the choice of total, air filled and water filled porosity and soil air permeability has surely an influence on the results. I suggest to carry out a sensitivity analysis on this parameters so to assess their influence on the calculated indoor air concentration.
Section 3.2: given the comment above, it would be useful to show the results obtained with different permeability and porosities. The authours did not add any kind of the sensitivity analysis, stating that they will be published in another work with reference to a case study. My request was more general, to have more information on the response of the model to different inputs on key parameters, such as water filled porosity and soil permeability.

Author response: I have acknowledged the reviewer's comment and the manuscript has been revised by including a sensitivity analysis section on page 23 (line 373). The effect of different soil types and change in soil porosity and moisture is discussed in this section.

Section 3.1.1 and 3.1.2: Both these sections deal with the comparison of the developed model with other models. Nevertheless, I do not understand the significance of this comparison. Before, you state that few models address the issue of lateral dispersion but here you assume lateral distance of the building equal to zero. Given my comment above, different models/data are needed for the validation of the new proposed model. For example Feng et al. (JCH, 2020) report an analytical solution of a model for a layered soil laterally away from the edge of the source. The authours did not include any further comparison on this key issue of the proposed model, i.e. how the model simulates lateral dispersion. I still think that further validation is required. For this reason, I ask the authours a further step to improve the paper.

Author response: Thank you for the suggestion. Previously, the lateral distance was considered zero to take into account commonly used CSMs where a building is directly over a contaminant plume. However, to stick to the CSM considered in this study, the model verification is conducted by comparing the results of the normalised sub-slab concentration obtained from the current model with the results of analytical approximation method (AAM)

(Yao et al., 2013) and Abreu and Johnson's 3-D model (Abreu and Johnson, 2005) for different values of source-building lateral separation (page 16; line 267). Further validation of the model is limited due to the lack of published data with highly permeable granular layer as preferential pathway.

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Abstract

Vapour Intrusion (VI) is the process through which volatile organic compounds migrate from the subsurface source to the soil predominantly by diffusion, entering the overlying buildings through joints, cracks or other openings. This activity poses potentially serious health hazards for the occupants. Because of these health risks, recommendations for site closure are often made by quantifying the VI risks using mathematical models known as 'Vapour Intrusion Models' (VIM). Most of these VIMs seem to overlook the role of preferred pathways like utility lines, high conductivity zones of soil or rocks, etc., which act as the path of least resistance for vapour transport thereby increasing vapour intrusion risks. This study presents a two-dimensional (2-D) chlorinated vapour intrusion (CVI) model which seeks to estimate the source-to-indoor air concentration attenuation. It takes into account the effects of a highly permeable utility line embedment as a preferential pathway. The transport of 2-D soil gas is described using the finite difference method where advection serves as the dominant transport mechanism in the preferential pathway layer, while diffusion applies to the rest of the vadose zone. The model returned results comparable with other models for the same input parameters, and was found to closely replicate the results of 3-D models. The simulations indicate that the presence of highly permeable utility line embedment and backfill layers do trigger a higher indoor air concentration compared to a no preferential pathway scenario.

Keywords: Vapour intrusion; two dimensional model; preferential pathway; chlorinated hydrocarbons.

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1. Introduction

The conceptual site models (CSMs) help in identifying the pathways for vapour transport in the vadose zone and its entry into buildings. Conventional CSMs assume a 'soil VI pathway' in which vapours from a subsurface source emanate and diffuse vertically and/or laterally through the subsurface soil, which then intrudes into the indoor air typically through foundation pores, cracks or openings (Guo et al., 2015). However, the presence of alternate exposure pathways in the vadose zone like utility lines, naturally occurring fractures or macro pores, highly permeable soil layers or backfills etc. had been generally overlooked until recently. These alternative exposure pathways, known as preferential pathways, intersect with the vapour source or vapour migration pathways offer least resistance to soil vapour flow, subsequently and significantly increasing the risk of vapour intrusion (VI) (USEPA, 2002). The majority of vapour intrusion models (VIMs) currently in use have been developed with conventional CSMs but have often ignored the potential for vapour entry into indoor air scenarios through utility corridors, plumbing systems, etc., during VI investigations and developing VIMs. Failure to incorporate the role of preferential pathways into VI results in inaccurate predictions of indoor air vapour concentrations and wrong clean-up strategies.

The United States Environmental Protection Agency (US EPA) recommended a buffer zone of about 100 feet (or 30 m) vertically and laterally from the contaminant source, beyond which buildings can be deemed safe since no significant indoor air concentration had been found in them at a distance greater than one house lot (USEPA, 2002). Yet, in recent studies, VI impacts were detected in buildings even outside the footprint of the contaminant plume (Yao et al., 2017a) due to the presence of preferential pathways which offer little vapour attenuation and this leads to high indoor air concentrations. Most of the VI through preferential pathways are related to the interception of compromised or deteriorated sewer systems, primarily designed to carry wastewater to treatment plants, with the contaminant plume in vadose zone ultimately resulting in unhindered transport of volatile organic compounds (VOCs) into the indoor air through connected plumbing systems (Jacobs et al., 2015). Several field studies have been conducted in recent times confirming the role of sewers acting as a preferential pathway for soil vapour transport, resulting in significant indoor air contaminant concentrations even in buildings outside the groundwater plume area (Distler and Mazierski, 2010, Riis et al., 2010, Vroblesky et al., 2011, Pennell et al., 2013, Guo et al., 2015, McHugh et al., 2017, Guo et al., 2020, Beckley and McHugh, 2021). Additionally, VI episodes without a vadose zone source can occur from VOCs volatilising from industrial discharges which are directly discharged into sewer systems which contribute to higher indoor air contaminant concentrations (Roghani et al., 2018).

Many studies conducted on preferential pathways in VI focus on contaminant transport through sewers, utility tunnels and their associated plumbing conduits. However, the role of highly permeable soil layers and backfill materials in VI have rarely been investigated. The presence of any high permeability region in the vadose zone - either natural or anthropogenic - can function as a preferential pathway in contaminant vapour transport. These regions of high permeability can occur naturally as gravel layers or fractured rocks which facilitate higher contaminant flux owing to their higher porosity (USEPA, 2015b). As well, granular fill materials laid as bedding and embedment to utility lines can cause high contaminant flux laterally and vertically to the ground surface, and thereby serve as preferential pathways (ITRC, 2014).

The aim of this study is to develop and evaluate a 2-D model in order to estimate the indoor air concentration at sites contaminated with chlorinated hydrocarbons (CHCs) with a highly permeable gravel layer acting as a preferential pathway. The numerical model depicts: i) two-dimensional vapour flux (lateral and vertical directions) of chlorinated hydrocarbon contaminants; ii) the building of concern laterally situated at a distance from the edge of the contaminant plume; and iii) the presence of a highly permeable course grained soil layer such as gravel used as bedding for utility lines which act as preferential pathway for vapour transport.

This model: firstly, solves partial differential equations of diffusion and advection in the vadose zone with preferential pathway to estimate the total vapour flux; secondly, has a modular subroutine for simulating the effect of preferential pathway in vapour transport; and thirdly, estimates the indoor air concentration by 'continuous stirred tank reactor method' as employed in Johnson and Ettinger's (hereafter J&E) model. Evaluating the model's performance was carried out by comparing it with 1-D, 2-D and 3-D models using hypothetical as well as field data obtained from particular studies (Holton et al., 2013, Guo et al., 2015, Yao et al., 2017b).

2. Methodology

2.1. Model development

The numerical model took two stages to develop. First, a conceptual model was devised considering: i) the system as two-dimensional; ii) the building of concern placed laterally at a distance from the edge of the CHC contaminant plume; iii) a coarse grained utility line bedding, such as gravel, sand or crushed stone with high permeability acting as the path of least resistance for the contaminant vapour flux; and iv) foundation of the building as slab-on-grade and simulating the interaction between the sub-surface and the building. The purpose of this conceptual model is to illustrate the role of highly permeable bedding layers of utility lines in exacerbating the risk of VI in buildings located laterally at a distance from the edge of the contaminant plume. The general CSM developed for this study is depicted in Figure 1.

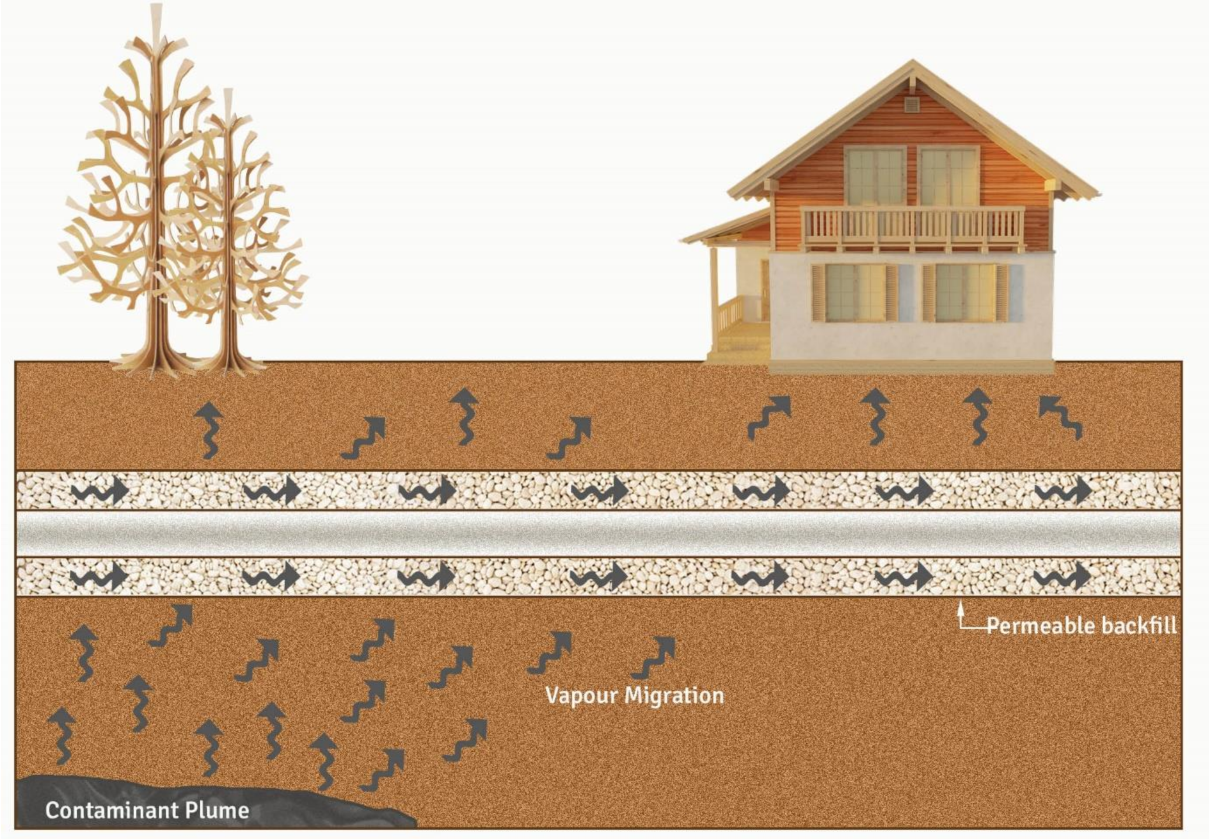
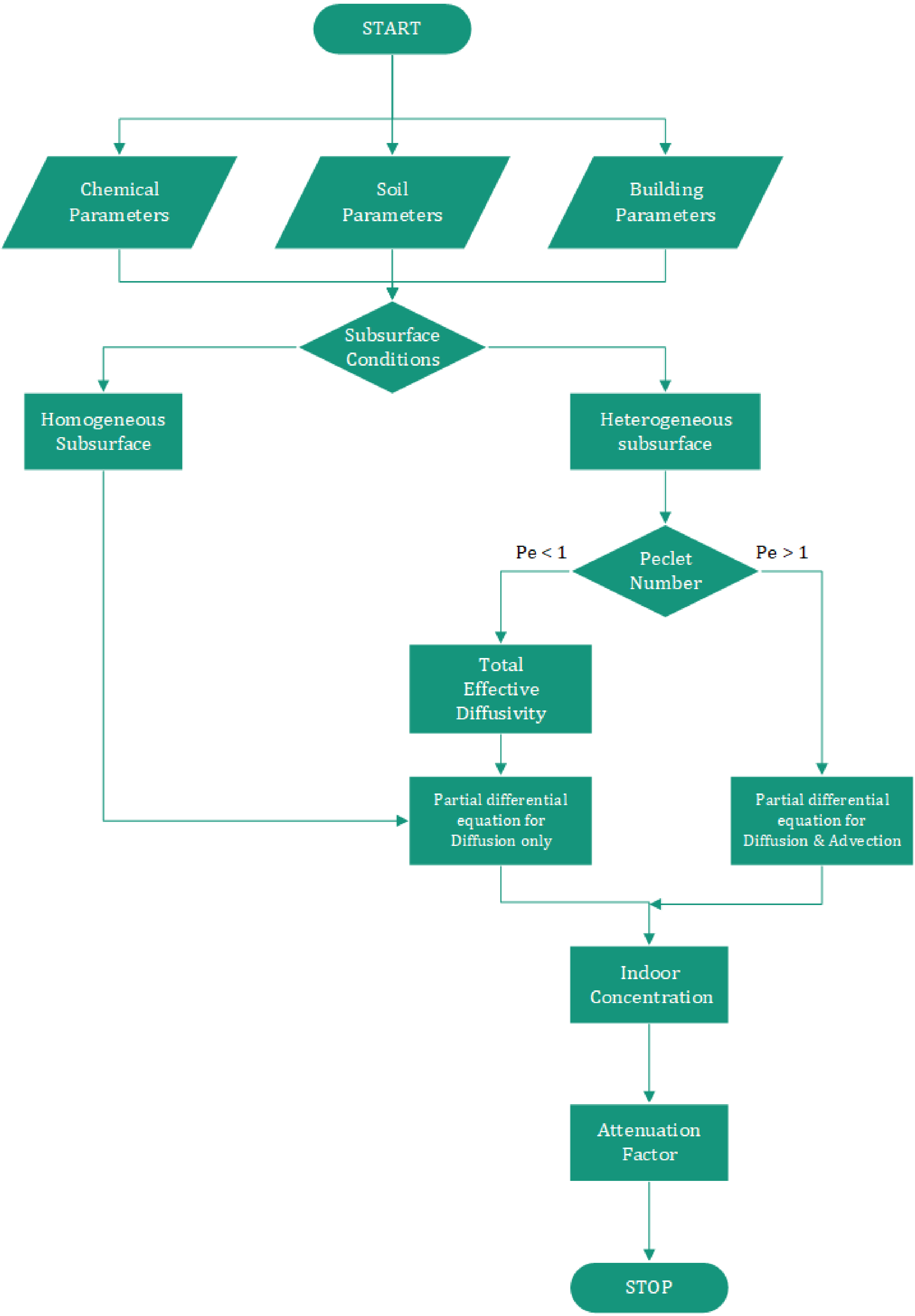


Figure 1. CSM developed for the study

In the second stage of model's development, governing equations were formulated and solved using the central difference scheme of the finite difference method and coded in Python programming language for simulating fate and transport of CHCs from source to the building foundations through sub-surface soil. The vapour entry into the building through the foundations and subsequent indoor air contaminant concentration is calculated using the 'continuous stirred tank reactor method' employed in the J&E model (Johnson and Ettinger, 1991).

Although there are several models which consider two-dimensional vapour transport, most of them assume diffusion is the dominant transport mechanism in the vadose zone but do not take into account the presence of a preferential pathway. Some guidance documents suggest the role of natural and induced high permeability zones in the vadose zone as preferential pathways, for instance gravel and sand lenses, vertically fractures rocks, etc., as well as highly permeable bedding or backfill layers of utility lines which are mostly situated close to the surface (USEPA, 2015a, ITRC, 2014). However, we know of few studies that have shown vapour migration through backfills or naturally occurring high permeability zones which this model seeks to address. When a significant pressure gradient is present, an upward advective soil gas transport might be induced which can be identified using Peclet number (Pe) (Yao et al., 2015). If $Pe > 1$, it is assumed that advection will be the dominant transport mechanism but it will be diffusion if $Pe < 1$. The flowchart shown in Figure 2 illustrates the steps involved in developing the 2-D model for simulation of CHC vapour transport in the presence of a highly permeable preferential pathway layer. This model calculates the indoor air concentration and attenuation factor by simulating the vapour transport in the vadose zone. It does this by considering diffusion as the dominant transport mechanism if $Pe<1$ and advection as the dominant transport mechanism if $Pe>1$ in the bedding and backfill layer.



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139 Figure 2: Overview of the 2-D model process with the preferential pathway

The major components involved in the model's methodology are: i) obtaining the vapour flux and contaminant concentration profile in the vadose zone; ii) determining the dominant transport mechanism in the backfill and bedding layer by computing Pe; iii) calculating vapour entry into the building using continuous stirred tank reactor method; and iv) computing indoor air concentration and attenuation factor based on the subsoil and building interaction. The effect of preferential pathways in three scenarios considered in this study are: i) preferential pathway closer to the source; ii) preferential pathway equidistant from the source and receptor; and iii) preferential pathway furthest from the source. Results of these simulations are then compared with a 'no-preferential pathway' scenario in order to fully understand the role of the highly permeable bedding layer in exacerbating the VI risk.

For refining the numerical model, the following assumptions are made. Firstly, the model operates under steady state conditions. The source concentration is considered to be constant and the vapour migration is deemed to be a steady-state process. Although the actual vapour migration is a transient process, the steady state scenario can express the most hazardous scenario. Secondly, the subsurface is assumed to be stratified due to the presence of the preferential pathway and each soil layer is homogeneous. Thirdly, the contaminant concentration decreases exponentially with lateral distance from the source. Fourthly, the utility line is leak-proof and does not act as preferential pathway. Fifthly, the effect of biodegradation is not taken into account since the rate of degradation of TCE is negligible without a growth substrate like methane (Choi et al., 2002). The vapour concentrations and subsequent indoor air concentration calculated under these assumptions can be overestimated compared to actual on-site measurement. Nevertheless, the model can be employed as a screening tool to address the VI problem with a preferential pathway.

2.2. Governing equations and boundary conditions

2.2.1. Transport by diffusion

The vapour transport in the vadose zone is assumed to be steady state diffusion except in the highly permeable preferential pathway layer. Since both lateral and vertical movement of the contaminant vapours are considered in a two-dimensional soil context, the governing equation for the transport of a non-reacting, non-adsorbing vapour through the vadose zone under steady state diffusion is explained by Laplace equation as given in eq. (1) (Yao et al., 2017b):

$$\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) = 0 \qquad \textbf{(1)}$$

where: x and y are lateral and vertical coordinates (m), respectively; and C denotes the contaminant vapour concentration (mg/L).

The effective vapour diffusion coefficient of the media, D_e (m^2/s), is calculated using the Millington-Quirk equation (1961) as given in eq. (2):

$$D_e = D_a \frac{\theta_a^{10/3}}{\theta_T^2} + \frac{D_w}{H}\frac{\theta_w^{10/3}}{\theta_T^2} \qquad \textbf{(2)}$$

where: D_a is the molecular diffusion coefficient in gas (m^2/s); D_w stands for the molecular diffusion coefficient in water (m^2/s); θ_T, θ_a & θ_w are total porosity, air filled porosity and water filled porosity, respectively; and H is the dimensionless Henry's law constant.

In a heterogeneous subsurface with *n* layers of soil, a total effective diffusion coefficient can be introduced ($D_{e,tot}$) as shown in eq. (3) which transforms the diffusion coefficients of individual soil layers of the subsurface into an equivalent homogeneous system (Johnson and Ettinger, 1991):

$$D_{e(tot)} = \frac{L}{\sum_{i=0}^{n} \frac{d_i}{D_{e(i)}}} \qquad (3)$$

where: L is the depth of vadose zone (m); d_i is the thickness of the *i*th layer (m); and $D_{e(i)}$ denotes the effective diffusion coefficient of the *i*th layer (m^2/s).

2.2.2. Transport by advection

In preferential subsurface pathways such as utility corridors, highly permeable soils or porous zones of rocks, the contaminant vapours tend to migrate via advection (USEPA, 2015a). A relatively small change in partial pressure can trigger significant advective vapour transport which is larger than the diffusive fluxes (Scanlon et al., 2002). The contaminant vapours reach the highly permeable granular fill in the vadose zone from the source. Meanwhile the pressure difference between the subsurface and open ground and the high soil permeability causes a change in vapour velocity. This can be calculated using eq. (4) as written below:

$$\boldsymbol{u_g = \frac{K_{bf}}{\mu}.\nabla P_w} \quad (4)$$

where: u_g is the average vapour phase velocity (m/s); K_{bf} is the soil air permeability of the granular backfill (m^2); μ stands for soil gas viscosity (Pa.s); and ∇P_w represents the vapour pressure gradient in the granular backfill (Pa), which is required as an independent input of the model.

Once the vapour velocity is obtained, the Peclet number can be computed using eq. (5) to confirm the dominant transport mechanism in the preferential pathway:

$$\boldsymbol{P_e = \frac{u_g.L}{D_{TCE}}} \quad (5)$$

where: u_g is the vapour velocity (m/s); L is the depth of preferential pathway layer (m); and D_{TCE} is the effective diffusivity of TCE in soil (m^2/s).

If Pe < 1, the dominant transport mechanism will be diffusion and the governing equation is given by eq. (1). If Pe > 1, the dominant transport mechanism will be advection for which the governing equation is given by eq. (6) as stated below:

$$\boldsymbol{-u_g\left(\frac{\partial C}{\partial x} + \frac{\partial C}{\partial y}\right) = 0} \quad (6)$$

For geological systems with permeability > 10^{-9} m^2, the contaminant transport can be simulated with advection equation (Yao et al., 2012).

2.2.3. Computation of indoor air concentration

The average indoor air concentration is calculated in this model using the 'continuous stirred tank reactor' method as employed in the J&E model. As per the technical VI guidance of US EPA (2015a), for a building laterally at a distance from the contaminant plume, the soil vapour concentration obtained from below the foundation closest to the source can help to describe the worst case scenario underneath the building. Hence the subslab concentration of vapours $C(x_{ck},d_s)$ closest to the edge of the contaminant plume is obtained from the simulations and is employed for the vapour entry and indoor air concentration calculations using eq. (7) to (14). The sub-slab crack concentration (C_{ck}) can be computed using eq. (7) as documented below:

$$\boldsymbol{C_{ck} = \frac{\pi D_e . d_s . t_{ck}}{D_a w_{ck}} C(x_{ck}, d_s)} \tag{7}$$

where: t_{ck} is the thickness of the foundation (m); w_{ck} is the width of the crack (m); x_{ck} is the distance of the foundation crack from the edge of contaminant plume and d_s is the depth of source from the foundation.

The indoor air contaminant concentration (C_{in}) can be calculated as a function of sub-slab crack concentration as given in eq. (8) using a series of empirical equations as stated in eq. (9) to eq. (14):

$$\boldsymbol{C_{in} = C_{ck} \left(\frac{R_{mix}}{R_{crack} + R_{mix}} \right)} \tag{8}$$

Where,

$$R_{mix} = \frac{1}{L_{mix} . ER} \tag{9}$$

and

$$R_{crack} = \left(R_{mix} - \frac{A_b}{Q_s}\right)(e^{-\varepsilon} - 1) \quad (10)$$

with

$$\varepsilon = \frac{Q_s}{A_b}\frac{t_{ck}}{D_a \eta} \quad (11)$$

$$\eta = \frac{w_{ck} l_{ck}}{A_b} \quad (12)$$

$$Q_s = \frac{2\pi K_a \Delta p l_{ck}}{\mu \ln\left(\frac{2d_f}{r_{ck}}\right)} \quad (13)$$

and

$$r_{ck} = \frac{\eta A_b}{l_{ck}} \quad (14)$$

where: L_{mix} (m) denotes the height of the building at which contaminant mixing occurs; ER (1/hr) is the building air exchange rate; A_b (m^2) stands for the foundation area in contact with the soil; Q_s (m^3/s) is the convective soil vapour entry rate into the building; d_f (m) is the depth of foundation below ground surface; η represents the foundation crack fraction; l_{ck} (m) is the foundation perimeter; K_a (m^2) is the soil air permeability; μ (Pa.s) is the soil gas viscosity; and Δp (Pa) is the pressure difference between building and soil.

The sub-slab-to-indoor air concentration attenuation factor (α), which relates indoor air vapour concentration (C_{in}) to the source vapour concentration (C_s) can be calculated using eq. (15):

$$\alpha = \frac{C_{in}}{C_s} \quad (15)$$

2.2.4. Boundary conditions

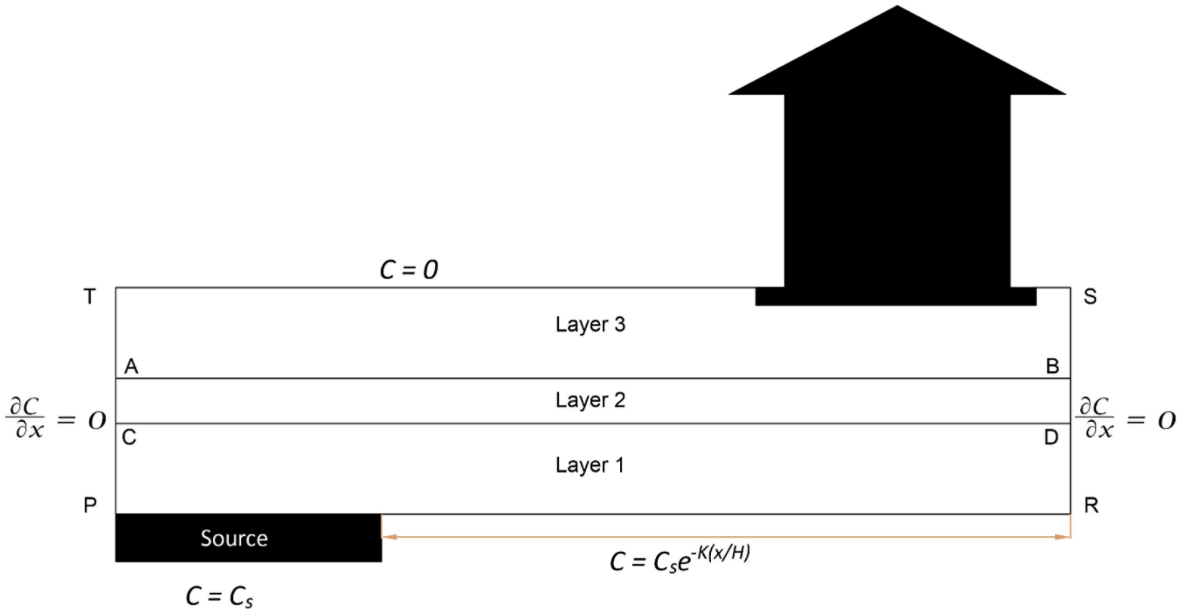


Figure 3. Boundary conditions employed for the CSM

Figure 3 depicts the boundary conditions for the solution of the transport equations in the vadose zone. The conceptual model assumes concentration at source to be C_s while the concentration at ground surface is zero. The left-hand and right-hand side boundaries of the domain are assumed to have no flux boundary condition, i.e. $\frac{\partial C}{\partial x} = 0$ where concentration attenuation is linear. Beyond the edge of the source, the concentration tends towards zero at large lateral distances and the concentration attenuation is exponential which is satisfied by $C_s e^{-K(\frac{x}{H})}$, where: x is the lateral distance from source (m); H is the depth of source (m); and K is the decay rate constant.

Boundary condition for advection process in the highly permeable preferential pathway is established by considering the system as three separate layers. The values obtained by solving eq. (1) in layer 1 with the corresponding boundary conditions becomes the boundary condition for layer 2 (CD in fig.3). With ∇P_w as independent input in the model, the calculated soil vapour velocity (u_g) will determine Pe which in turn determines the vapour transport mechanism in layer 2. If Pe>1, the transport mechanism will be advection and the system will solve for eq.

(6) for the whole layer (until AB in fig. 3). This in turn will serve as the boundary condition for layer 3 which will solve for diffusion equation for that layer.

3. Results and Discussion

3.1. Comparison with existing models

The capability of VI assessment by the developed model is conducted by comparing the results of the normalised sub-slab concentration obtained from the current model with the results of analytical approximation method (AAM) (Yao et al., 2013) and Abreu and Johnson's 3-D model (Abreu and Johnson, 2005). The calculated vapour concentration at the near edge of the foundation bottom is regarded as the sub-slab concentration. The data adopted for model comparison is obtained from Yao et al., (2013) for a building foundation depth of 0.2 m and source depth 8 m for different values of source-building separation. The results of the three methods are compared in figure 4. With respect to the change in contaminant sub-slab concentration in lateral direction, the developed model follows the trend of other models, particularly when compared with the 3-D model, which implies that the developed model may provide an alternative method of assessing VI risk.

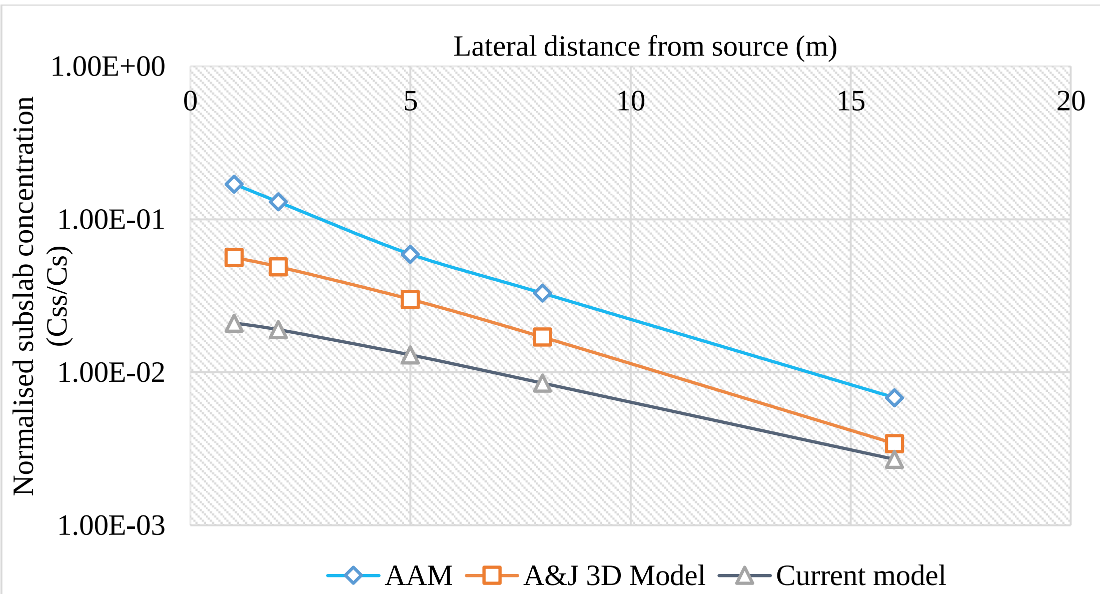


Figure 4. The plot of normalised sub-slab concentration (C_{ss}/C_s) vs Lateral distance from the edge of the source for AAM, 3-DM and current model.

3.2. Simulated scenarios

3.2.1. Effect of preferential pathway

To understand the effect of highly permeable granular fill in the vadose zone in exacerbating VI risks, a scenario is simulated by using a granular backfill comprising well graded gravel that is 0.5 m in depth. It functions as the preferential pathway at a depth of 1 m from the ground surface, where the primary transport mechanism is advection. The building of concern has its closest point from the edge of the contaminant plume of concentration 1 g/m^3 at an arbitrarily chosen distance of 3 m. The rest of the vadose zone other than the preferential pathway is assumed to consist of sandy clay where diffusion is assumed to be the primary transport mechanism. The specifications related to pipe embedment and backfilling is consistent with Standard drawings SCP-1000 and SCP-1001 of the Standard Technical Specifications for Construction of Sewer Rising Mains by Hunter Water Corporation (2005).This is then compared to a 'no-preferential pathway' scenario where the vadose zone is considered homogeneous with sandy clay soil where diffusion is the only soil transport mechanism. Biodegradation is not accounted for in the simulations since the contaminant of interest is TCE which is normally difficult to biodegrade in soil. The input parameters used in the simulations are reported in Table 1.

Table 1. Input parameters for the model simulations.

Chemical Parameters		***Unit***	***Value***
Source vapour concentration	C_s	g/m3	1
Diffusion coefficient in air	D_a	m2/s	7.90E-06
Diffusion coefficient in water	D_w	m2/s	9.10E-10
Henry's law constant	H	-	0.403
Soil gas viscosity	μ	Pa.s	5.32E-04
Soil Parameters			
Total Porosity	Θ_T	-	0.385
Air filled porosity	Θ_a	-	0.188
Water filled porosity	Θ_w	-	0.197
Soil air permeability	K_a	m^2	1.70E-13
Granular backfill soil parameters			

Depth of backfill	ds	m	0.5
Total Porosity	Θ_T	-	0.5
Air filled porosity	Θ_a	-	0.49
Water filled porosity	Θ_w	-	0.01
Soil air permeability	K_a	m^2	1.00E-09
Building parameters			
Width of foundation slab		m	10
Foundation footprint area	A_b	m2	100
Depth of foundation below grade	d_f	m	0.3
Thickness of foundation crack	t_{ck}	m	0.1
Width of foundation crack	w_{ck}	m	0.001
Foundation perimeter	l_{ck}	m	40
Building height	L_{mix}	m	3
Building Air exchange rate	ER	h^{-1}	0.5
Soil and building pressure difference	Δp	Pa	5

From the simulations, it was observed that there was a considerable increase, virtually double the amount, in sub-slab as well as indoor air concentrations in the presence of a highly permeable preferential pathway layer when compared to the 'no-preferential pathway' scenario. Table 2 shows the contrasts in vapour concentration in the sub-slab and indoor air and the attenuation factor with and without the preferential pathway. Based on these results, it is clearly evident that the presence of preferential pathway indeed increases the potential risk of VI.

Table 2. Comparison of sub-slab concentration, indoor air concentration and attenuation factor with and without the preferential pathway for different scenarios.

	Without preferential pathway	*With preferential pathway*
Source concentration (g/m^3)	1	1
Sub-slab concentration (g/m^3)	0.025	0.048
Indoor air concentration (g/m^3)	3.86E-05	7.40E-05
Attenuation factor (α)	3.86E-05	7.40E-05

This increase in indoor air contaminant concentration can be attributed to the limited attenuation occurring in the preferential pathway. Advection is assumed to be the dominant transport mechanism in the preferential pathway layer, so the vapour movement occurs at a faster rate.

This is comparable to the rest of the vadose zone where vapour transport occurs due to diffusion, hence offering the least resistance for soil gas transport and subsequently less attenuation. Figure 5 presents the vapour concentration profile in the vadose zone which shows the increase in vapour concentration in the preferential pathway layer as opposed to that of a ‘no-preferential pathway’ scenario. It proves that the preferential pathway offers the least resistance to vapour transport in the vadose zone and ultimately results in exacerbation of VI.

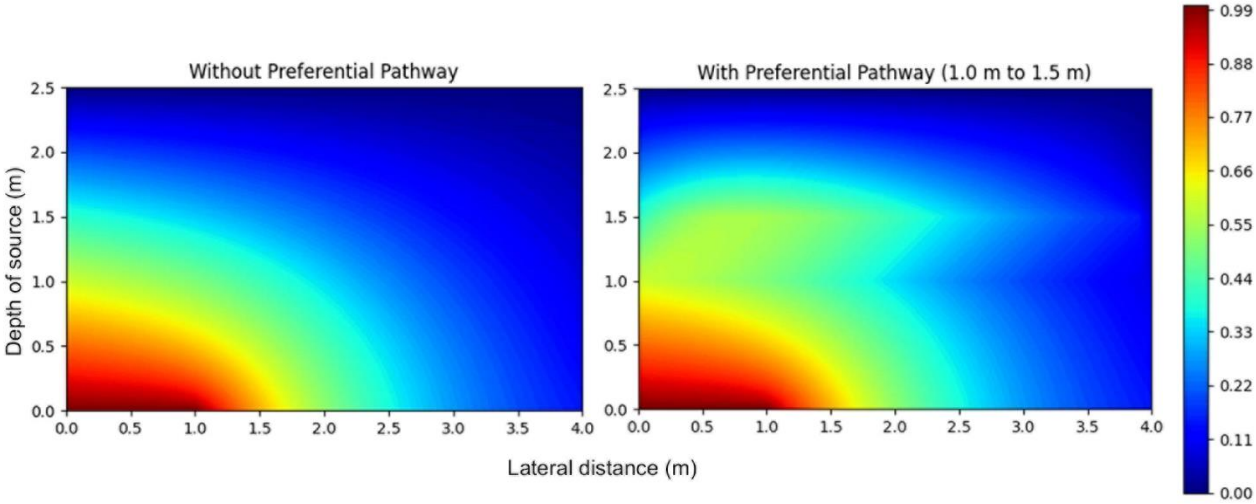


Fig. 5: Comparison of vapour concentration profile in the vadose zone with and without the preferential pathway for the same scenario.

3.2.2. Influence of depth of source from preferential pathway

Simulations were conducted to understand the effect of proximity of the source to the preferential pathway by varying the depth of source (0.5 m, 1 m, 2 m, 4 m & 8 m) from the preferential pathway, retaining the remainder of the vadose zone conditions and the input parameters the same as that of the previous simulation. The closer the source is to the preferential pathway, the distance of vapour transport in soil before reaching the preferential pathway diminishes, resulting in less vapour attenuation. This causes a high vapour concentration to enter the preferential pathway which then travels with comparatively least resistance till the upper layer of soil with lesser attenuation, leading to an increase in indoor air concentration. Similarly, when the source is further away from the preferential pathway, more vapour travels through the soil resulting in more vapour attenuation before reaching the preferential pathway. As a result of this, comparatively less vapour concentration enters the preferential pathway and the increase in indoor air vapour concentration abates when compared to the scenario where the source is close to the preferential pathway. In Figure 6 it can be observed that when the source was at a depth of 0.5 m from the preferential pathway, a 200% increase in indoor air concentration was obtained when compared to the same scenario without preferential pathway which then gradually fell to almost 150% when the depth was increased to 8 m.

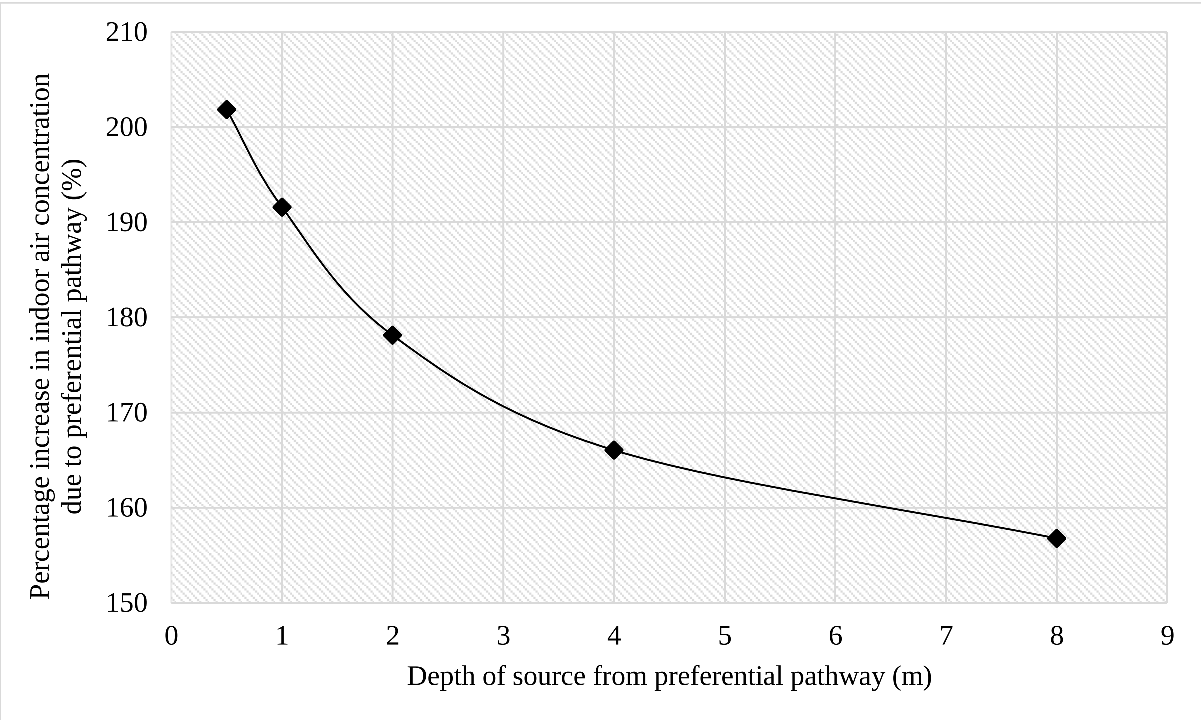


Fig. 6. Increase in indoor air concentration with preferential pathway for different depths of source to preferential pathways.

The reduction in indoor air concentration can be attributed to the higher vapour attenuation occurring in the soil before reaching the preferential pathway due to an increase in depth. As the depth increases, the vapour concentration entering the preferential pathway decreases and vice versa. Figure 7 demonstrates the concentration profile of the vadose zone for different depths of source from the preferential pathway.

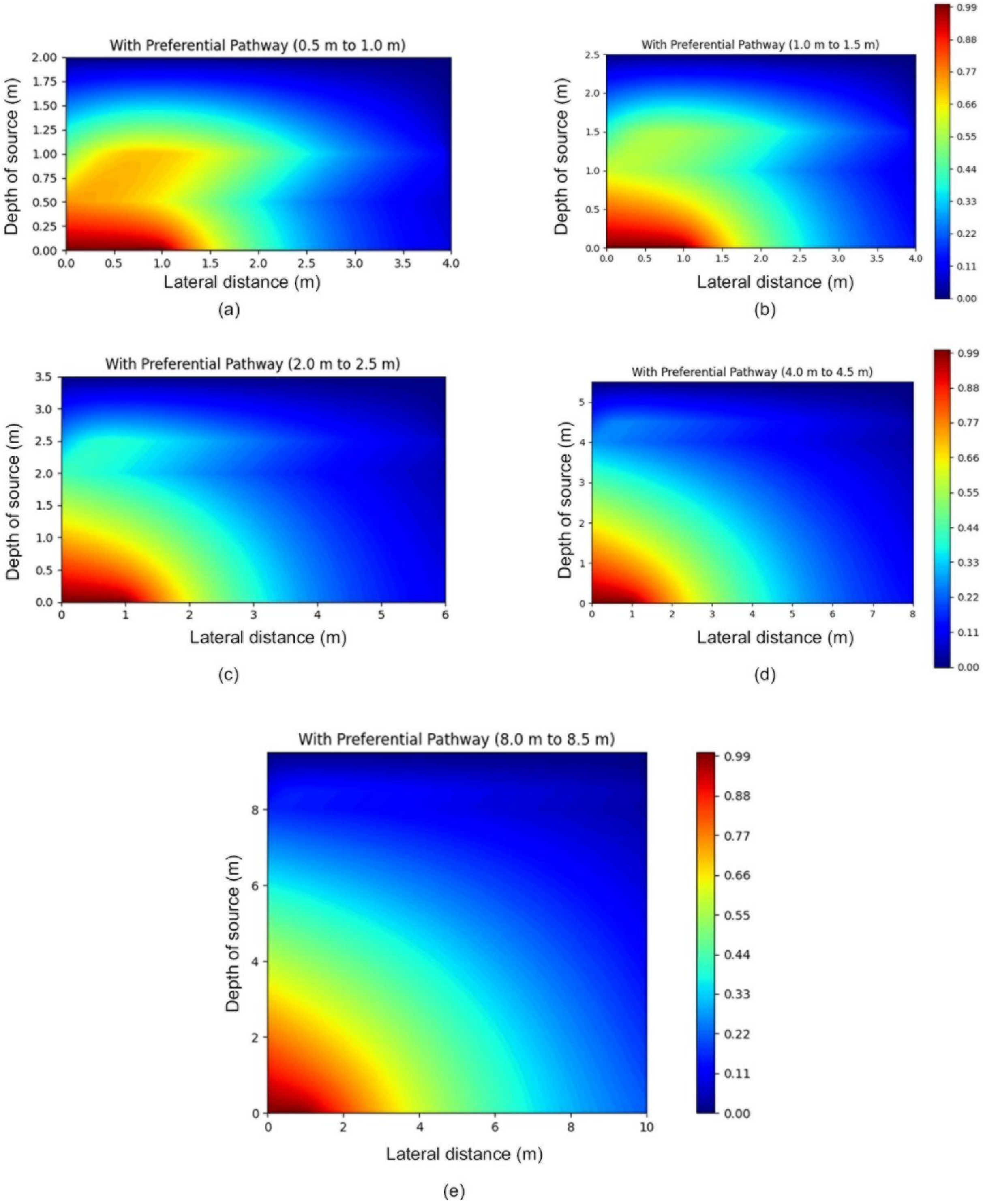


Figure 7. Vapour concentration profiles of the vadose zone for different depths of source from preferential pathway

3.2.3. Effect of lateral distance of building from the source

In order to understand the effect of lateral distance in vapour attenuation when preferential pathway was present, simulations were conducted to compare the indoor air concentrations with and without preferential pathway. Taken into account here was the building of concern at varied lateral distances from the edge of the contaminant plume. The simulations were executed considering the scenario similar to that of the first simulation but with different source to building lateral distances. A vadose zone of sandy clay soil had a depth of 2.5 m with a highly permeable preferential pathway of thickness 0.5 m at a depth of 1 m from the ground surface and the contaminant source of concentration 1 g/m^3 at a depth further 1 m from the bottom of the preferential pathway layer. For the scenario without preferential pathway, the vadose zone is considered homogeneous with sandy clay soil at a depth of 2.5 m from the ground surface. The input parameters for the simulations are same as those reported in Table 3.

It was observed that the indoor air concentration was larger in the presence of the preferential pathway as expected, but the latter's effect was significant only for a few meters laterally as shown in Figure 8. As the source to building distance increases, the effect of preferential pathway in exacerbation of VI reduces until it plays no consequential role in increasing the indoor air concentration at large lateral distances. This can be attributed to the general tendency of the vapour to move rapidly in a vertical direction, and thereby crossing the preferential pathway with least resistance vertically than laterally.

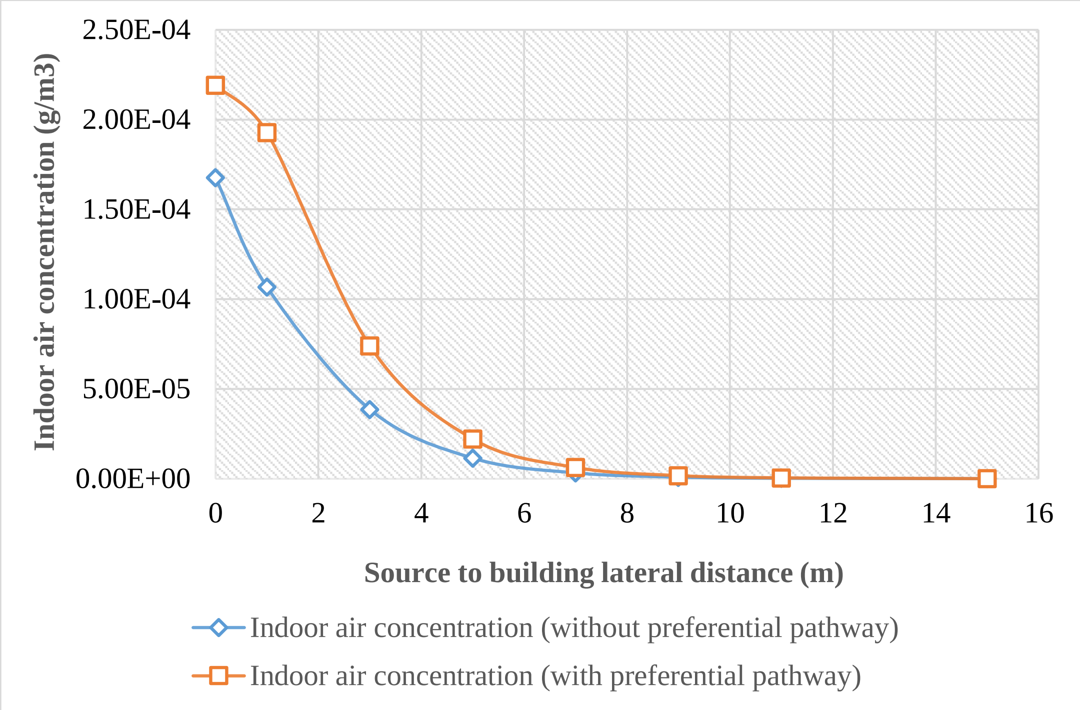


Figure 8. Indoor air concentration with and without preferential pathway vs source to building lateral distances.

3.3. Sensitivity Analysis

The influence of different types of soil texture on the indoor air concentration is investigated with the characteristics of 12 typical soils summarised in US EPA database (2012). The total porosity, water-filed porosity and intrinsic permeability used for the simulations for 12 typical soils are listed in Table 3. Simulations for sensitivity analysis were conducted using a CSM where a 0.5 m granular backfill comprising of well graded gravel acting as the preferential pathway is at a depth of 1 m below ground surface (bgs) and a TCE contaminant source 1g/m^3 at a depth of 1 m from the preferential pathway.

Table 3. Soil characteristics for 12 typical soils summarised in US EPA database

Soil Type	*Total Porosity*	*Water-filled porosity*	*Soil permeability (m^2)*
Clay	0.459	0.215	2.32×10^{-13}
Clay Loam	0.442	0.168	1.29×10^{-13}
Loam	0.399	0.148	1.90×10^{-13}
Loamy sand	0.390	0.076	1.67×10^{-12}

Sand	0.375	0.054	1.02×10^{-11}
Sandy clay	0.385	0.197	1.79×10^{-13}
Sandy clay loam	0.384	0.146	2.09×10^{-13}
Sandy loam	0.387	0.103	6.09×10^{-13}
Silt	0.489	0.167	6.92×10^{-13}
Silt loam	0.439	0.180	2.89×10^{-13}
Silty clay	0.481	0.216	1.52×10^{-13}
Silty clay loam	0.482	0.198	1.75×10^{-13}

Figure 9 shows the indoor air contaminant concentration corresponding to the various types of soil with different intrinsic permeability in the vadose zone with and without the preferential pathway. Soils with poor permeability like clay and sandy clay lead to lower indoor air contaminant concentration as opposed to sand which causes an increased indoor air contaminant concentration due to its high permeability. An increase of more than one order of magnitude in indoor air vapour concentration was observed with highly permeable soils in the vadose zone as compared to soils with low permeability. The presence of highly permeable preferential pathway of 0.5 m causes almost a two-fold increase in indoor air concentration for all soil types.

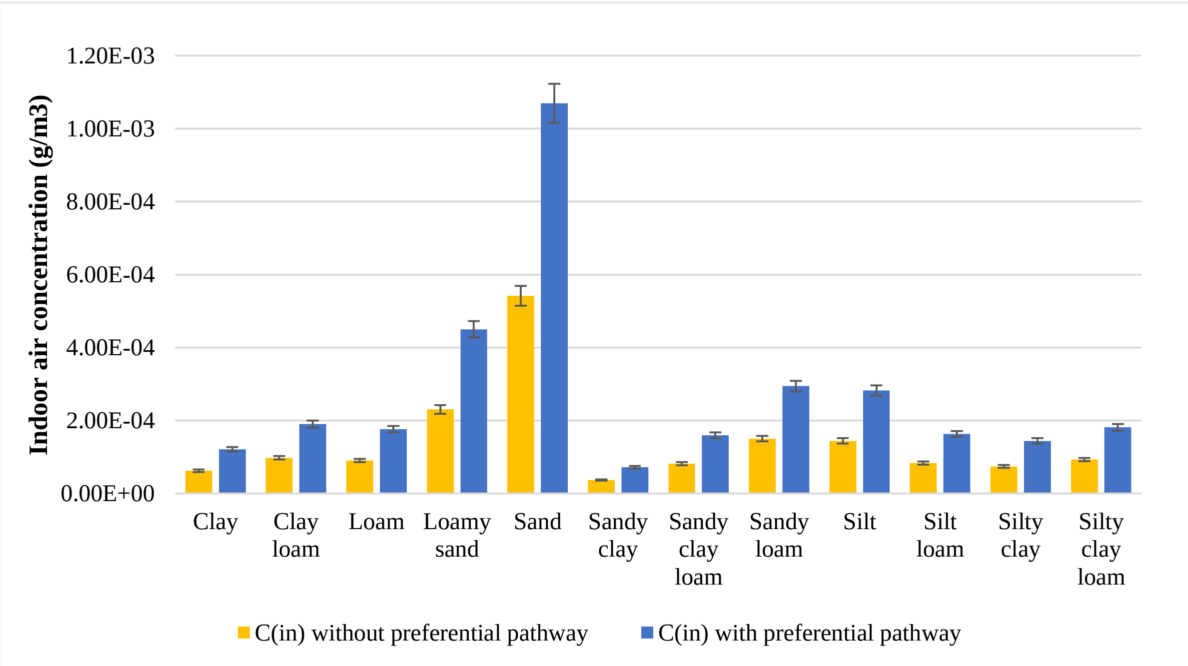
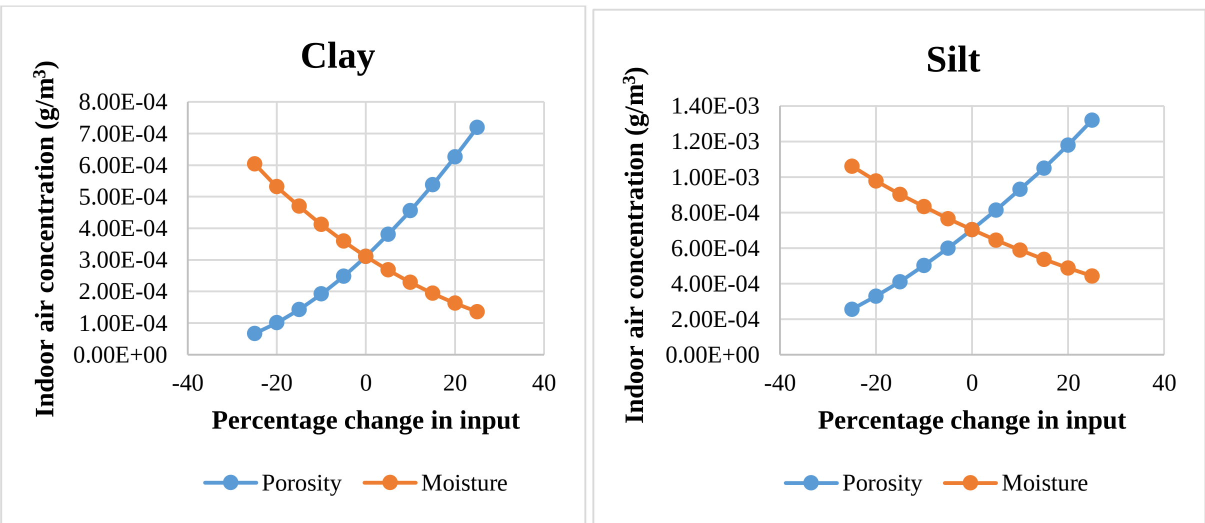
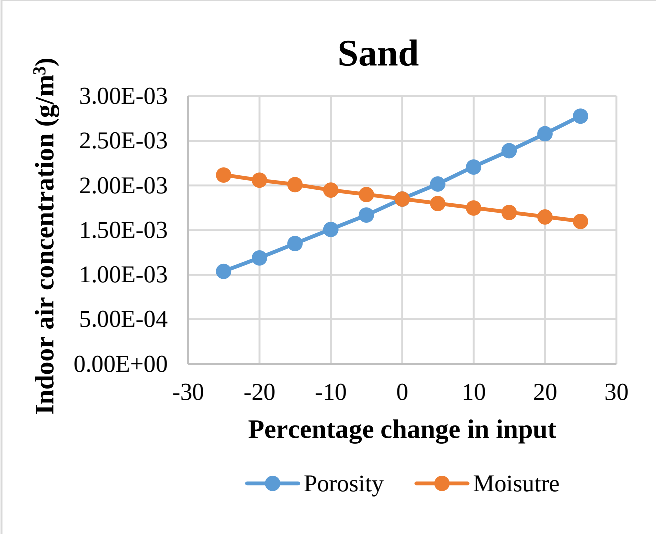


Figure 9. Simulated indoor air concentrations for 12 typical soils summarised in US EPA database.

To understand the effect of soil porosity and moisture, a one-at-a-time (OAT) sensitivity analysis technique was conducted in three different types of soils (clay, silt and sand). The outputs were obtained and compared by varying the input parameters by ±25% (Ma et al., 2016) from the default values of clay, silt and sand (given in table 3). Figures 10 (a) (b) and (c) shows the sensitivity behaviour of soil moisture and soil porosity in this model for clay, silt and sand, respectively. The sensitivity behaviour of soil moisture and soil porosity is observed to depend on the soil type. The change in indoor air concentration is almost exponential in clay when compared to a linear change in sand. So it can be stated here that changes in soil porosity and moisture content are more sensitive in soils with low permeability. Increase in soil porosity provides greater passageways for vapour migration, resulting in increased diffusive flux in the sub-surface and subsequently higher indoor air vapour concentration. Concurrently, an increase in soil moisture acts as a large resistance to diffusion. As the moisture content in the soil increases, the effective air diffusivity wanes, resulting in additional partitioning into liquid phase. Hence the soil gas concentration is reduced which ultimately lowers the indoor air vapour concentration.



(a) (b)



(c)

Figure 10. Changes in indoor air vapour concentration with variations in soil porosity and moisture in (a) clay, (b) silt and (c) sand.

3.4. Effect of depth of preferential pathway

The presence of any kind of high permeability region in the vadose zone – either natural or anthropogenic – can facilitate higher contaminant flux both vertically and laterally owing to its high permeability than the surrounding soils. Figure 11 shows a significant increase in indoor air contaminant concentration for different depths of highly permeable layer in the vadose zone acting as the preferential pathway. From the simulations, a 1 m deep preferential pathway can lead to an almost 70% increase in indoor air contaminant concentration compared to a no preferential pathway scenario. As the depth of preferential pathway increases, the contaminant vapour has more room for migration with least resistance in the vadose zone resulting in lower attenuation and hence higher indoor air vapour concentration.

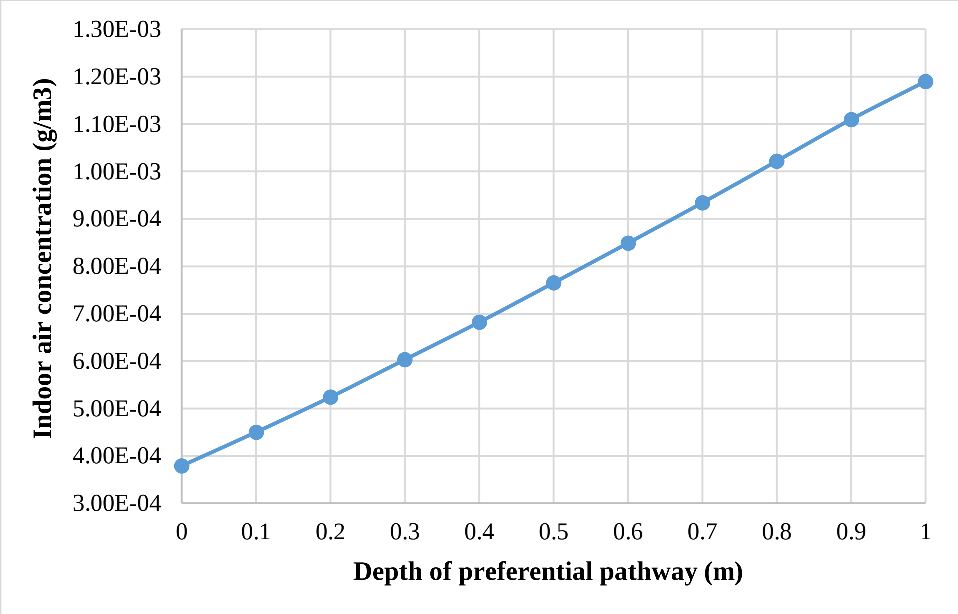


Figure 11**.** Simulated indoor air contaminant concentration for varying depths of preferential pathway.

4. Conclusion

Detecting the impacts of VI outside the contaminant plume footprint has led to research seeking to understand the role of preferential pathways in VI. Though the majority of studies involving preferential pathways focused on sewer VI investigations, the roles of highly permeable soil layers and backfill materials have rarely been examined. This model was developed to illustrate the role of highly permeable granular soil layers like gravel or crushed rocks used as beddings and backfills for utility lines in exacerbating the indoor air vapour concentrations.

Despite some guidance documents suggesting highly permeable soil zones may act as preferential pathways, it is not documented anywhere with sufficient importance suggesting that these pathways might well be addressed by standard VI investigation measures. However from this study, these preferential pathways were found to exacerbate the indoor air concentration depending on the depth of the contaminant plume from the preferential pathway layer. The close proximity of the source to the preferential pathway resulted in an increase of indoor air concentration as high as 200% compared to a no-preferential pathway scenario which then decreased to about 150% as the depth of source to preferential pathway increased with respect to the simulations' parameters. Although it can be considered not a significant increase in evaluating VI risks, such an increase in indoor air concentration can influence the screening criteria and response levels of the affected sites by considering it safe or whether an investigation or intervention is necessary. In the lateral direction, despite the presence of preferential pathway causing an increased risk of VI, the impact in indoor air concentration is evident only until a few meters from the plume's edge. As the source to building distance increases, the preferential pathway seems to play no substantial role in increasing indoor air concentration at very large lateral distances.

Natural soil varies widely in permeability which greatly influences the rate of vapour entry into buildings. Soils with high permeability like sand result in higher indoor air concentration, of a greater than one order of magnitude, than soils with low permeability like clay. The presence of a highly permeable preferential pathway aggravated (in fact doubled) the vapour transport increasing the indoor air vapour concentration. Vapour transport in the vadose zone is largely influenced by soil porosity and soil moisture as they influence the effective diffusivity of the vapour in soil. The sensitivity of these soil parameters is more pronounced in soils with low permeability.

Since the proposed model is based on a CSM scenario of CVI where the building is located laterally at a distance from the edge of an infinite and uniform contaminant plume, a proper evaluation of the site needs to be conducted for this model to have feasible applications. This model can be implemented in places where a highly permeable preferential pathway is prevalent in the vadose zone which exacerbates VI in the building. As far as limitations are concerned, this model cannot be used for sites with PVI since biodegradation is not considered here. The subsurface heterogeneity and the effect of rainfall, snow and changes in groundwater levels were ignored during the model's development. Hence a proper evaluation is necessary to understand whether these assumptions are reasonable for sites under consideration.

Declaration of Competing Interests

We declare that we have no financial and personal relationships with other people or organisations of any kind that could be influencing our work presented in the manuscript titled, "Two-dimensional vapour intrusion model involving advective transport of vapours with a highly permeable granular layer in the vadose zone serving as the preferential pathway".

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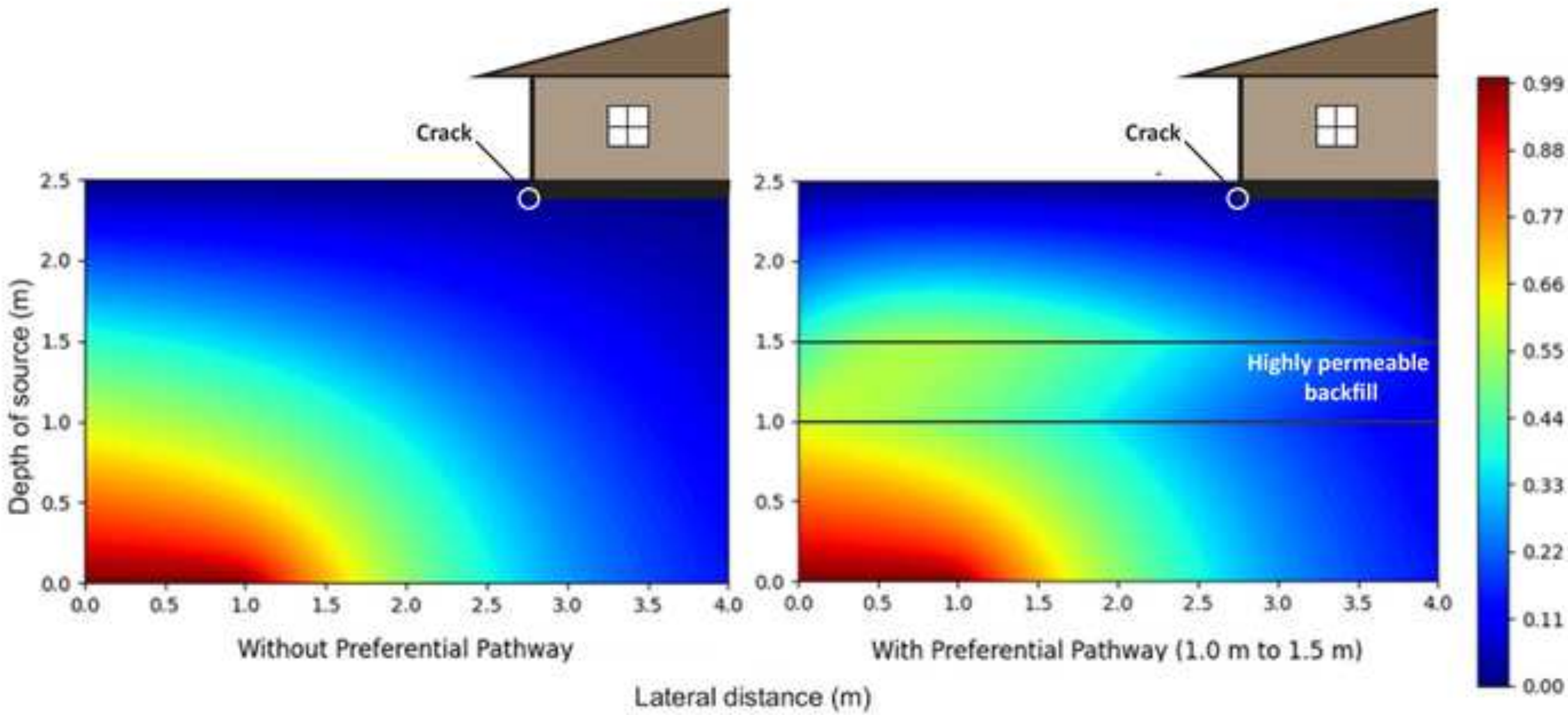
Graphical Abstract



Two-dimensional vapour intrusion model involving advective transport of vapours with a highly permeable granular layer in the vadose zone serving as the preferential pathway

Highlights

- A 2-D vapour intrusion model to estimate the indoor air concentration is developed
- Effects of highly permeable backfill layers as preferential pathway is considered
- Advection serves the dominant transport mechanism in the preferential pathway layer
- Proximity of the source to preferential pathway affects the indoor air concentration

Two-dimensional chlorinated vapour intrusion model involving advective transport of vapours with a highly permeable granular layer in the vadose zone serving as the preferential pathway

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Abstract

Vapour Intrusion (VI) is the process through which volatile organic compounds migrate from the subsurface source to the soil predominantly by diffusion, entering the overlying buildings through joints, cracks or other openings. This activity poses potentially serious health hazards for the occupants. Because of these health risks, recommendations for site closure are often made by quantifying the VI risks using mathematical models known as 'Vapour Intrusion Models' (VIM). Most of these VIMs seem to overlook the role of preferred pathways like utility lines, high conductivity zones of soil or rocks, etc., which act as the path of least resistance for vapour transport thereby increasing vapour intrusion risks. This study presents a two-dimensional (2-D) chlorinated vapour intrusion (CVI) model which seeks to estimate the source-to-indoor air concentration attenuation. It takes into account the effects of a highly permeable utility line embedment as a preferential pathway. The transport of 2-D soil gas is described using the finite difference method where advection serves as the dominant transport mechanism in the preferential pathway layer, while diffusion applies to the rest of the vadose zone. The model returned results comparable with other models for the same input parameters, and was found to closely replicate the results of 3-D models. The simulations indicate that the presence of highly permeable utility line embedment and backfill layers do trigger a higher indoor air concentration compared to a no preferential pathway scenario.

Keywords: Vapour intrusion; two dimensional model; preferential pathway; chlorinated hydrocarbons.

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1. Introduction

The conceptual site models (CSMs) help in identifying the pathways for vapour transport in the vadose zone and its entry into buildings. Conventional CSMs assume a 'soil VI pathway' in which vapours from a subsurface source emanate and diffuse vertically and/or laterally through the subsurface soil, which then intrudes into the indoor air typically through foundation pores, cracks or openings (Guo et al., 2015). However, the presence of alternate exposure pathways in the vadose zone like utility lines, naturally occurring fractures or macro pores, highly permeable soil layers or backfills etc. had been generally overlooked until recently. These alternative exposure pathways, known as preferential pathways, intersect with the vapour source or vapour migration pathways offer least resistance to soil vapour flow, subsequently and significantly increasing the risk of vapour intrusion (VI) (USEPA, 2002). The majority of vapour intrusion models (VIMs) currently in use have been developed with conventional CSMs but have often ignored the potential for vapour entry into indoor air scenarios through utility corridors, plumbing systems, etc., during VI investigations and developing VIMs. Failure to incorporate the role of preferential pathways into VI results in inaccurate predictions of indoor air vapour concentrations and wrong clean-up strategies.

The United States Environmental Protection Agency (US EPA) recommended a buffer zone of about 100 feet (or 30 m) vertically and laterally from the contaminant source, beyond which buildings can be deemed safe since no significant indoor air concentration had been found in them at a distance greater than one house lot (USEPA, 2002). Yet, in recent studies, VI impacts were detected in buildings even outside the footprint of the contaminant plume (Yao et al., 2017a) due to the presence of preferential pathways which offer little vapour attenuation and this leads to high indoor air concentrations. Most of the VI through preferential pathways are related to the interception of compromised or deteriorated sewer systems, primarily designed to carry wastewater to treatment plants, with the contaminant plume in vadose zone ultimately resulting in unhindered transport of volatile organic compounds (VOCs) into the indoor air through connected plumbing systems (Jacobs et al., 2015). Several field studies have been conducted in recent times confirming the role of sewers acting as a preferential pathway for soil vapour transport, resulting in significant indoor air contaminant concentrations even in buildings outside the groundwater plume area (Distler and Mazierski, 2010, Riis et al., 2010, Vroblesky et al., 2011, Pennell et al., 2013, Guo et al., 2015, McHugh et al., 2017, Guo et al., 2020, Beckley and McHugh, 2021). Additionally, VI episodes without a vadose zone source can occur from VOCs volatilising from industrial discharges which are directly discharged into sewer systems which contribute to higher indoor air contaminant concentrations (Roghani et al., 2018).

Many studies conducted on preferential pathways in VI focus on contaminant transport through sewers, utility tunnels and their associated plumbing conduits. However, the role of highly permeable soil layers and backfill materials in VI have rarely been investigated. The presence of any high permeability region in the vadose zone - either natural or anthropogenic - can function as a preferential pathway in contaminant vapour transport. These regions of high permeability can occur naturally as gravel layers or fractured rocks which facilitate higher contaminant flux owing to their higher porosity (USEPA, 2015b). As well, granular fill materials laid as bedding and embedment to utility lines can cause high contaminant flux laterally and vertically to the ground surface, and thereby serve as preferential pathways (ITRC, 2014).

The aim of this study is to develop and evaluate a 2-D model in order to estimate the indoor air concentration at sites contaminated with chlorinated hydrocarbons (CHCs) with a highly permeable gravel layer acting as a preferential pathway. The numerical model depicts: i) two-dimensional vapour flux (lateral and vertical directions) of chlorinated hydrocarbon contaminants; ii) the building of concern laterally situated at a distance from the edge of the contaminant plume; and iii) the presence of a highly permeable course grained soil layer such as gravel used as bedding for utility lines which act as preferential pathway for vapour transport.

This model: firstly, solves partial differential equations of diffusion and advection in the vadose zone with preferential pathway to estimate the total vapour flux; secondly, has a modular subroutine for simulating the effect of preferential pathway in vapour transport; and thirdly, estimates the indoor air concentration by ‘continuous stirred tank reactor method’ as employed in Johnson and Ettinger’s (hereafter J&E) model. Evaluating the model’s performance was carried out by comparing it with 1-D, 2-D and 3-D models using hypothetical as well as field data obtained from particular studies (Holton et al., 2013, Guo et al., 2015, Yao et al., 2017b).

2. Methodology

2.1. Model development

The numerical model took two stages to develop. First, a conceptual model was devised considering: i) the system as two-dimensional; ii) the building of concern placed laterally at a distance from the edge of the CHC contaminant plume; iii) a coarse grained utility line bedding, such as gravel, sand or crushed stone with high permeability acting as the path of least resistance for the contaminant vapour flux; and iv) foundation of the building as slab-on-grade and simulating the interaction between the sub-surface and the building. The purpose of this conceptual model is to illustrate the role of highly permeable bedding layers of utility lines in exacerbating the risk of VI in buildings located laterally at a distance from the edge of the contaminant plume. The general CSM developed for this study is depicted in Figure 1.

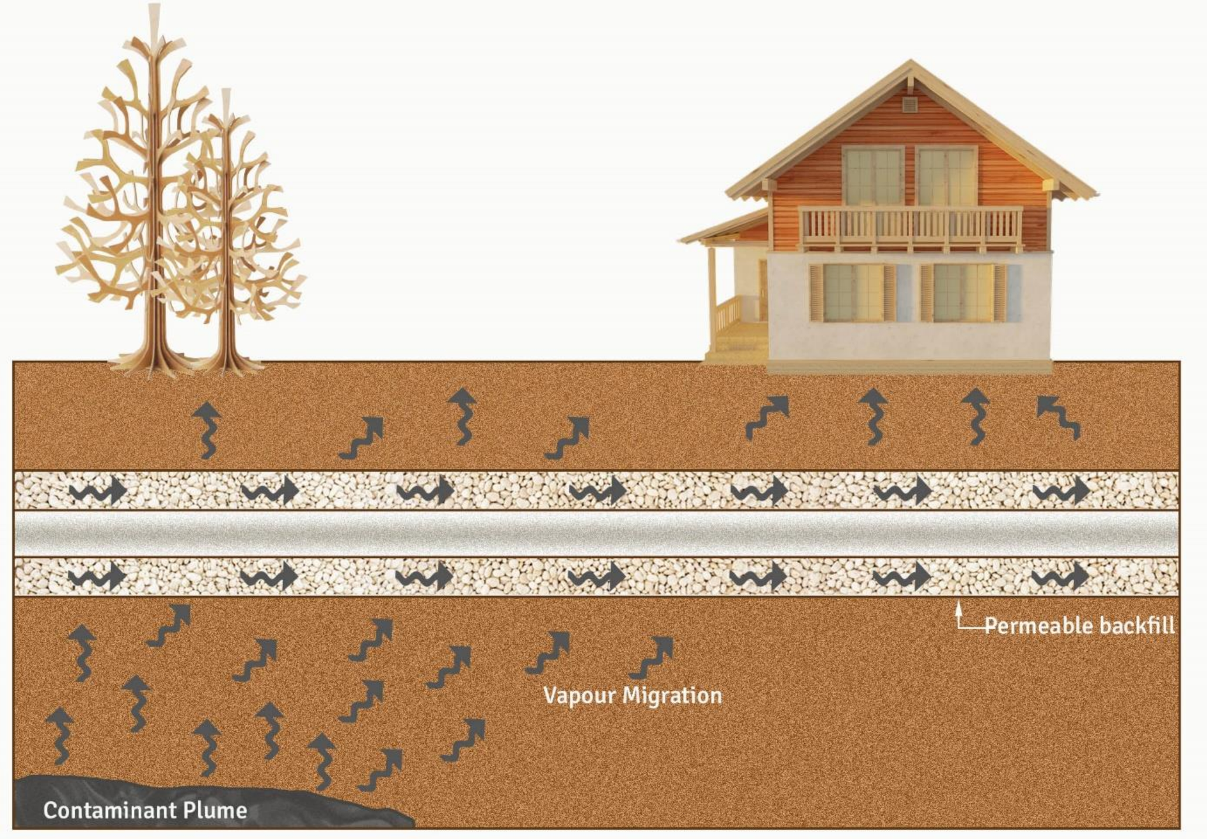


Figure 1. CSM developed for the study

In the second stage of model's development, governing equations were formulated and solved using the central difference scheme of the finite difference method and coded in Python programming language for simulating fate and transport of CHCs from source to the building foundations through sub-surface soil. The vapour entry into the building through the foundations and subsequent indoor air contaminant concentration is calculated using the 'continuous stirred tank reactor method' employed in the J&E model (Johnson and Ettinger, 1991).

Although there are several models which consider two-dimensional vapour transport, most of them assume diffusion is the dominant transport mechanism in the vadose zone but do not take into account the presence of a preferential pathway. Some guidance documents suggest the role of natural and induced high permeability zones in the vadose zone as preferential pathways, for instance gravel and sand lenses, vertically fractures rocks, etc., as well as highly permeable bedding or backfill layers of utility lines which are mostly situated close to the surface (USEPA, 2015a, ITRC, 2014). However, we know of few studies that have shown vapour migration through backfills or naturally occurring high permeability zones which this model seeks to address. When a significant pressure gradient is present, an upward advective soil gas transport might be induced which can be identified using Peclet number (Pe) (Yao et al., 2015). If Pe >1, it is assumed that advection will be the dominant transport mechanism but it will be diffusion if Pe < 1. The flowchart shown in Figure 2 illustrates the steps involved in developing the 2-D model for simulation of CHC vapour transport in the presence of a highly permeable preferential pathway layer. This model calculates the indoor air concentration and attenuation factor by simulating the vapour transport in the vadose zone. It does this by considering diffusion as the dominant transport mechanism if Pe<1 and advection as the dominant transport mechanism if Pe>1 in the bedding and backfill layer.

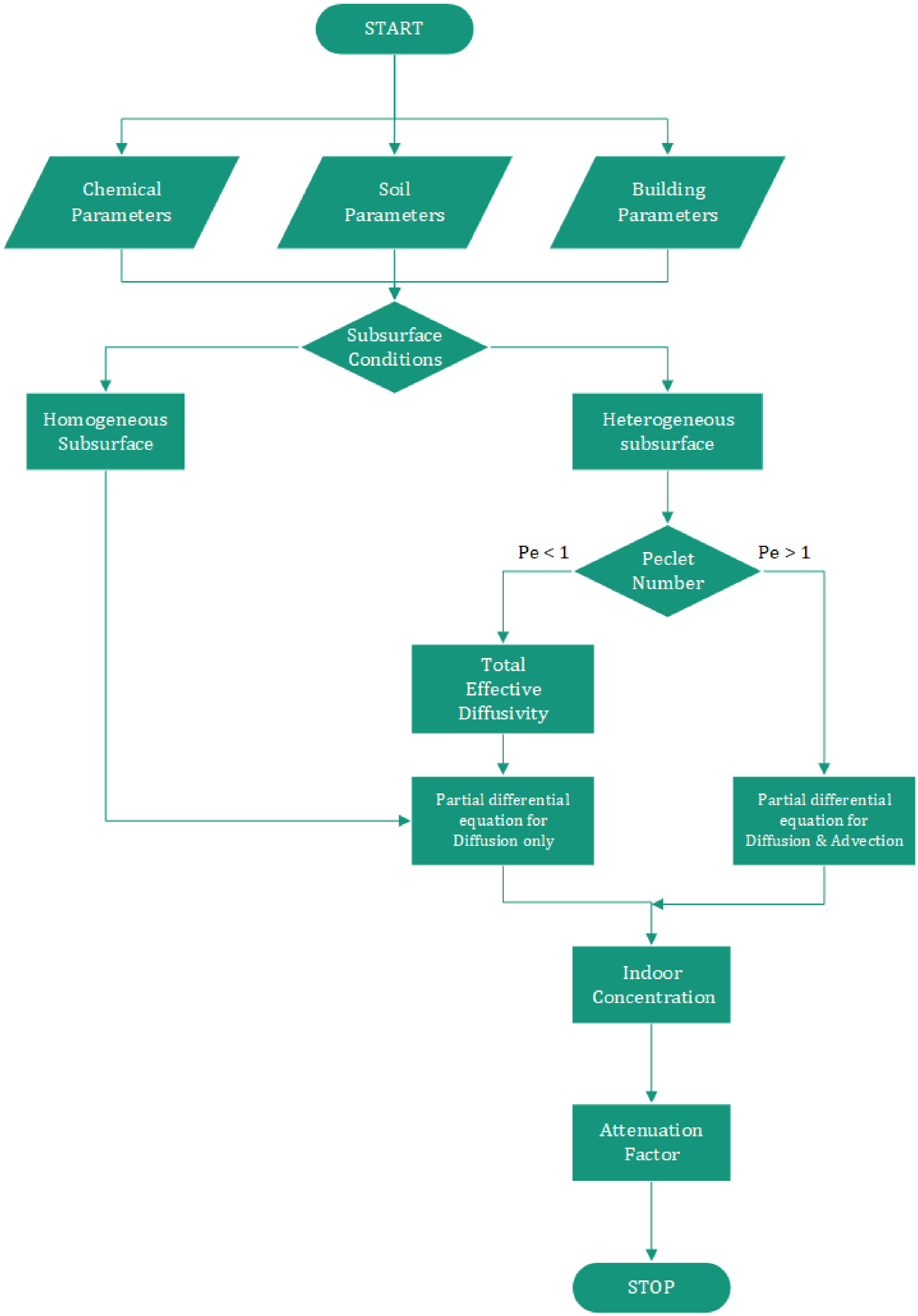


Figure 2: Overview of the 2-D model process with the preferential pathway

The major components involved in the model's methodology are: i) obtaining the vapour flux and contaminant concentration profile in the vadose zone; ii) determining the dominant transport mechanism in the backfill and bedding layer by computing Pe; iii) calculating vapour entry into the building using continuous stirred tank reactor method; and iv) computing indoor air concentration and attenuation factor based on the subsoil and building interaction. The effect of preferential pathways in three scenarios considered in this study are: i) preferential pathway closer to the source; ii) preferential pathway equidistant from the source and receptor; and iii) preferential pathway furthest from the source. Results of these simulations are then compared with a 'no-preferential pathway' scenario in order to fully understand the role of the highly permeable bedding layer in exacerbating the VI risk.

For refining the numerical model, the following assumptions are made. Firstly, the model operates under steady state conditions. The source concentration is considered to be constant and the vapour migration is deemed to be a steady-state process. Although the actual vapour migration is a transient process, the steady state scenario can express the most hazardous scenario. Secondly, the subsurface is assumed to be stratified due to the presence of the preferential pathway and each soil layer is homogeneous. Thirdly, the contaminant concentration decreases exponentially with lateral distance from the source. Fourthly, the utility line is leak-proof and does not act as preferential pathway. Fifthly, the effect of biodegradation is not taken into account since the rate of degradation of TCE is negligible without a growth substrate like methane (Choi et al., 2002). The vapour concentrations and subsequent indoor air concentration calculated under these assumptions can be overestimated compared to actual on-site measurement. Nevertheless, the model can be employed as a screening tool to address the VI problem with a preferential pathway.

2.2. Governing equations and boundary conditions

2.2.1. Transport by diffusion

The vapour transport in the vadose zone is assumed to be steady state diffusion except in the highly permeable preferential pathway layer. Since both lateral and vertical movement of the contaminant vapours are considered in a two-dimensional soil context, the governing equation for the transport of a non-reacting, non-adsorbing vapour through the vadose zone under steady state diffusion is explained by Laplace equation as given in eq. (1) (Yao et al., 2017b):

$$\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) = 0 \qquad \textbf{(1)}$$

where: x and y are lateral and vertical coordinates (m), respectively; and C denotes the contaminant vapour concentration (mg/L).

The effective vapour diffusion coefficient of the media, D_e (m^2/s), is calculated using the Millington-Quirk equation (1961) as given in eq. (2):

$$D_e = D_a \frac{\theta_a^{10/3}}{\theta_T^2} + \frac{D_w}{H} \frac{\theta_w^{10/3}}{\theta_T^2} \qquad \textbf{(2)}$$

where: D_a is the molecular diffusion coefficient in gas (m^2/s); D_w stands for the molecular diffusion coefficient in water (m^2/s); θ_T, θ_a & θ_w are total porosity, air filled porosity and water filled porosity, respectively; and H is the dimensionless Henry's law constant.

In a heterogeneous subsurface with *n* layers of soil, a total effective diffusion coefficient can be introduced ($D_{e,tot}$) as shown in eq. (3) which transforms the diffusion coefficients of individual soil layers of the subsurface into an equivalent homogeneous system (Johnson and Ettinger, 1991):

$$D_{e(tot)} = \frac{L}{\sum_{i=0}^{n} \frac{d_i}{D_{e(i)}}} \qquad (3)$$

where: L is the depth of vadose zone (m); d_i is the thickness of the *i*th layer (m); and $D_{e(i)}$ denotes the effective diffusion coefficient of the *i*th layer (m^2/s).

2.2.2. Transport by advection

In preferential subsurface pathways such as utility corridors, highly permeable soils or porous zones of rocks, the contaminant vapours tend to migrate via advection (USEPA, 2015a). A relatively small change in partial pressure can trigger significant advective vapour transport which is larger than the diffusive fluxes (Scanlon et al., 2002). The contaminant vapours reach the highly permeable granular fill in the vadose zone from the source. Meanwhile the pressure difference between the subsurface and open ground and the high soil permeability causes a change in vapour velocity. This can be calculated using eq. (4) as written below:

$$\boldsymbol{u_g = \frac{K_{bf}}{\mu}.\nabla P_w} \tag{4}$$

where: u_g is the average vapour phase velocity (m/s); K_{bf} is the soil air permeability of the granular backfill (m^2); μ stands for soil gas viscosity (Pa.s); and ∇P_w represents the vapour pressure gradient in the granular backfill (Pa), which is required as an independent input of the model.

Once the vapour velocity is obtained, the Peclet number can be computed using eq. (5) to confirm the dominant transport mechanism in the preferential pathway:

$$\boldsymbol{P_e = \frac{u_g.L}{D_{TCE}}} \tag{5}$$

where: u_g is the vapour velocity (m/s); L is the depth of preferential pathway layer (m); and D_{TCE} is the effective diffusivity of TCE in soil (m^2/s).

If Pe < 1, the dominant transport mechanism will be diffusion and the governing equation is given by eq. (1). If Pe > 1, the dominant transport mechanism will be advection for which the governing equation is given by eq. (6) as stated below:

$$\boldsymbol{-u_g\left(\frac{\partial C}{\partial x}+\frac{\partial C}{\partial y}\right) = 0} \tag{6}$$

For geological systems with permeability > 10^{-9} m^2, the contaminant transport can be simulated with advection equation (Yao et al., 2012).

2.2.3. Computation of indoor air concentration

The average indoor air concentration is calculated in this model using the ‘continuous stirred tank reactor’ method as employed in the J&E model. As per the technical VI guidance of US EPA (2015a), for a building laterally at a distance from the contaminant plume, the soil vapour concentration obtained from below the foundation closest to the source can help to describe the worst case scenario underneath the building. Hence the subslab concentration of vapours $C(x_{ck},d_s)$ closest to the edge of the contaminant plume is obtained from the simulations and is employed for the vapour entry and indoor air concentration calculations using eq. (7) to (14). The sub-slab crack concentration (C_{ck}) can be computed using eq. (7) as documented below:

$$\boldsymbol{C_{ck} = \frac{\pi D_e . d_s . t_{ck}}{D_a w_{ck}} C(x_{ck}, d_s)} \tag{7}$$

where: t_{ck} is the thickness of the foundation (m); w_{ck} is the width of the crack (m); x_{ck} is the distance of the foundation crack from the edge of contaminant plume and d_s is the depth of source from the foundation.

The indoor air contaminant concentration (C_{in}) can be calculated as a function of sub-slab crack concentration as given in eq. (8) using a series of empirical equations as stated in eq. (9) to eq. (14):

$$\boldsymbol{C_{in} = C_{ck}\left(\frac{R_{mix}}{R_{crack}+R_{mix}}\right)} \tag{8}$$

Where,

$$R_{mix} = \frac{1}{L_{mix}.ER} \tag{9}$$

and

$$R_{crack} = \left(R_{mix} - \frac{A_b}{Q_s}\right)(e^{-\varepsilon} - 1) \quad (10)$$

with

$$\varepsilon = \frac{Q_s}{A_b}\frac{t_{ck}}{D_a \eta} \quad (11)$$

$$\eta = \frac{w_{ck} l_{ck}}{A_b} \quad (12)$$

$$Q_s = \frac{2\pi K_a \Delta p l_{ck}}{\mu \ln\left(\frac{2d_f}{r_{ck}}\right)} \quad (13)$$

and

$$r_{ck} = \frac{\eta A_b}{l_{ck}} \quad (14)$$

where: L_{mix} (m) denotes the height of the building at which contaminant mixing occurs; ER (1/hr) is the building air exchange rate; A_b (m^2) stands for the foundation area in contact with the soil; Q_s (m^3/s) is the convective soil vapour entry rate into the building; d_f (m) is the depth of foundation below ground surface; η represents the foundation crack fraction; l_{ck} (m) is the foundation perimeter; K_a (m^2) is the soil air permeability; μ (Pa.s) is the soil gas viscosity; and Δp (Pa) is the pressure difference between building and soil.

The sub-slab-to-indoor air concentration attenuation factor (α), which relates indoor air vapour concentration (C_{in}) to the source vapour concentration (C_s) can be calculated using eq. (15):

$$\alpha = \frac{C_{in}}{C_s} \quad (15)$$

2.2.4. Boundary conditions

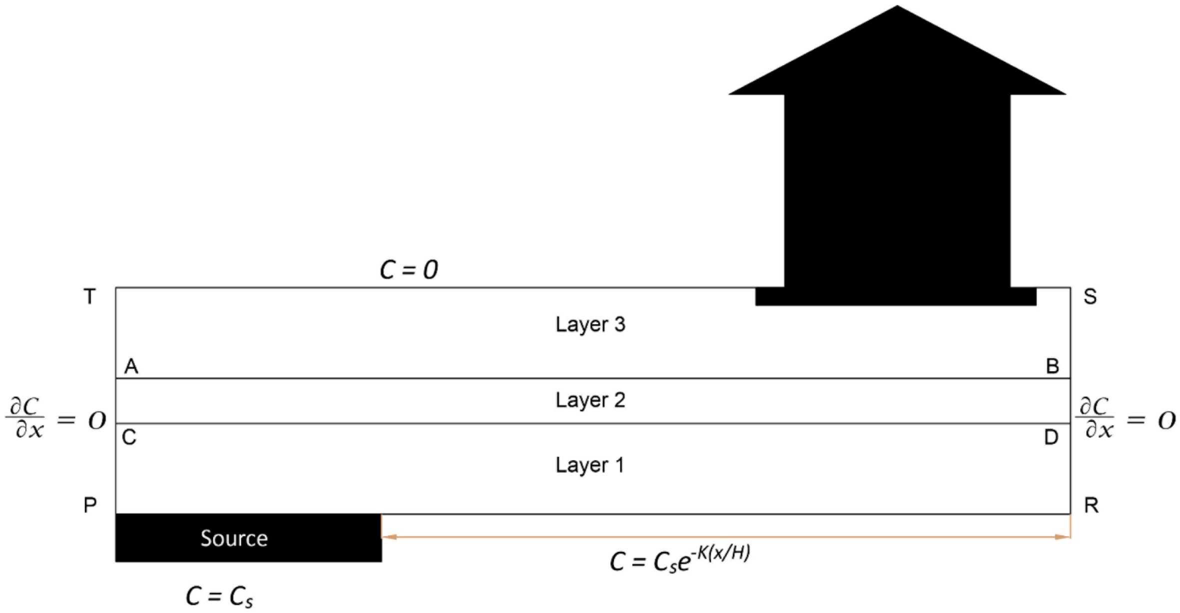


Figure 3. Boundary conditions employed for the CSM

Figure 3 depicts the boundary conditions for the solution of the transport equations in the vadose zone. The conceptual model assumes concentration at source to be C_s while the concentration at ground surface is zero. The left-hand and right-hand side boundaries of the domain are assumed to have no flux boundary condition, i.e. $\frac{\partial C}{\partial x} = 0$ where concentration attenuation is linear. Beyond the edge of the source, the concentration tends towards zero at large lateral distances and the concentration attenuation is exponential which is satisfied by $C_s e^{-K(\frac{x}{H})}$, where: x is the lateral distance from source (m); H is the depth of source (m); and K is the decay rate constant.

Boundary condition for advection process in the highly permeable preferential pathway is established by considering the system as three separate layers. The values obtained by solving eq. (1) in layer 1 with the corresponding boundary conditions becomes the boundary condition for layer 2 (CD in fig.3). With ∇P_w as independent input in the model, the calculated soil vapour velocity (u_g) will determine Pe which in turn determines the vapour transport mechanism in layer 2. If Pe>1, the transport mechanism will be advection and the system will solve for eq.

(6) for the whole layer (until AB in fig. 3). This in turn will serve as the boundary condition for layer 3 which will solve for diffusion equation for that layer.

3. Results and Discussion

3.1. Comparison with existing models

The capability of VI assessment by the developed model is conducted by comparing the results of the normalised sub-slab concentration obtained from the current model with the results of analytical approximation method (AAM) (Yao et al., 2013) and Abreu and Johnson's 3-D model (Abreu and Johnson, 2005). The calculated vapour concentration at the near edge of the foundation bottom is regarded as the sub-slab concentration. The data adopted for model comparison is obtained from Yao et al., (2013) for a building foundation depth of 0.2 m and source depth 8 m for different values of source-building separation. The results of the three methods are compared in figure 4. With respect to the change in contaminant sub-slab concentration in lateral direction, the developed model follows the trend of other models, particularly when compared with the 3-D model, which implies that the developed model may provide an alternative method of assessing VI risk.

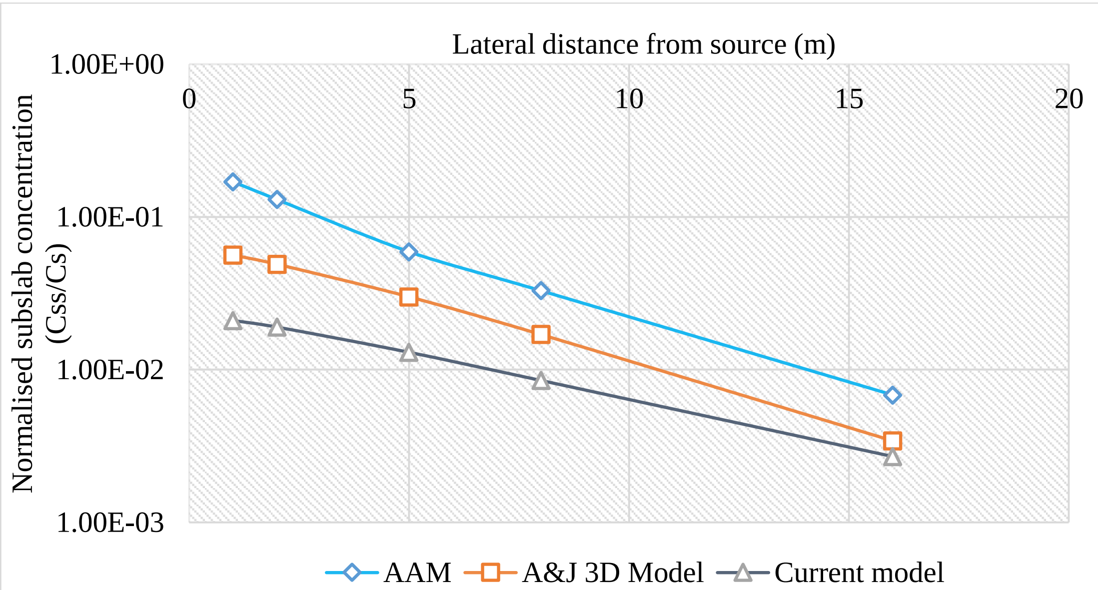


Figure 4. The plot of normalised sub-slab concentration (C_{ss}/C_s) vs Lateral distance from the edge of the source for AAM, 3-DM and current model.

3.2. Simulated scenarios

3.2.1. Effect of preferential pathway

To understand the effect of highly permeable granular fill in the vadose zone in exacerbating VI risks, a scenario is simulated by using a granular backfill comprising well graded gravel that is 0.5 m in depth. It functions as the preferential pathway at a depth of 1 m from the ground surface, where the primary transport mechanism is advection. The building of concern has its closest point from the edge of the contaminant plume of concentration 1 g/m^3 at an arbitrarily chosen distance of 3 m. The rest of the vadose zone other than the preferential pathway is assumed to consist of sandy clay where diffusion is assumed to be the primary transport mechanism. The specifications related to pipe embedment and backfilling is consistent with Standard drawings SCP-1000 and SCP-1001 of the Standard Technical Specifications for Construction of Sewer Rising Mains by Hunter Water Corporation (2005).This is then compared to a 'no-preferential pathway' scenario where the vadose zone is considered homogeneous with sandy clay soil where diffusion is the only soil transport mechanism. Biodegradation is not accounted for in the simulations since the contaminant of interest is TCE which is normally difficult to biodegrade in soil. The input parameters used in the simulations are reported in Table 1.

Table 1. Input parameters for the model simulations.

Chemical Parameters		***Unit***	***Value***
Source vapour concentration	C_s	g/m3	1
Diffusion coefficient in air	D_a	m2/s	7.90E-06
Diffusion coefficient in water	D_w	m2/s	9.10E-10
Henry's law constant	H	-	0.403
Soil gas viscosity	μ	Pa.s	5.32E-04
Soil Parameters			
Total Porosity	Θ_T	-	0.385
Air filled porosity	Θ_a	-	0.188
Water filled porosity	Θ_w	-	0.197
Soil air permeability	K_a	m^2	1.70E-13
Granular backfill soil parameters			

Depth of backfill	ds	m	0.5
Total Porosity	Θ_T	-	0.5
Air filled porosity	Θ_a	-	0.49
Water filled porosity	Θ_w	-	0.01
Soil air permeability	K_a	m^2	1.00E-09
Building parameters			
Width of foundation slab		m	10
Foundation footprint area	A_b	m2	100
Depth of foundation below grade	d_f	m	0.3
Thickness of foundation crack	t_{ck}	m	0.1
Width of foundation crack	w_{ck}	m	0.001
Foundation perimeter	l_{ck}	m	40
Building height	L_{mix}	m	3
Building Air exchange rate	ER	h^{-1}	0.5
Soil and building pressure difference	Δp	Pa	5

From the simulations, it was observed that there was a considerable increase, virtually double the amount, in sub-slab as well as indoor air concentrations in the presence of a highly permeable preferential pathway layer when compared to the 'no-preferential pathway' scenario. Table 2 shows the contrasts in vapour concentration in the sub-slab and indoor air and the attenuation factor with and without the preferential pathway. Based on these results, it is clearly evident that the presence of preferential pathway indeed increases the potential risk of VI.

Table 2. Comparison of sub-slab concentration, indoor air concentration and attenuation factor with and without the preferential pathway for different scenarios.

	Without preferential pathway	*With preferential pathway*
Source concentration (g/m^3)	1	1
Sub-slab concentration (g/m^3)	0.025	0.048
Indoor air concentration (g/m^3)	3.86E-05	7.40E-05
Attenuation factor (α)	3.86E-05	7.40E-05

This increase in indoor air contaminant concentration can be attributed to the limited attenuation occurring in the preferential pathway. Advection is assumed to be the dominant transport mechanism in the preferential pathway layer, so the vapour movement occurs at a faster rate.

This is comparable to the rest of the vadose zone where vapour transport occurs due to diffusion, hence offering the least resistance for soil gas transport and subsequently less attenuation. Figure 5 presents the vapour concentration profile in the vadose zone which shows the increase in vapour concentration in the preferential pathway layer as opposed to that of a 'no-preferential pathway' scenario. It proves that the preferential pathway offers the least resistance to vapour transport in the vadose zone and ultimately results in exacerbation of VI.

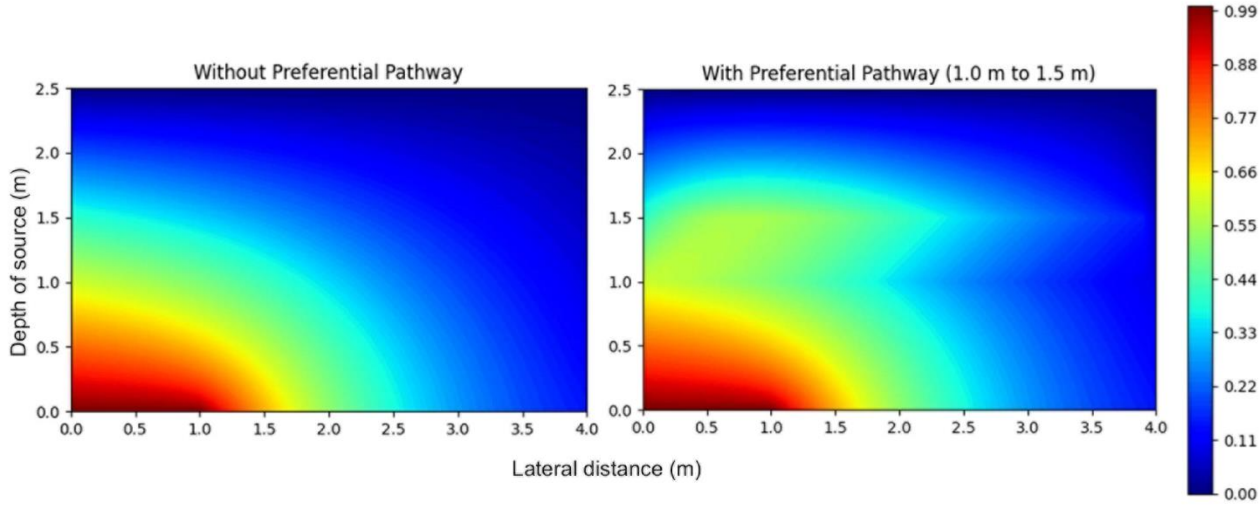


Fig. 5: Comparison of vapour concentration profile in the vadose zone with and without the preferential pathway for the same scenario.

3.2.2. Influence of depth of source from preferential pathway

Simulations were conducted to understand the effect of proximity of the source to the preferential pathway by varying the depth of source (0.5 m, 1 m, 2 m, 4 m & 8 m) from the preferential pathway, retaining the remainder of the vadose zone conditions and the input parameters the same as that of the previous simulation. The closer the source is to the preferential pathway, the distance of vapour transport in soil before reaching the preferential pathway diminishes, resulting in less vapour attenuation. This causes a high vapour concentration to enter the preferential pathway which then travels with comparatively least resistance till the upper layer of soil with lesser attenuation, leading to an increase in indoor air concentration. Similarly, when the source is further away from the preferential pathway, more vapour travels through the soil resulting in more vapour attenuation before reaching the preferential pathway. As a result of this, comparatively less vapour concentration enters the preferential pathway and the increase in indoor air vapour concentration abates when compared to the scenario where the source is close to the preferential pathway. In Figure 6 it can be observed that when the source was at a depth of 0.5 m from the preferential pathway, a 200% increase in indoor air concentration was obtained when compared to the same scenario without preferential pathway which then gradually fell to almost 150% when the depth was increased to 8 m.

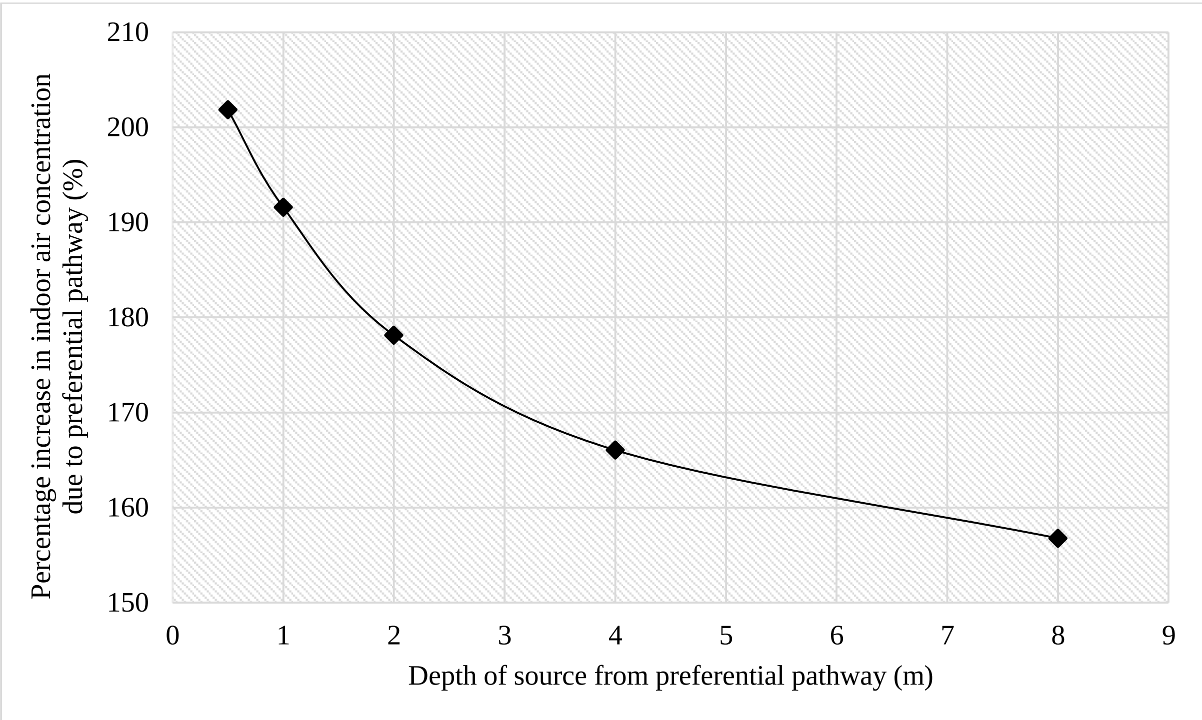


Fig. 6. Increase in indoor air concentration with preferential pathway for different depths of source to preferential pathways.

The reduction in indoor air concentration can be attributed to the higher vapour attenuation occurring in the soil before reaching the preferential pathway due to an increase in depth. As the depth increases, the vapour concentration entering the preferential pathway decreases and vice versa. Figure 7 demonstrates the concentration profile of the vadose zone for different depths of source from the preferential pathway.

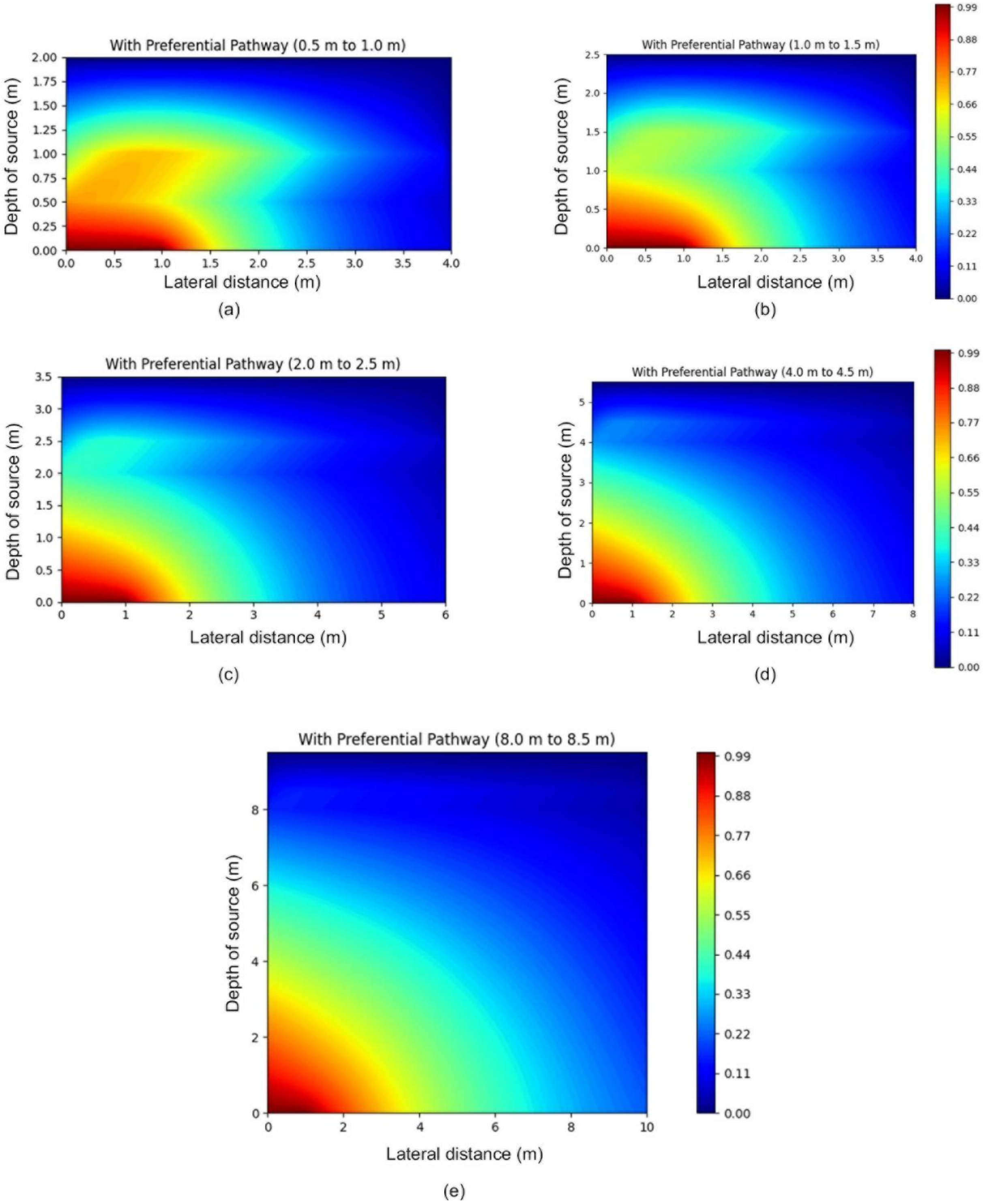


Figure 7. Vapour concentration profiles of the vadose zone for different depths of source from preferential pathway

3.2.3. Effect of lateral distance of building from the source

In order to understand the effect of lateral distance in vapour attenuation when preferential pathway was present, simulations were conducted to compare the indoor air concentrations with and without preferential pathway. Taken into account here was the building of concern at varied lateral distances from the edge of the contaminant plume. The simulations were executed considering the scenario similar to that of the first simulation but with different source to building lateral distances. A vadose zone of sandy clay soil had a depth of 2.5 m with a highly permeable preferential pathway of thickness 0.5 m at a depth of 1 m from the ground surface and the contaminant source of concentration 1 g/m^3 at a depth further 1 m from the bottom of the preferential pathway layer. For the scenario without preferential pathway, the vadose zone is considered homogeneous with sandy clay soil at a depth of 2.5 m from the ground surface. The input parameters for the simulations are same as those reported in Table 3.

It was observed that the indoor air concentration was larger in the presence of the preferential pathway as expected, but the latter's effect was significant only for a few meters laterally as shown in Figure 8. As the source to building distance increases, the effect of preferential pathway in exacerbation of VI reduces until it plays no consequential role in increasing the indoor air concentration at large lateral distances. This can be attributed to the general tendency of the vapour to move rapidly in a vertical direction, and thereby crossing the preferential pathway with least resistance vertically than laterally.

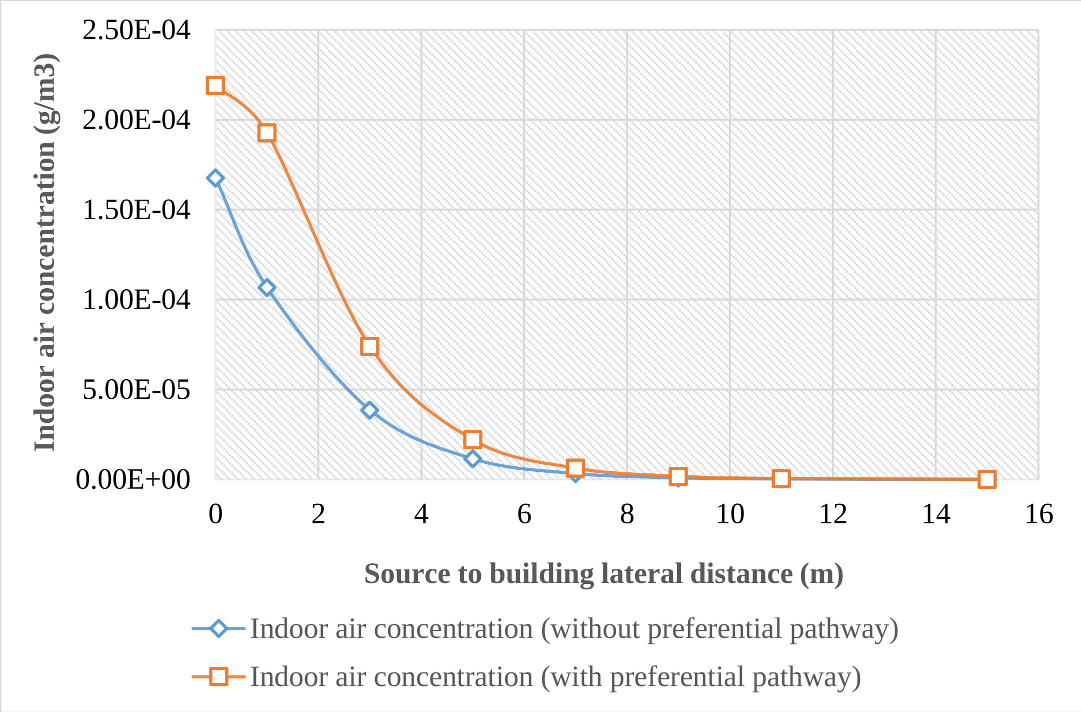


Figure 8. Indoor air concentration with and without preferential pathway vs source to building lateral distances.

3.3. Sensitivity Analysis

The influence of different types of soil texture on the indoor air concentration is investigated with the characteristics of 12 typical soils summarised in US EPA database (2012). The total porosity, water-filed porosity and intrinsic permeability used for the simulations for 12 typical soils are listed in Table 3. Simulations for sensitivity analysis were conducted using a CSM where a 0.5 m granular backfill comprising of well graded gravel acting as the preferential pathway is at a depth of 1 m below ground surface (bgs) and a TCE contaminant source 1g/m^3 at a depth of 1 m from the preferential pathway.

Table 3. Soil characteristics for 12 typical soils summarised in US EPA database

Soil Type	*Total Porosity*	*Water-filled porosity*	*Soil permeability (m^2)*
Clay	0.459	0.215	2.32×10^{-13}
Clay Loam	0.442	0.168	1.29×10^{-13}
Loam	0.399	0.148	1.90×10^{-13}
Loamy sand	0.390	0.076	1.67×10^{-12}

Sand	0.375	0.054	1.02×10^{-11}
Sandy clay	0.385	0.197	1.79×10^{-13}
Sandy clay loam	0.384	0.146	2.09×10^{-13}
Sandy loam	0.387	0.103	6.09×10^{-13}
Silt	0.489	0.167	6.92×10^{-13}
Silt loam	0.439	0.180	2.89×10^{-13}
Silty clay	0.481	0.216	1.52×10^{-13}
Silty clay loam	0.482	0.198	1.75×10^{-13}

Figure 9 shows the indoor air contaminant concentration corresponding to the various types of soil with different intrinsic permeability in the vadose zone with and without the preferential pathway. Soils with poor permeability like clay and sandy clay lead to lower indoor air contaminant concentration as opposed to sand which causes an increased indoor air contaminant concentration due to its high permeability. An increase of more than one order of magnitude in indoor air vapour concentration was observed with highly permeable soils in the vadose zone as compared to soils with low permeability. The presence of highly permeable preferential pathway of 0.5 m causes almost a two-fold increase in indoor air concentration for all soil types.

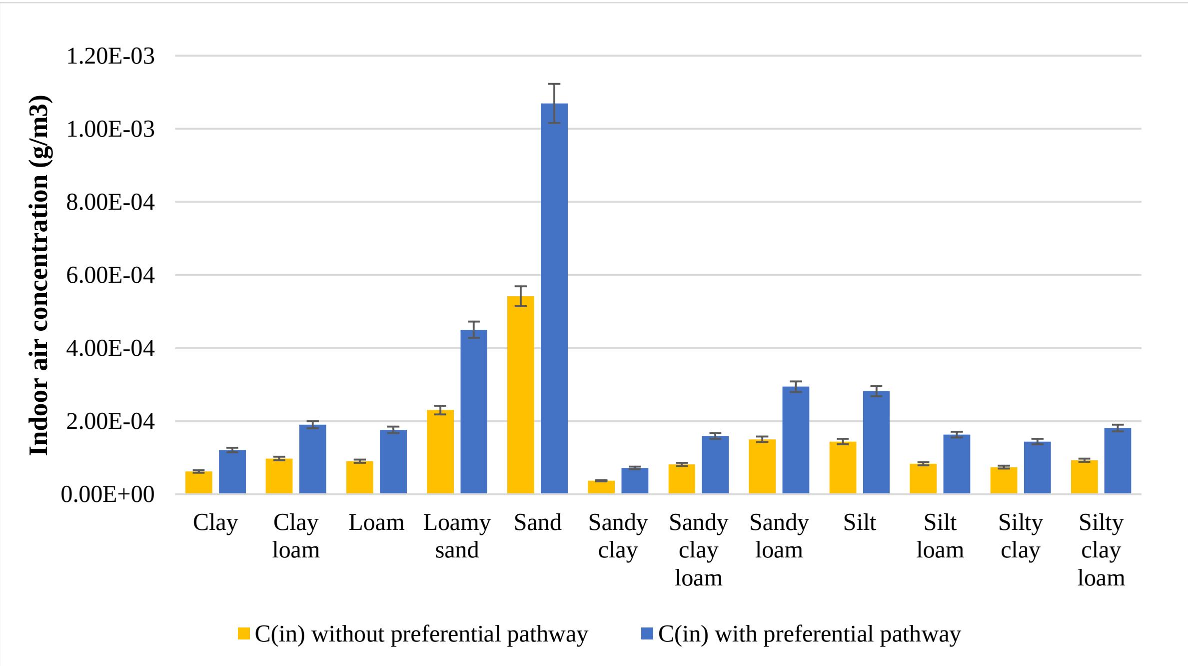
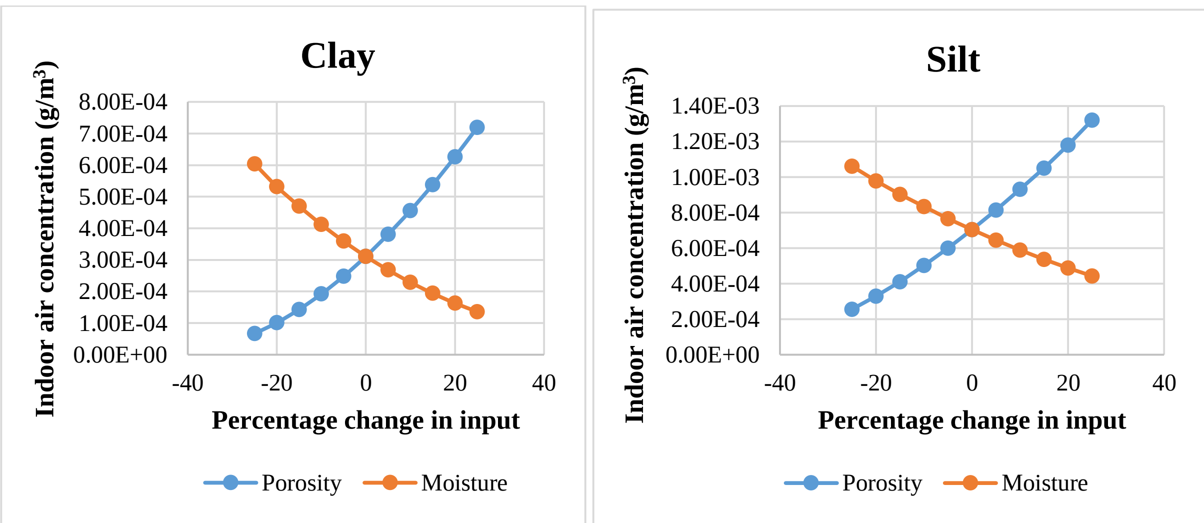
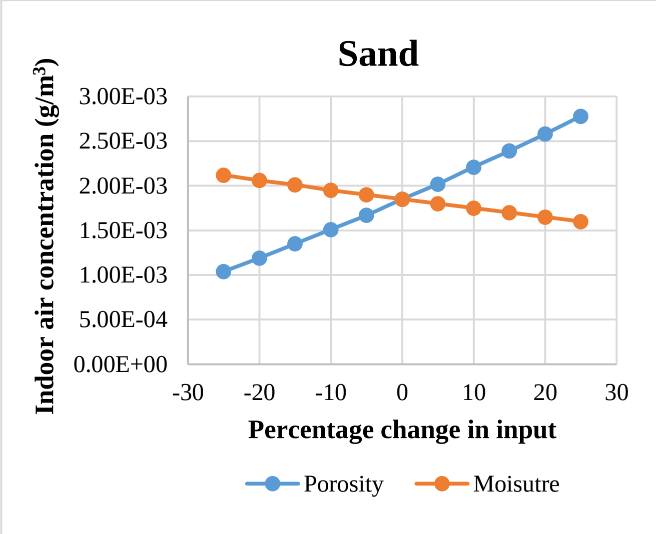


Figure 9. Simulated indoor air concentrations for 12 typical soils summarised in US EPA database.

To understand the effect of soil porosity and moisture, a one-at-a-time (OAT) sensitivity analysis technique was conducted in three different types of soils (clay, silt and sand). The outputs were obtained and compared by varying the input parameters by ±25% (Ma et al., 2016) from the default values of clay, silt and sand (given in table 3). Figures 10 (a) (b) and (c) shows the sensitivity behaviour of soil moisture and soil porosity in this model for clay, silt and sand, respectively. The sensitivity behaviour of soil moisture and soil porosity is observed to depend on the soil type. The change in indoor air concentration is almost exponential in clay when compared to a linear change in sand. So it can be stated here that changes in soil porosity and moisture content are more sensitive in soils with low permeability. Increase in soil porosity provides greater passageways for vapour migration, resulting in increased diffusive flux in the sub-surface and subsequently higher indoor air vapour concentration. Concurrently, an increase in soil moisture acts as a large resistance to diffusion. As the moisture content in the soil increases, the effective air diffusivity wanes, resulting in additional partitioning into liquid phase. Hence the soil gas concentration is reduced which ultimately lowers the indoor air vapour concentration.



(a) (b)



(c)

Figure 10. Changes in indoor air vapour concentration with variations in soil porosity and moisture in (a) clay, (b) silt and (c) sand.

3.4. Effect of depth of preferential pathway

The presence of any kind of high permeability region in the vadose zone – either natural or anthropogenic – can facilitate higher contaminant flux both vertically and laterally owing to its high permeability than the surrounding soils. Figure 11 shows a significant increase in indoor air contaminant concentration for different depths of highly permeable layer in the vadose zone acting as the preferential pathway. From the simulations, a 1 m deep preferential pathway can lead to an almost 70% increase in indoor air contaminant concentration compared to a no preferential pathway scenario. As the depth of preferential pathway increases, the contaminant vapour has more room for migration with least resistance in the vadose zone resulting in lower attenuation and hence higher indoor air vapour concentration.

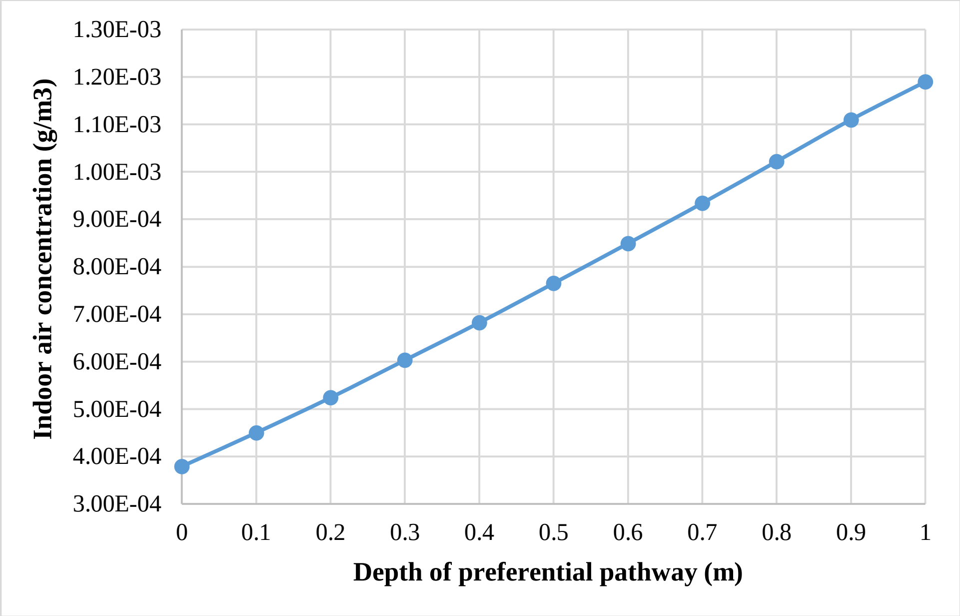


Figure 11**.** Simulated indoor air contaminant concentration for varying depths of preferential pathway.

4. Conclusion

Detecting the impacts of VI outside the contaminant plume footprint has led to research seeking to understand the role of preferential pathways in VI. Though the majority of studies involving preferential pathways focused on sewer VI investigations, the roles of highly permeable soil layers and backfill materials have rarely been examined. This model was developed to illustrate the role of highly permeable granular soil layers like gravel or crushed rocks used as beddings and backfills for utility lines in exacerbating the indoor air vapour concentrations.

Despite some guidance documents suggesting highly permeable soil zones may act as preferential pathways, it is not documented anywhere with sufficient importance suggesting that these pathways might well be addressed by standard VI investigation measures. However from this study, these preferential pathways were found to exacerbate the indoor air concentration depending on the depth of the contaminant plume from the preferential pathway layer. The close proximity of the source to the preferential pathway resulted in an increase of indoor air concentration as high as 200% compared to a no-preferential pathway scenario which then decreased to about 150% as the depth of source to preferential pathway increased with respect to the simulations' parameters. Although it can be considered not a significant increase in evaluating VI risks, such an increase in indoor air concentration can influence the screening criteria and response levels of the affected sites by considering it safe or whether an investigation or intervention is necessary. In the lateral direction, despite the presence of preferential pathway causing an increased risk of VI, the impact in indoor air concentration is evident only until a few meters from the plume's edge. As the source to building distance increases, the preferential pathway seems to play no substantial role in increasing indoor air concentration at very large lateral distances.

Natural soil varies widely in permeability which greatly influences the rate of vapour entry into buildings. Soils with high permeability like sand result in higher indoor air concentration, of a greater than one order of magnitude, than soils with low permeability like clay. The presence of a highly permeable preferential pathway aggravated (in fact doubled) the vapour transport increasing the indoor air vapour concentration. Vapour transport in the vadose zone is largely influenced by soil porosity and soil moisture as they influence the effective diffusivity of the vapour in soil. The sensitivity of these soil parameters is more pronounced in soils with low permeability.

Since the proposed model is based on a CSM scenario of CVI where the building is located laterally at a distance from the edge of an infinite and uniform contaminant plume, a proper evaluation of the site needs to be conducted for this model to have feasible applications. This model can be implemented in places where a highly permeable preferential pathway is prevalent in the vadose zone which exacerbates VI in the building. As far as limitations are concerned, this model cannot be used for sites with PVI since biodegradation is not considered here. The subsurface heterogeneity and the effect of rainfall, snow and changes in groundwater levels were ignored during the model's development. Hence a proper evaluation is necessary to understand whether these assumptions are reasonable for sites under consideration.

Declaration of Competing Interests

We declare that we have no financial and personal relationships with other people or organisations of any kind that could be influencing our work presented in the manuscript titled, "Two-dimensional vapour intrusion model involving advective transport of vapours with a highly permeable granular layer in the vadose zone serving as the preferential pathway".

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LIST OF TABLES

Table 1. Input parameters for the model simulations.

Chemical Parameters		*Unit*	*Value*
Source vapour concentration	C_s	g/m3	1
Diffusion coefficient in air	D_a	m2/s	7.90E-06
Diffusion coefficient in water	D_w	m2/s	9.10E-10
Henry's law constant	H	-	0.403
Soil gas viscosity	μ	Pa.s	5.32E-04
Soil Parameters			
Total Porosity	Θ_T	-	0.385
Air filled porosity	Θ_a	-	0.188
Water filled porosity	Θ_w	-	0.197
Soil air permeability	K_a	m^2	1.70E-13
Granular backfill soil parameters			
Depth of backfill	ds	m	0.5
Total Porosity	Θ_T	-	0.5
Air filled porosity	Θ_a	-	0.49
Water filled porosity	Θ_w	-	0.01
Soil air permeability	K_a	m^2	1.00E-09
Building parameters			
Width of foundation slab		m	10
Foundation footprint area	A_b	m2	100
Depth of foundation below grade	d_f	m	0.3
Thickness of foundation crack	t_{ck}	m	0.1
Width of foundation crack	w_{ck}	m	0.001
Foundation perimeter	l_{ck}	m	40
Building height	L_{mix}	m	3
Building Air exchange rate	ER	h^{-1}	0.5
Soil and building pressure difference	Δp	Pa	5

Table 2. Comparison of sub-slab concentration, indoor air concentration and attenuation factor with and without the preferential pathway for different scenarios.

	Without preferential pathway	*With preferential pathway*
Source concentration (g/m^3)	1	1
Sub-slab concentration (g/m^3)	0.025	0.048
Indoor air concentration (g/m^3)	3.86E-05	7.40E-05
Attenuation factor (α)	3.86E-05	7.40E-05

Table 3. Soil characteristics for 12 typical soils summarised in US EPA database

Soil Type	***Total Porosity***	***Water-filled porosity***	***Soil permeability (m^2)***
Clay	0.459	0.215	2.32×10^{-13}
Clay Loam	0.442	0.168	1.29×10^{-13}
Loam	0.399	0.148	1.90×10^{-13}
Loamy sand	0.390	0.076	1.67×10^{-12}
Sand	0.375	0.054	1.02×10^{-11}
Sandy clay	0.385	0.197	1.79×10^{-13}
Sandy clay loam	0.384	0.146	2.09×10^{-13}
Sandy loam	0.387	0.103	6.09×10^{-13}
Silt	0.489	0.167	6.92×10^{-13}
Silt loam	0.439	0.180	2.89×10^{-13}
Silty clay	0.481	0.216	1.52×10^{-13}
Silty clay loam	0.482	0.198	1.75×10^{-13}

Figure 1

Click here to access/download;Figure;Figure 1.tif

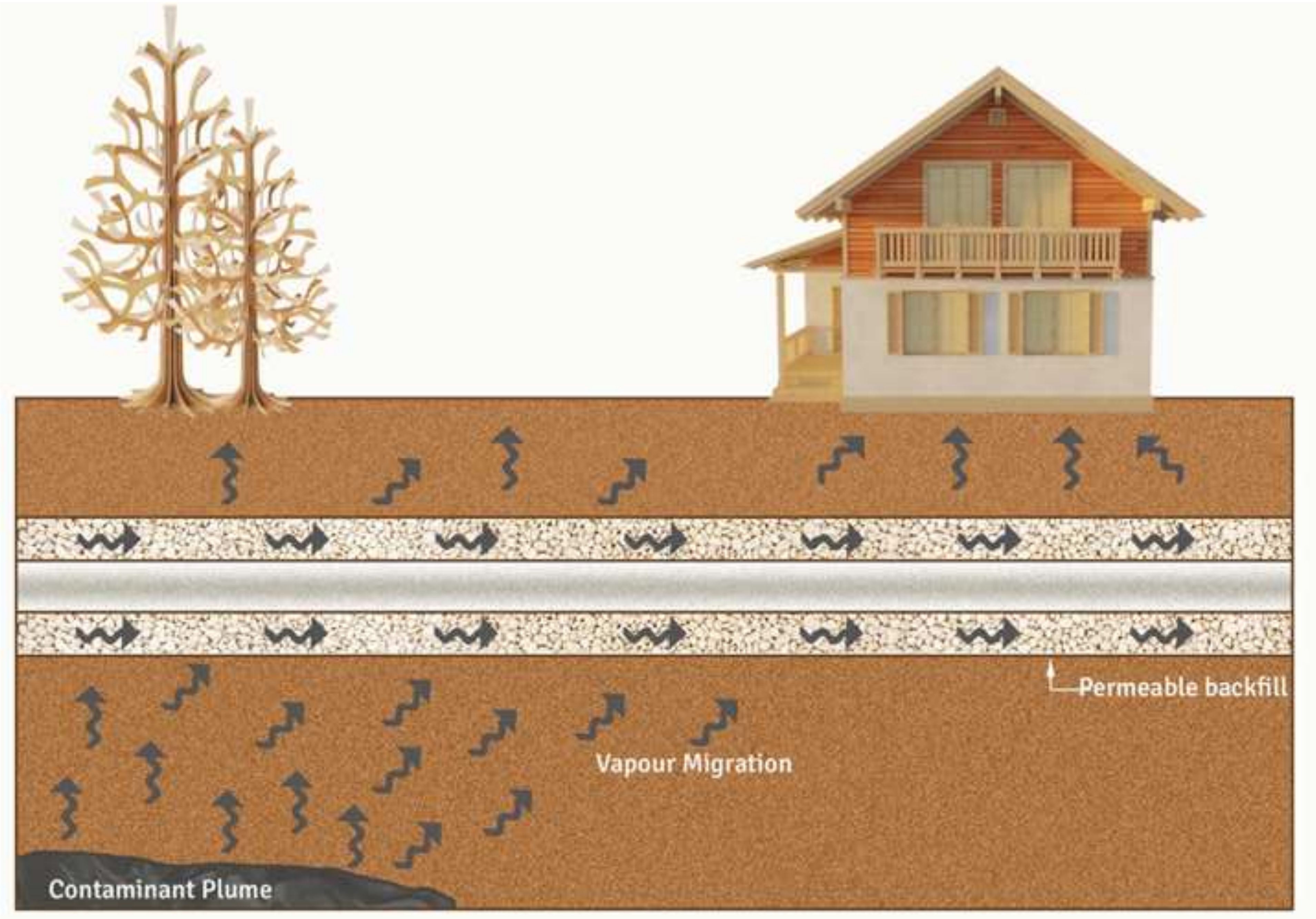


Figure 2

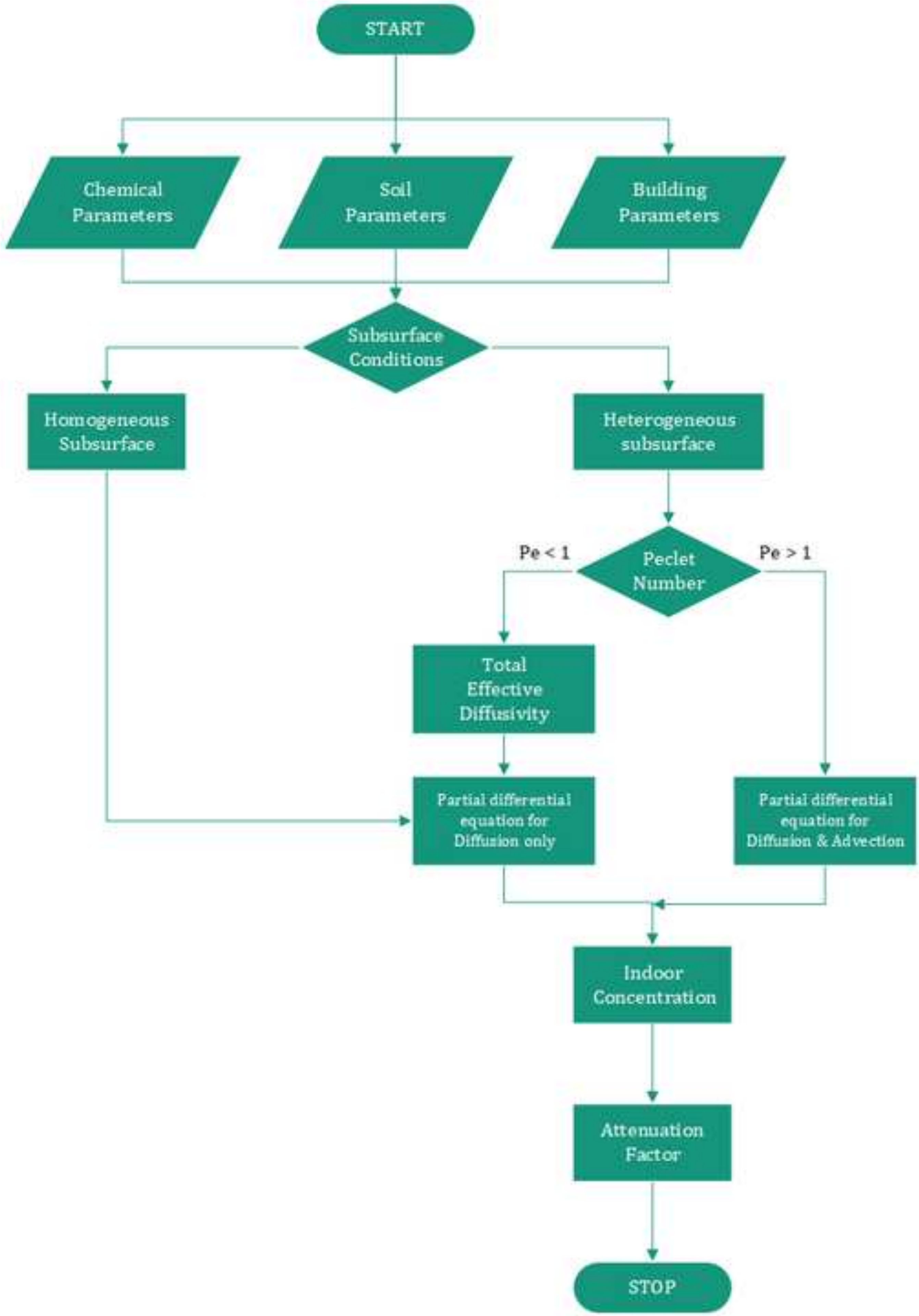
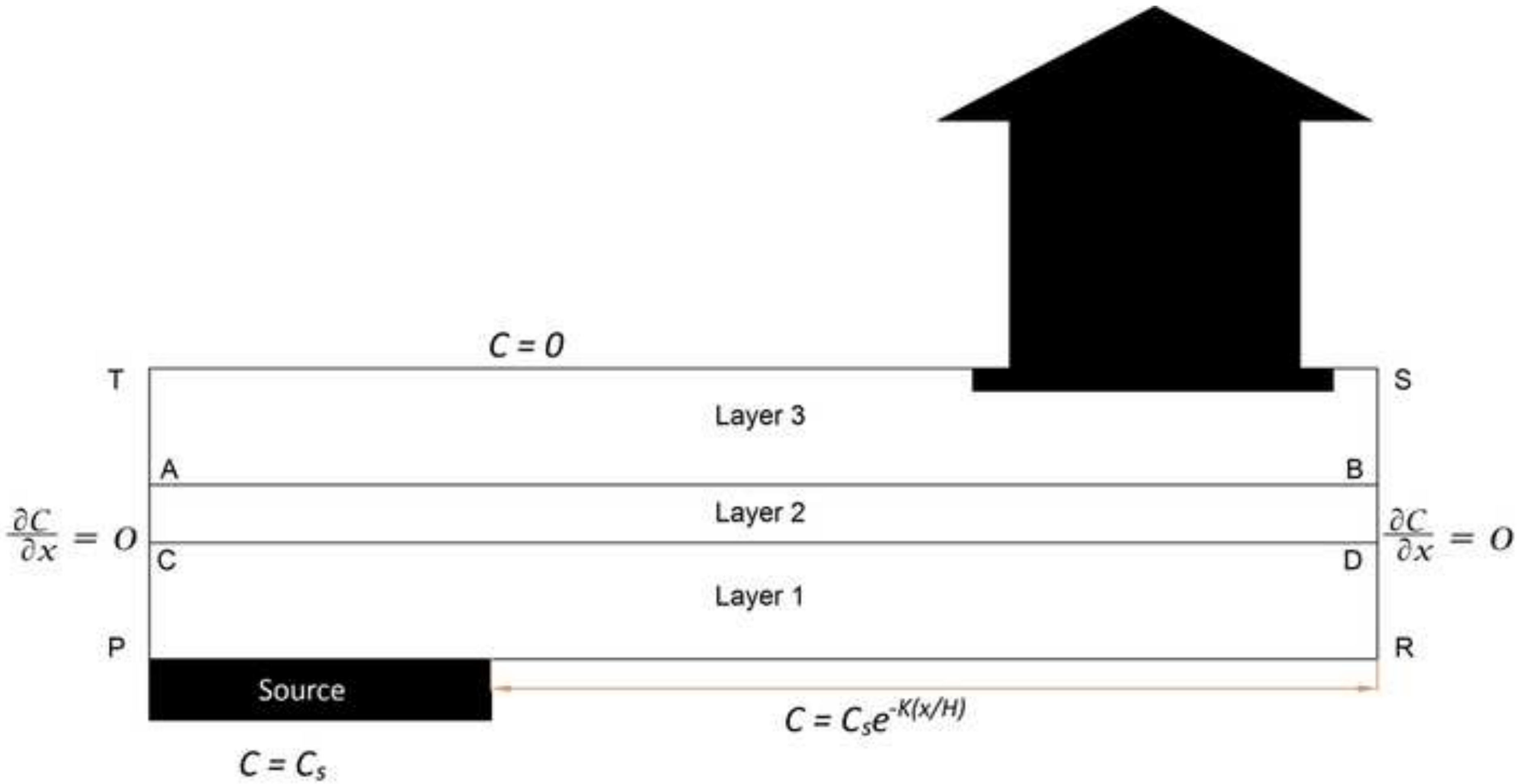

START
Chemical Parameters
Soil Parameters
Building Parameters
Subsurface Conditions
Homogeneous Subsurface
Heterogeneous subsurface
Pe < 1
Peclet Number
Pe > 1
Total Effective Diffusivity
Partial differential equation for Diffusion only
Partial differential equation for Diffusion & Advection
Indoor Concentration
Attenuation Factor
STOP

Figure 3



C = 0
T
S
Layer 3
A
B
Layer 2
$\frac{\partial C}{\partial x} = O$
$\frac{\partial C}{\partial x} = O$
C
D
Layer 1
P
R
Source
$C = C_s e^{-K(x/H)}$
$C = C_s$

Figure 4

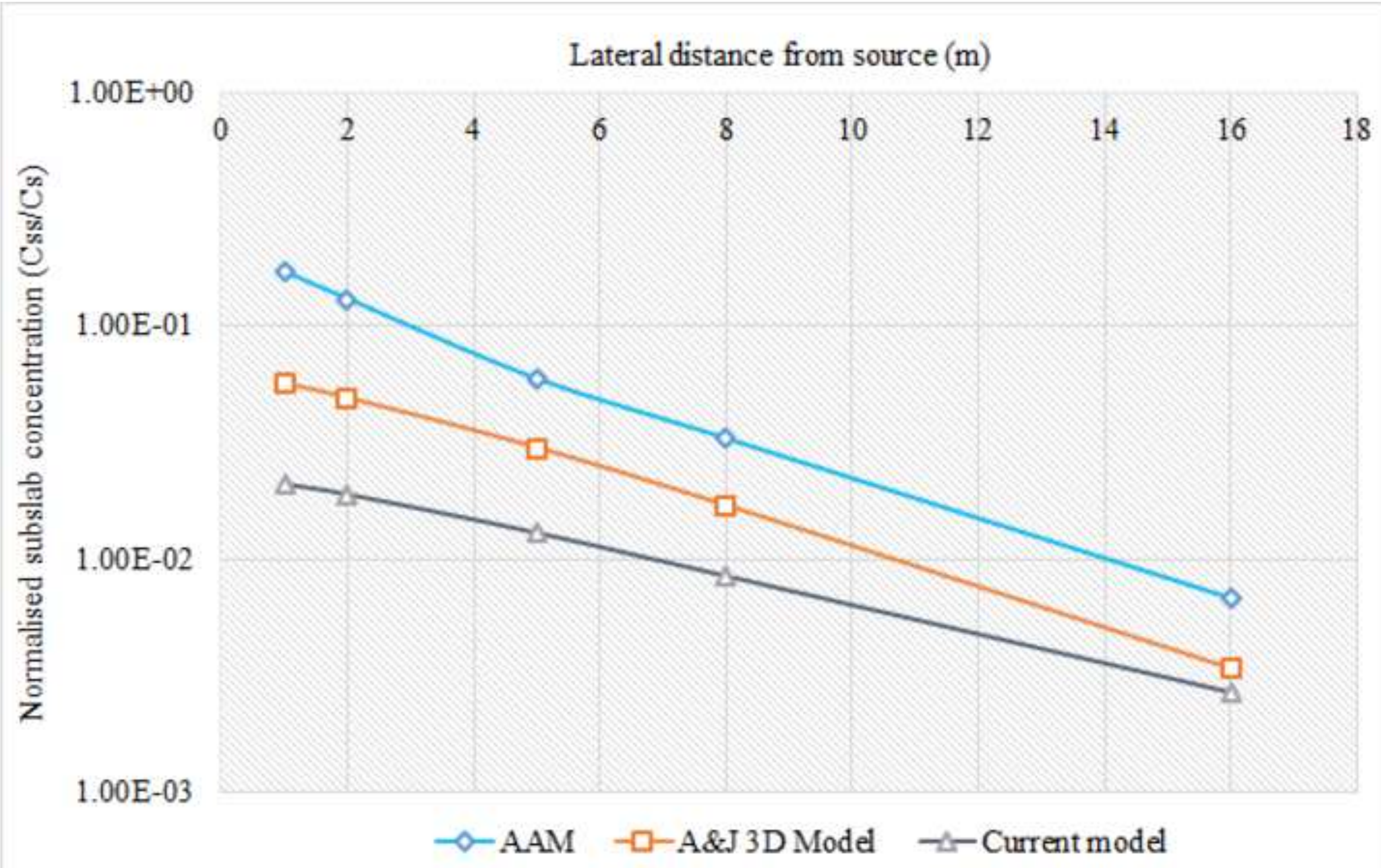

Lateral distance from source (m)
0
2
4
6
8
10
12
14
16
18
1.00E+00
1.00E-01
1.00E-02
1.00E-03
Normalised subslab concentration (Css/Cs)
AAM
A&J 3D Model
Current model

Figure 5

Click here to access/download;Figure;Figure 5.tif

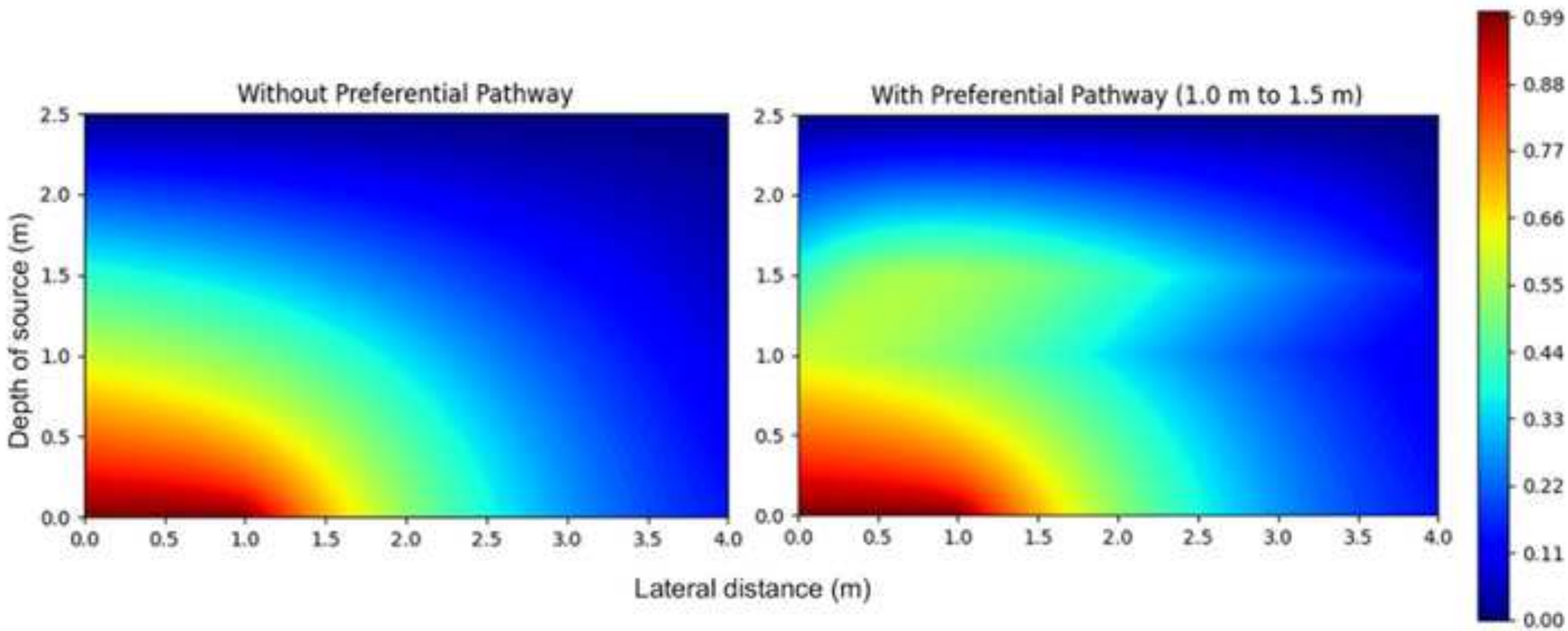


Figure 6

Click here to access/download;Figure;Figure 6.tif

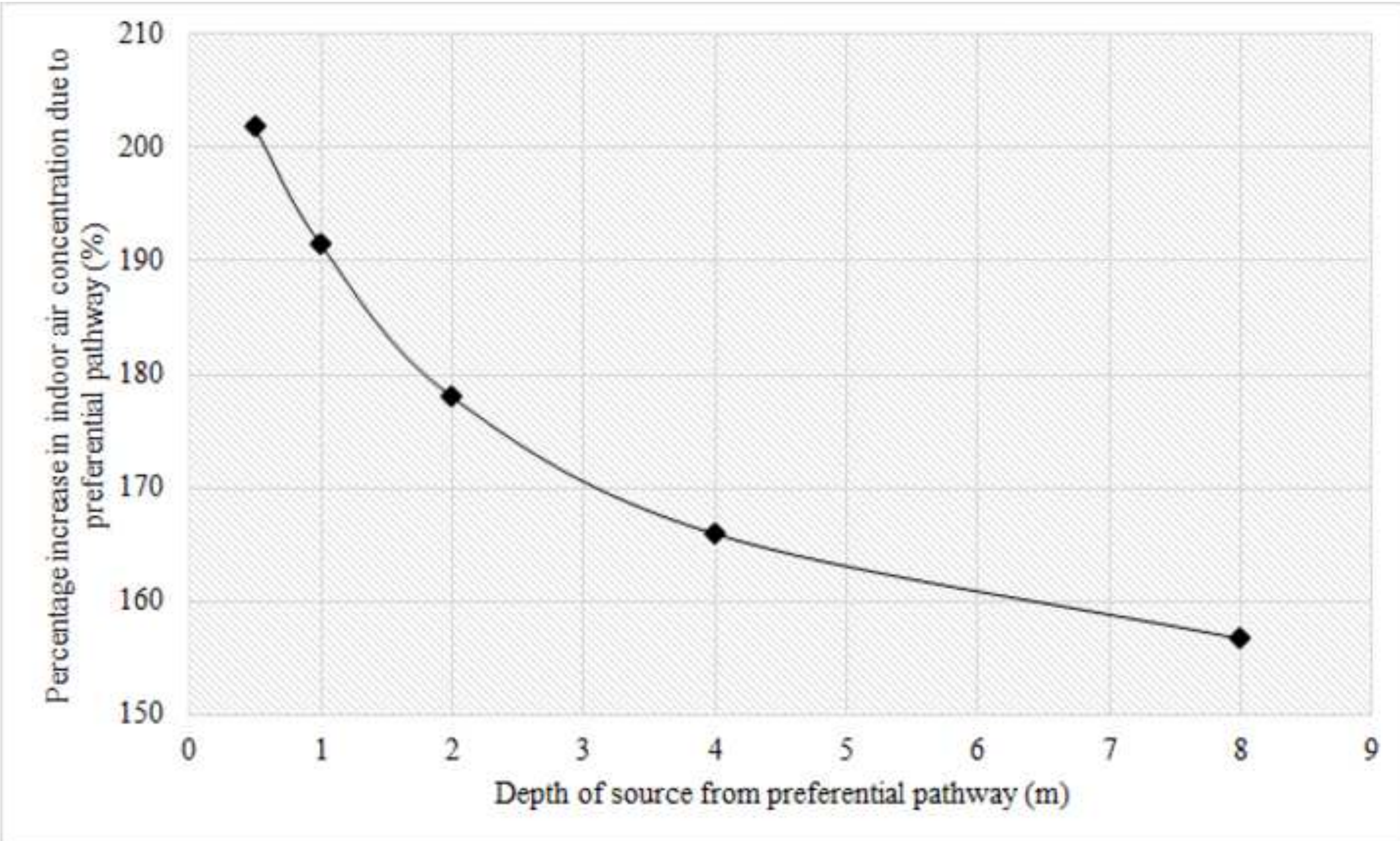


Figure 7 Click here to access/download;Figure;Figure 7.tif

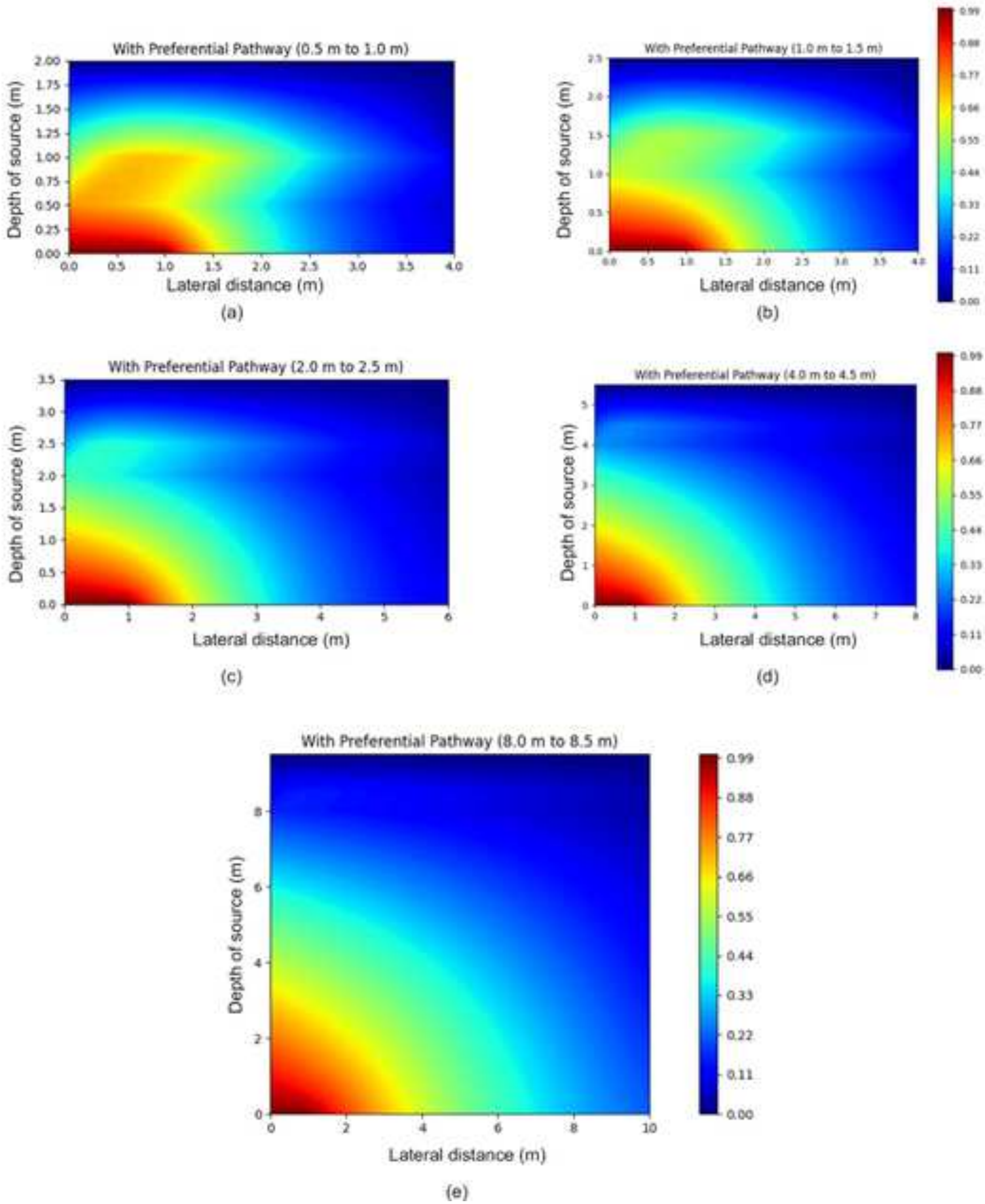
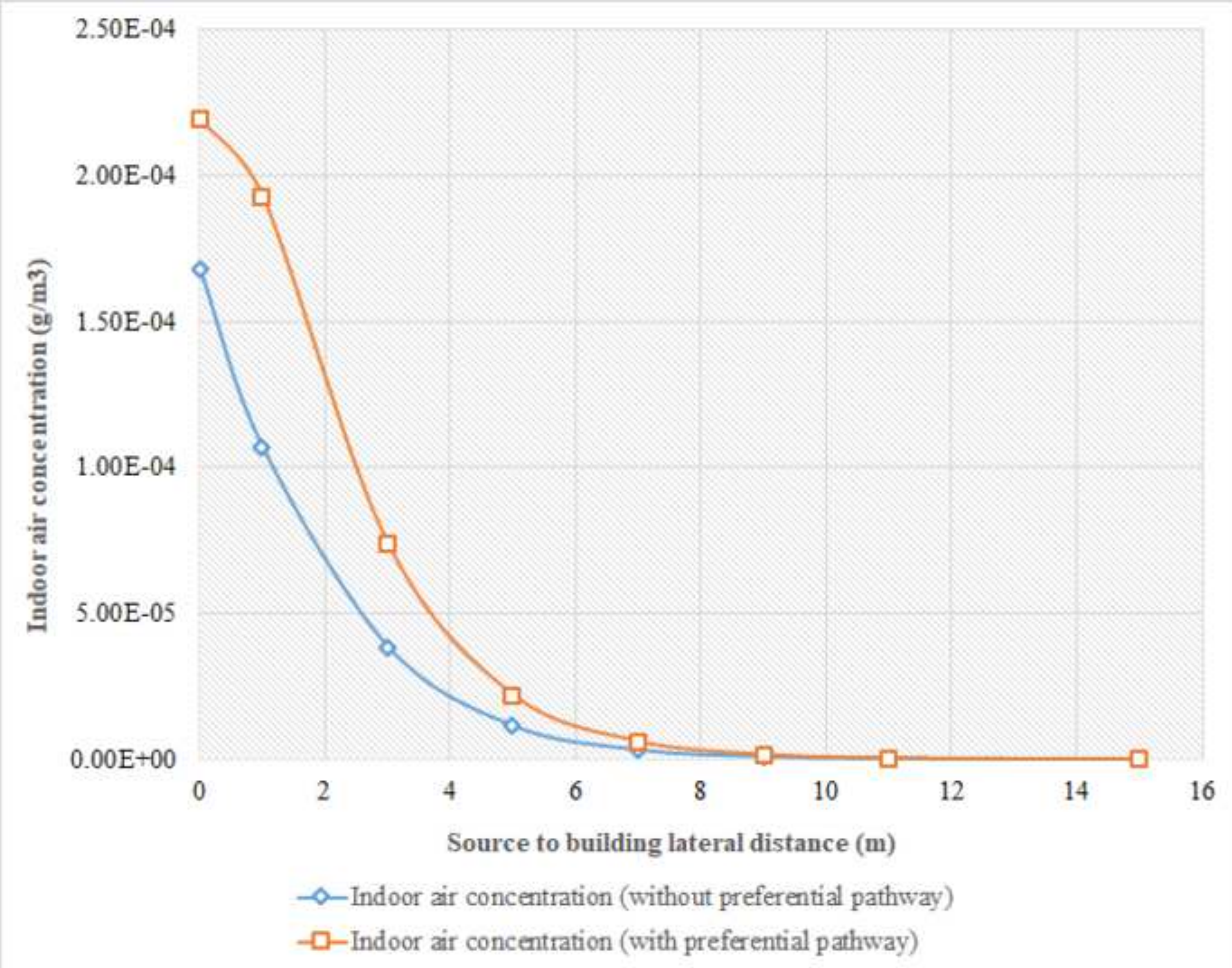
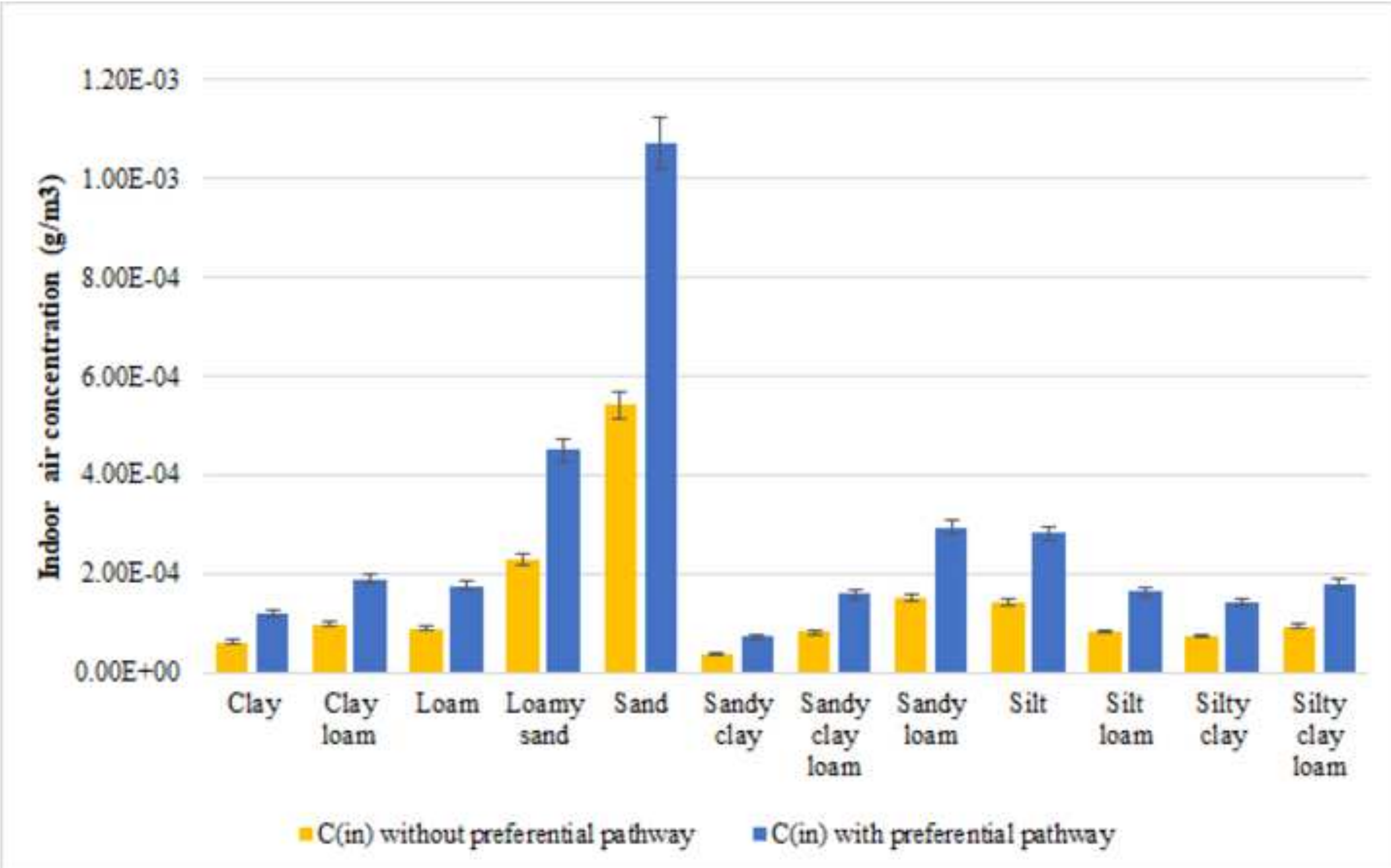


Figure 8

Click here to access/download;Figure;Figure 8.tif





1.20E-03
1.00E-03
8.00E-04
6.00E-04
4.00E-04
2.00E-04
0.00E+00
Indoor air concentration (g/m3)
Clay
Clay loam
Loam
Loamy sand
Sand
Sandy clay
Sandy clay loam
Sandy loam
Silt
Silt loam
Silty clay
Silty clay loam
C(in) without preferential pathway
C(in) with preferential pathway

Figure 10 a

Click here to access/download;Figure;Figure 10 a.tif

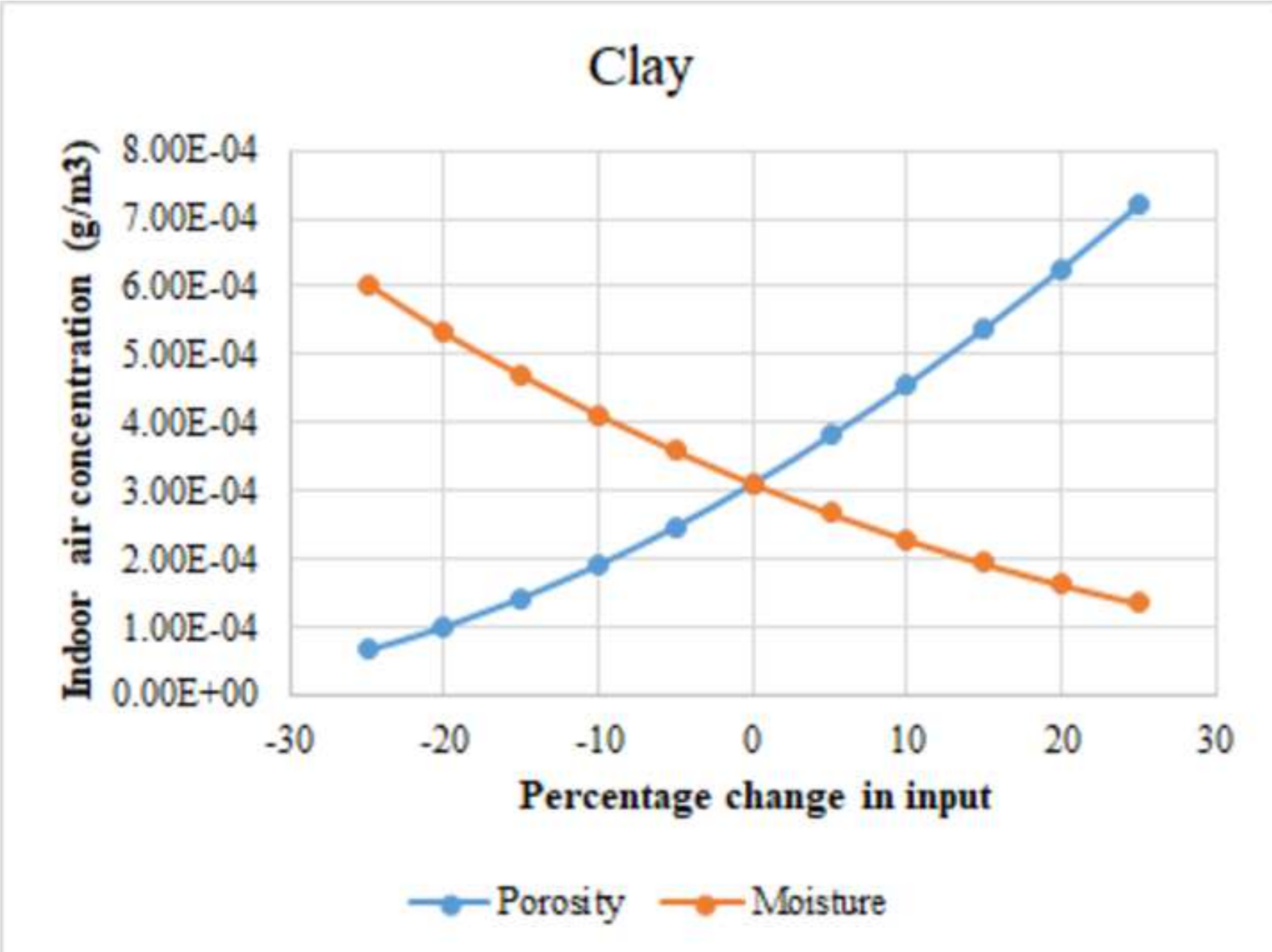


Figure 10 b

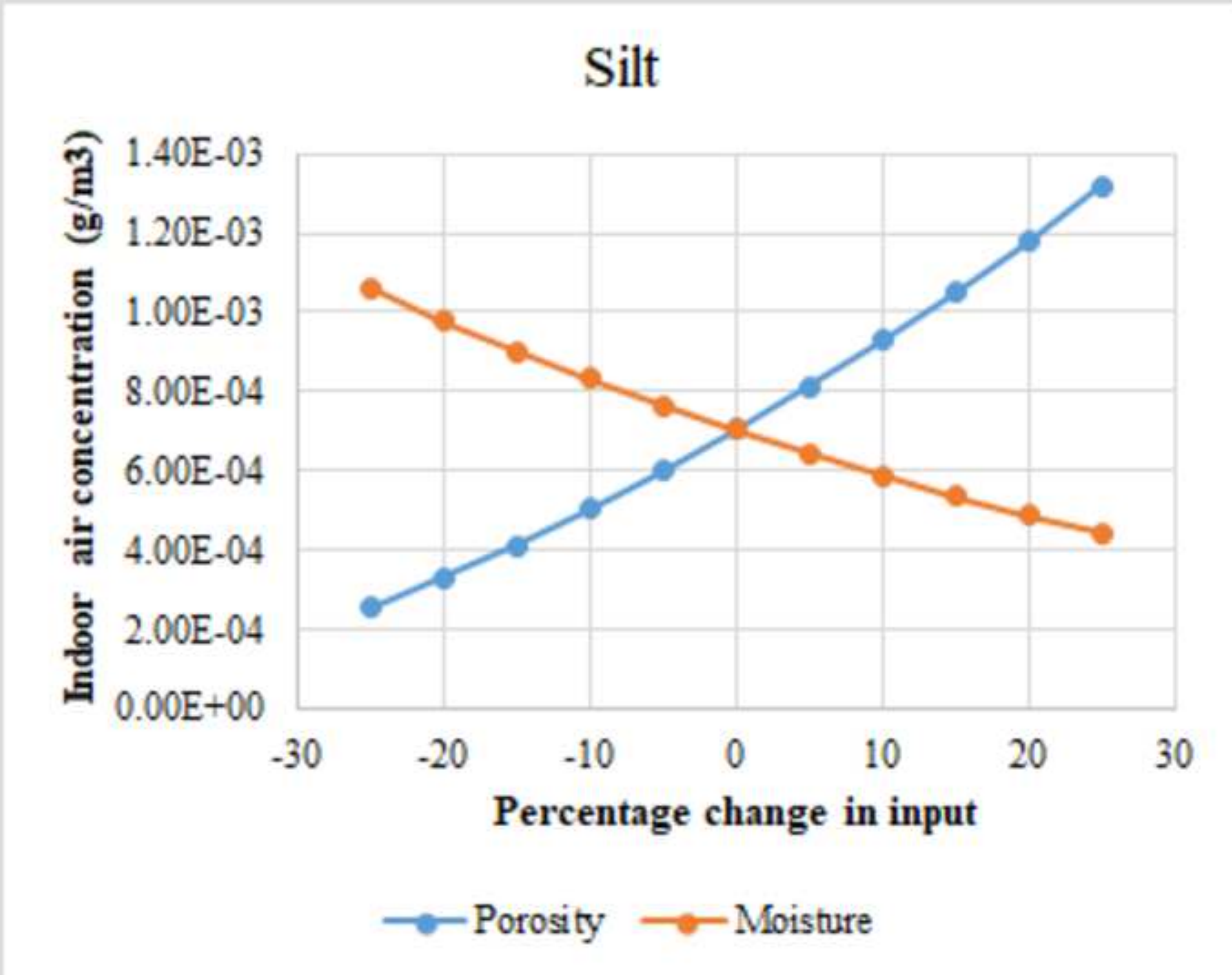

Silt
Indoor air concentration (g/m3)
1.40E-03
1.20E-03
1.00E-03
8.00E-04
6.00E-04
4.00E-04
2.00E-04
0.00E+00
-30
-20
-10
0
10
20
30
Percentage change in input
Porosity
Moisture

Figure 10 c

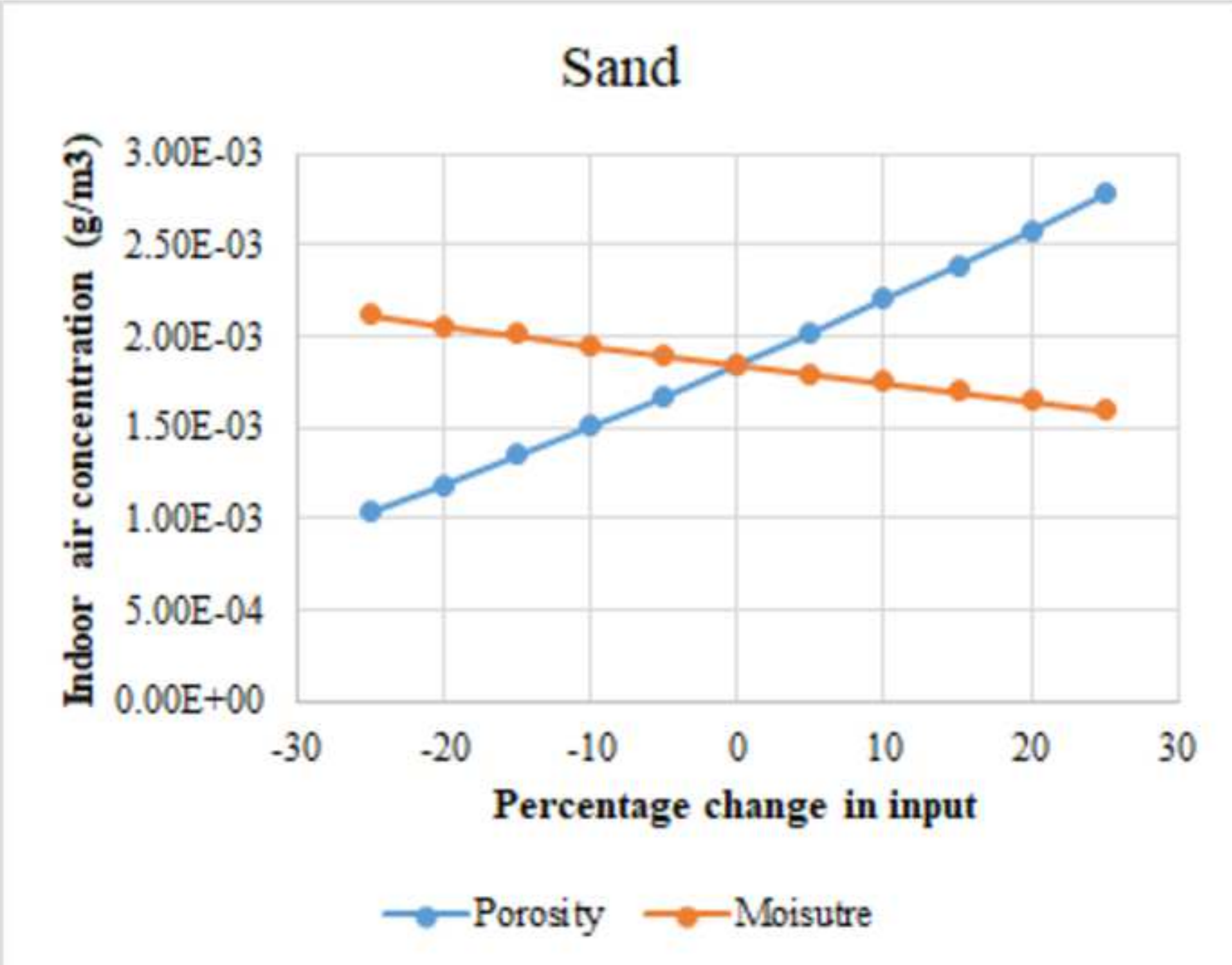
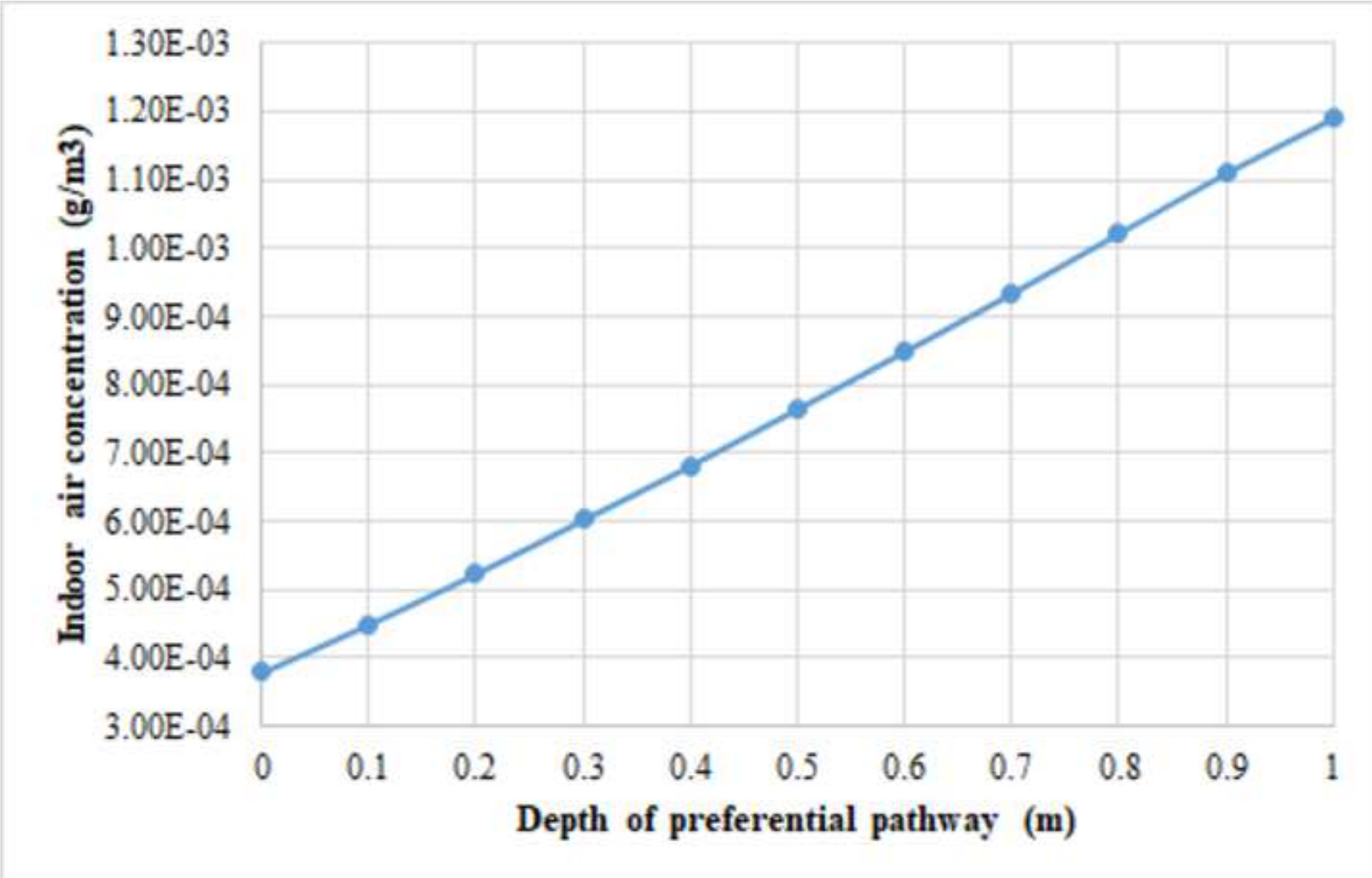

Sand
Indoor air concentration (g/m3)
3.00E-03
2.50E-03
2.00E-03
1.50E-03
1.00E-03
5.00E-04
0.00E+00
-30
-20
-10
0
10
20
30
Percentage change in input
Porosity
Moisutre

Figure 11

Click here to access/download;Figure;Figure 11.tif



Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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Aravind Unnithan, Methodology, Investigation, Formal analysis, Writing - Original Draft; Dawit Nega Bekele, Methodology, Formal analysis, Supervision, Writing - Review & Editing; Sreenivasulu Chadalavada, Methodology, Supervision, Resources, Writing - Review & Editing; Ravi Naidu, Conceptualization, Writing - Review & Editing, Supervision, Funding acquisition;