Influence of the lateral source/building separation on vapour intrusion: A numerical study

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Abstract. Various vapour intrusion (VI) models have been proposed in order to predict indoor concentration of Volatile Organic Compounds (VOCs) in buildings. However, these models tend to be conservative, and overestimate or underestimate vapour flux emissions due to several assumptions. Particularly, most of these VI models only consider an infinite uniform contaminated groundwater as the principal source of VOCs in the soil, and lateral pollution source in the vadose zone are disregarded. It has been shown that ignoring the lateral source position may lead to uncertainties on the estimations. In this paper, a numerical model is developed in order to better understand the relationship between the lateral source position in the soil, including both a source in the vadose zone and a source located at the groundwater level, and the resulting indoor air concentration. Results show that source position plays a significant role on vapour intrusion attenuation. In fact, indoor concentration of VOCs decreases with increasing lateral separation. Finally, it is shown that considering the source position can significantly improve the quality of VI predictions.

1 Introduction

VOCs can migrate from the subsurface (contaminated groundwater or soil) into buildings (vapour intrusion) by the difference in concentrations (diffusion) and air pressure between the subsurface contaminated areas and the indoor spaces (advection) [1]. In the soil distant from the building, vapours are transported mainly by diffusion, however in the subsurface near the building, the vapour entry into the building is due to both diffusion and advection (Figure 1). Vapour intrusion (VI) occurs essentially through the cracks and/or openings existing in the building foundation and may cause human health problems associated with the exposure of VOCs in the indoor environments [1].

Various numerical and analytical models have been proposed to predict VI [2]–[5]. Numerical models are useful for their capacity to capture precise characteristics of VI scenarios, but a significant computational effort is required and measured parameters from the studied site are needed. For this reason, analytical screening tools are much more used in practice. Nevertheless, analytical models present uncertainties mainly due to the assumptions made in their development [6], [7].

Most of VI models consider the contaminated plume is directly underneath the building (infinite homogeneous distribution of the contaminant source beneath the building). However, in reality, contaminant-source distribution is generally not uniform except in some certain localized area. Then, the application of classic VI models happens to be unrealistic in many cases [8].

![Fig. 1. Schematic modelling of vapour intrusion mechanisms and pathways.](image-url)

The issue of finite sources has received less attention and thus only few studies consider lateral migrations [2], [9]–[12]. The authors agree that lateral diffusion and...
soil/atmosphere interface play a significant role in indoor gas concentration attenuation. In fact, if the subsurface source is shallow and the ground surface is open to the atmosphere, vapour migration is mainly upwards toward the atmosphere [2]. Thus, the atmosphere, having a much larger area than vapour intrusion pathways, serves as a much more important sink than the foundation porosity and cracks [12].

In this context, the main objective of this work is to propose a numerical study to better understand the relationship between the lateral source position in the soil, including both a source in the vadose zone (unsaturated zone from the top of the ground surface to the water table) and a source located at the groundwater level, and the resulting indoor air concentration.

## 2 Model Development

OpenFOAM is used as the modelling tool. It is a Computational Fluid Dynamics (CFD) open source software based on C++ programming language for the development of numerical solvers in continuum mechanics. Finite element method is employed to solve continuity and general transport equations in order to calculate the vapour intrusion.

The 3-D model proposed in this work simulates the vapour transport in the vadose zone and its entry into the building through the vapour intrusion pathways (foundation porosity and existing cracks).

This model is based on the following hypotheses:

- Stationary pollutant transport.
- Soil considered as a homogeneous and isotropic porous media.
- Vapour source constant and infinite.
- No transfer towards the groundwater allowed.
- Pollutant entering into the building mixes immediately and homogeneously [4].
- Pollutant supposed to be completely diluted as soon as it reaches the atmosphere.
- Biodegradation and chemical interactions with the media not considered.

The transport of pollutants from the source of pollution to the building is governed by the continuity equation (1) and the general transport equation (2):

\[
\nabla \cdot (\rho \phi_d \mu_d \nabla p) = 0 
\]  

\[
\nabla \cdot F_i = 0 
\]  

where \( p \) is the pressure of the soil gas [M/L/T²]; obtained from Eq. 1 and Darcy’s law (\( q_g = (k_g/\mu_d) \nabla p \)), \( F^p \) is the pressure to the relative atmospheric conditions [M/L/T²], \( \nabla \) is the vector operator [L⁻¹], \( \phi_g \) is the gas-filled porosity [L³/L³], \( k_g \) is the soil gas permeability [L²], \( \mu_g \) is the soil gas dynamic viscosity [M/L/T], and \( C_i \) is the total concentration of the pollutant \( i \) in the soil [M/L³] and \( F_i \) is the mass flux vector (\( F_i = C_i \phi_d \mu_d - D_g \nabla C_i \)) [M/L²/T].

### 2.1 Model Domain and Boundary Conditions

A schematic of the modelling scenario is shown in Figure 2. The domain extension was chosen to be large enough to avoid the impact of lateral boundary conditions on the calculations [2], [5], [8], [13].

![Fig. 2. Schematic and boundary conditions of the modelling scenario.](image)

No flow boundary conditions are assigned at the lateral and at the lower horizontal boundaries (Eq. 3).

\[
\nabla \cdot \mathbf{n} = 0 
\]  

where \( \mathbf{n} \) is the normal vector to the surface of interest.

Pressure at the ground surface, \( p_{atm} \), and in the building, \( p_{indoore} \), are constant. For simulation results presented below, \( p_{atm} = 0 \) and \( p_{indoore} = constant \).

No vapour flux boundary conditions are assigned at the lateral, and at the lower horizontal boundaries (Eq. 4).

\[
\nabla C_{ig,n} = 0 
\]  

The vapour concentration at the ground surface (soil/atmosphere interface) is prescribed to be their atmospheric concentration (generally approximated to be zero):

\[
C_{ig} = C_{ig, atm} 
\]  

### 2.2 Vapour Source Concentration

A volume is generated in the domain in order to simulate the corresponding vapour source zone (Eq. 6).

\[
C_{ig} = C_{ig, source} 
\]  

### 2.3 Indoor Air Concentration

The indoor air concentration is determined from a steady-state mass balance in the enclosed space:

\[
C_{ig, indoor} = J / A_{ex} V_b 
\]  

where \( J \) is the total flux across the building foundation [M/L²/T], \( V_b \) is the enclosed space volume [M³], and \( A_{ex} \) is the air change rate of the building [1/T]. The values of \( C_{ig, indoor} \) and \( J \) are obtained iteratively. The iterations stop when the convergence criteria (10⁻⁶) is reached.

### 3 Considered Pollution Scenarios
Numerical models are proposed in order to simulate the different pollution scenarios and to better understand the transfer of soil gas pollutants in the vadose zone and into the buildings. The modelling of these scenarios is made by simplified representations according to the characteristics of each configuration (positioning of the source, boundary conditions, etc.). Among the different pollution configurations, three representative scenarios have been identified:

- Infinite homogeneous source: contaminated groundwater or soil.
- Finite source: at the groundwater level or soil stratification.
- Finite source: diffuse source in the vadose zone.

Table 1 summarizes the characteristics of the different pollution configurations.

Table 1. Description of the three studied configurations.

| POLLUTION SCENARIO | DESCRIPTION | NUMERICAL MODELISATION |
|--------------------|-------------|-----------------------|
| Spreading spills... | Spills storage sites... | Spills, storage sites or soil stratifications. |
| Spills, storage sites... | Entering into the vadose zone scenario. |
| Gas leaks, storage sites, mine tailings... | Soil stratifications... |

The model inputs are summarized in Table 2.

Table 2. Input parameters of the model.

| Building/foundation properties | |
|-------------------------------|---|
| Length                        | 10 m |
| Width                         | 10 m |
| Foundation type               | Crawl space |
| Enclosed space volume (V_b)   | 250 m³ |
| Air exchange rate (A_e)       | 0.5 h⁻¹ |
| Indoor pressure (p_inh)       | 4 Pa |
| Contaminant vapour source properties | |
| Source size                   | 1 x 1 m |
| Source vapour concentration (C_{source}^v) | 1 mol/m³ |
| Overall effective diffusivity in the soil (D_{source}^v) | 8.68 10⁻⁷ m²/s |
| Source depth (H)              | 4 - 20 m |
| Source lateral separation (L) | 0 - 20 m |

Soil properties

- Soil permeability (k_{soil}) | 10⁻¹¹ m² |
- Dynamic viscosity (µ_g) | 10⁻⁵ Pa.s |

These inputs (dimension, air exchange rate, pressure, foundation features) are based on the values reported in the literature [2], [5], [8], [13], [14].

4 Results and Discussion

The numerical accuracy of the code was assessed in several ways. First, the output was compared with semi-empirical models [14], [15] for simplistic two-dimensional steady-state of pressure and concentration profiles in homogeneous and layered setting. Second, the numerical model output was compared with published solutions from other numerical codes [2], [12]. Finally, overall mass balance checks were conducted (e.g., vapour influxes across all boundaries). The results were satisfying and showed that the code is capable of fitting vapour intrusion process.

All the results are presented in terms of normalized indoor air concentration, the so-called attenuation factor [4], defined as the ratio between the indoor pollutant concentration and the concentration of the source:

\[ α = \frac{C_{ig,\text{in}}}{C_{ig,\text{source}}} \]  

4.1 VOCs Source in the Vadose Zone

Firstly, a study of the impact of the source position on the normalized indoor air concentration for different depths is proposed (Figure 3). For reference, L = 0 m corresponds to the central axe of the building.

![Schematic modelling of a VOCs source in the vadose zone scenario.](image)

Results (Figure 4) show that the attenuation factor varies as a function of source position in the soil (lateral distance and depth).

Underneath the building (L < 5 m), the attenuation factor decreases with increasing source depth and is less influenced by the lateral source/building distance. In this case, the indoor pollution is higher when the source is closer to the building.
When the source is no longer underneath the building (L > 5 m), the attenuation factor decreases rapidly with increasing lateral distance, being more important for shallow source (H = 4 m).

For example, comparing a source below the building with a source at 20 m lateral distance from the building, with both sources at 4 m depth below ground surface, the difference between the normalized indoor air concentrations is about two orders of magnitude. Although, comparing a source at 20 m lateral distance from the building, the attenuation is about four order of magnitude when the source is positioned at 4 m of depth and about three orders of magnitude when the source is at 8 m or deeper. Vapour attenuation is more important for shallow sources, where vapours migrate mainly straight towards the atmosphere.

### 4.2 VOCs Source at the Groundwater Level

This analysis aims at identifying the impact of the source position, located at the groundwater level, on the attenuation factor for different depths (Figure 5).

As in the former case, two phases are identified from the results (Figure 6). Firstly, underneath the building (L < 5 m), the attenuation factor varies slightly with increasing lateral separation, decreasing mostly with an increase of the source depth.

Secondly, when the source is no longer underneath the building (L > 5 m), indoor concentration decreases more significantly with the lateral separation.

For example, comparing a source below the building with a source at 20 m lateral distance from the building, with both sources at 4 m depth below ground surface, the difference between the attenuation factors is about six orders of magnitude. However, comparing a source at 20 m lateral distance from the building, the attenuation is about six orders of magnitude lower when the source is positioned at 4 m of depth and about four orders of magnitude when the source is at 8 m or deeper being more important for shallow sources as explained before.

### 4.3 Comparison of Different Pollution Scenarios

Depending on the pollution configuration, vapour migrations have a different behaviour. For example, a vapour source in the vadose zone may diffuse vapours in all directions, unlike a contaminated groundwater that diffuses vapours only vertically towards the ground surface [1].

#### 4.3.1 Contaminated Groundwater Pollution versus Finite Source Located in the Vadose Zone

A comparison is made, including both a contaminated groundwater and a finite vapour source in the vadose zone (Figure 7). Both sources are at 8 m of depth from the edge of a building, and the groundwater depth is 20 m for the source located in the vadose zone.

The Figure 8 shows that the attenuation factor for a contaminated groundwater scenario is about 10 times
higher than that induced by a finite source in the vadose zone under the building.

Moreover, the difference is greater when the lateral distance from the building increases, being about two orders of magnitude lower. As described earlier, vapour attenuation increases with lateral separation.

4.3.2 Finite Source Location

Most VI models including lateral separation are specific to groundwater vapour sources at the groundwater level [2], [9]–[12]. However, variations from this assumption may affect their results and conclusions.

A confrontation is thus made between a vapour source located in the vadose zone scenario and another one located at the groundwater level (Figure 9) for two different depths.

![Fig. 9. Comparison between finite sources located at the groundwater level (a) and in the vadose zone (b).](image)

Firstly, both sources are located at a depth of 4 m from the soil surface (Figure 10).

![Fig. 10. Attenuation factor evolution as a function of the source/building lateral distance (H = 4 m).](image)

Underneath the building, the attenuation factor is about 10 times higher for a vapour source positioned at the groundwater level than a source located in the vadose zone. This difference is principally associated with the modelling of the source. In fact, the former configuration promotes upward transport due to the lower limit that blocks the transfer to the groundwater increasing vapour migration to the upper boundaries. However, the space between the source and the water table, when the source in the vadose zone, allows the vapours to migrate in all the directions and not just preferentially upwards.

The attenuation factor decreases with the increase of the lateral distance as discussed earlier. The vapour attenuation with increasing lateral separation is more important when the source is located at the groundwater level. In this case, vapours migrate straight into the atmosphere generating a greater vapour attenuation, while a radial migration promoting lateral transfer produces a higher vapour entry into the building.

![Fig. 11. Attenuation factor evolution as a function of the source/building lateral distance (H = 8 m).](image)

Secondly, both sources are positioned at a depth of 8 m from the soil surface (Figure 11). In this case, the source located at the groundwater level produces a higher indoor pollution. As shown before, this configuration promotes upward migration generating a higher indoor pollution. On the other hand, increasing the source depth enlarges lateral vapours migration into the building and consequently indoor air pollution (migration less influenced by the atmosphere).

5. Conclusion

A numerical analysis was proposed to better understand the relationship between the source location in the soil and the resulting indoor air concentration, including both a source in the vadose zone and a source located at the groundwater level.

Results show that indoor concentration decreases significantly with the lateral source/building distance, attenuation being more important for shallow sources.

However, depending on the location of the polluting source, vapour migrates differently. For sources in the vadose zone (residual or mobile non-aqueous phase liquid or in organic phase), the vapours migrate radially in all directions, vertically towards the ground surface (atmosphere or buildings) or to the groundwater, possibly leading to contamination of the groundwater.
On the other hand, vapours from an infinite homogenous source (e.g. contaminated groundwater) only migrate vertically towards the ground surface.

Finally, the results show that considering the lateral source location can significantly improve the quality of the indoor air pollution predictions. Then, it is important to consider the influence of this factor in VI models.

All the results presented here were limited to homogeneous soils and recalcitrant contaminants. Thus, as perspectives, it seems pertinent to include the impacts of stratified soils, natural barriers or paved areas and chemical reactions on vapour intrusion scenarios including lateral source/building distance.

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