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A numerical investigation of oxygen concentration dependence on biodegradation rate laws in vapor intrusion

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Abstract

In subsurface vapor intrusion, aerobic biodegradation has been considered as a major environmental factor that determines the soil gas concentration attenuation factors for contaminants such as petroleum hydrocarbons. The site investigation showed that oxygen could play an important role in this biodegradation rate, and this paper explores the influence of oxygen concentration in biodegradation reactions included in vapor intrusion (VI) models. Two different three dimensional (3-D) numerical models of vapor intrusion were explored for their sensitivity to the form of the biodegradation rate law. A second order biodegradation rate law, explicitly including oxygen concentration dependence, was introduced into one model. The results indicate that the aerobic/anoxic interface depth is determined by the ratio of contaminant source vapor to atmospheric oxygen concentration, and that the contaminant concentration profile in the aerobic zone was significantly influenced by the choice of rate law.

1. Introduction

Vapor intrusion (VI) is the process of the contaminant vapor released by subsurface source, transports in the soil and intrudes into the enclosed space of the building on the surface. The biodegradation of contaminants in VI scenarios has become a focus of recent research interest, especially for petroleum hydrocarbons (1–5). There have been reports of research on biodegradation rates from both lab and field site studies and there have been several VI models developed that include biodegradation (6–11). In most of the earlier studies, the biodegradation of petroleum hydrocarbons has been considered as a first order (in hydrocarbon) aerobic reaction (1, 2, 12–18). This raises some questions as it may seem inappropriate for these models not to include the influence of oxygen concentration in reaction rate, insofar as it is aerobic biodegradation that is being modeled. It has however at the same time been realized that oxygen does limit the aerobic biodegradation of contaminants such as petroleum hydrocarbon. While a recent study (19) employed the

Monod equation to describe reaction kinetics, this paper explicitly explores a second order biodegradation, i.e. the rate is a function of both oxygen and contaminant concentrations. Rather than implying that this absolutely needs to be the approach, this work explores how the choice of form of rate equation influences predictions of contaminant concentrations.

Figure 1 presents actual, typical benzene and oxygen concentration profiles from Hers et al. (3), which studied cases with and without building foundation cover. It shows that the concentration profiles can be divided into three sections. In the bottom section, below 0.8 m bgs (below-ground-surface), the oxygen concentration is relatively low and does not decrease with depth, while the benzene concentration is relatively high and does not change much with depth. In other words, little reaction between benzene and oxygen takes place in this largely anoxic zone. In the middle zone, between 0.6 and 0.8 m bgs, the oxygen concentration sharply decreases and benzene concentration sharply increases with depth. This means benzene is aerobically biodegraded in a fairly narrow reaction zone, as reported by Davis et al. (20). In Roggemans et al. (21, 22), where an instant reaction is assumed, the concept of an aerobic/anoxic interface is employed to represent this narrow reaction zone, the depth of which can be obtained by solving the equation of hydrocarbon vapor and oxygen diffusive transport in stoichiometric proportions. In the upper zone, above 0.6 m bgs, the oxygen concentration is relatively high and the decay rate with depth becomes quite small, due to low benzene concentration. Hence it is seen that consideration of transport of both species is necessary to fully understand the process.

2. Development of a 3-D model with second order biodegradation

The VI scenario simulated here uses a previously presented 3-D vapor intrusion model, but now including a biodegradation rate equation. The remainder of the model is that used in previous research by our group (23–28). In short, they all focus on nonbiodegradable contaminants, such as PCE and TCE. The case discussed here is similar to the earlier discussed steady-state “base case”, in which a single structure is located atop an otherwise flat, open field, underlain by a homogeneous soil between the open ground surface and a groundwater table serving as an infinite contaminant vapor source. All contaminant vapor is assumed to originate from the groundwater source, and there is no contaminant source within the soil itself. The “chimney effect” induces the depressurization of the building air and therefore soil gas advection through a perimeter crack at the building foundation. This is also main pathway for contaminant to enter the enclosed space. The differences between the model used here and that described earlier (23–34) include:

- The prototypical contaminant assumed here was benzene, which is aerobically biodegradable.
- Oxygen transport in the soil was now included in the model.
- A second order biodegradation rate expression, a function of both the contaminant and oxygen concentration, is added to the existing transport part of the model (see below). The governing equations for the transport of oxygen and contaminants are solved simultaneously to obtain the concentration profiles of both the contaminant and oxygen.

As before, we considered only steady state cases, and the same method was used to calculate indoor air concentration. The biodegradation rate expression was assumed to be of the following form:

$$R_c = \frac{\lambda_2 \varphi_w}{H_c \varphi_g} c_c c_o \quad (1)$$

where R_c is the biodegradation rate of the hydrocarbon contaminant [M/L^3_{gas}], c_c and c_o are the hydrocarbon contaminant and oxygen soil vapor concentrations [M/L^3_{gas}], respectively, φ_g is the gas filled porosity [$L^3_{\text{gas}}/L^3_{\text{soil}}$]; λ_2 is the second order reaction rate constant [$L^3_{\text{gas}}/M/T$], H_c is the contaminant air/water partition (Henry's) coefficient [$L^3_{\text{water}}/L^3_{\text{gas}}$], and φ_w is the moisture filled porosity [$L^3_{\text{water}}/L^3_{\text{soil}}$]. In most cases, biodegradation is believed to take place in a water film on the soil particles, so the larger the value of H_c , the lower the effective rate, for a given c_c . The constant λ_2 also includes the partitioning of oxygen into the water phase.

The chemical transport equation in steady state cases including biodegradation becomes:

$$0 = -\nabla \cdot (q_g c_{ig}) + \nabla \cdot (D_i \nabla c_{ig}) - R_i \quad (2)$$

where $-\nabla \cdot (q_g c_{ig})$ represents the advection term, $\nabla \cdot (D_i \nabla c_{ig})$ represents the diffusion term, and $-R_i$ is the reaction term, R_i is the reaction rate of chemical i per unit volume of soil

[$M_i/L^3_{\text{soil}}/T$], which is $R_c = \frac{\lambda_2 \varphi_w}{H_c} c_c c_o$ for contaminant and $R_o = \beta \frac{\lambda_2 \varphi_w}{H_c} c_c c_o$ for oxygen. β is the stoichiometric parameter [M_o/M_c], q_g is the soil gas advection rate per unit area [$L^3_{\text{gas}}/L^2/T$], c_{ig} is the concentration of contaminant i in the gas phase [M_i/L^3_{gas}], and D_i is overall effective diffusion coefficient for transport of chemical i in the soil [L^2/T]. The value for β used in this work was 3, as suggested by Roggemans et al. (22). Consider for benzene the complete oxidation reaction:

In this case, the stoichiometric ratio is used, meaning that 78 g of benzene react with 240 g of oxygen, giving $\beta = [M_o/M_c] \approx 3$.

Except for the fact that the governing transport equation includes a second order biodegradation term in (2), all other model attributes are the same as described in previous research by our group. Table 1 gives the key input parameters explored in this study. The rate constants used here were based on the results of Abreu and Johnson's 3-D model (16), to permit comparison with those results.

In Abreu and Johnson's paper (17), a biodegradation reaction, of first order form in hydrocarbon, was assumed wherever oxygen concentration in soil gas was higher than 5% of atmospheric concentration.

$$R_c = \frac{\lambda_1 \varphi_w}{H_c} c_c \text{ if } c_o > 5\% c_o^{atm} \quad (4)$$

where λ_1 is the first order reaction rate constant [1/T] based on the contaminant concentration in water, per unit volume of water. In that work (17), 0.018 h^{-1} , 0.18 h^{-1} and 1.8 h^{-1} were used for λ_1 . Here λ_2 , the second order reaction rate constant [$\text{L}^3_{\text{gas}}/\text{M}/\text{T}$], is also based on the contaminant concentration in water per unit volume of water, but was obtained in an oxygen concentration explicit form by dividing the λ_1 in Abreu and Johnson (17) by the atmospheric concentration of oxygen, $\lambda_2 = \frac{\lambda_1}{c_o^{atm}}$, where c_o^{atm} is the oxygen concentration (20°C and 1 atm) in atmosphere [M/L^3]

For example,

$$\lambda_2 = \frac{\lambda_1}{c_o^{atm}} \frac{0.18 \text{ h}^{-1} * \frac{1}{3600} \text{ h/s}}{279 \text{ mg/L}} = 1.79 \times 10^{-7} \text{ L/mg/s} \quad (5)$$

Strictly speaking, the two rate constants λ_1 and λ_2 are not simply related one to the other, by virtue of the fact that the constant λ_1 now becomes part of a rate that depends on oxygen concentration. What the present approach does is to allow comparing the predictions given similar orders of magnitude in biodegradation rate. Though the present expression is more complicated, the kinetics involving an oxygen concentration dependence could be important and this influence was explored here.

3. Results and Discussion

3.1 Comparison with Abreu and Johnson's 3-D model

The biodegradation issue has been considered in several earlier VI models. A typical example involves the use of “piecewise kinetics” as in the Abreu and Johnson model (16) and Devaull's analytical 1-D model (13). In the first case, the details of the intrusion pathway are represented by contaminant entry through a perimeter crack, while in the latter, the subslab contaminant concentration is assumed to be the same as the indoor air concentration. The “piecewise kinetics” assumption involves assuming $R_c = -(\frac{\lambda_1 \varphi_w}{H_c \varphi_g}) c_c$ when $c_o > 0.05 c_o^{atm}$, and zero otherwise.

In this section, the piecewise first order biodegradation rate model (as used by Abreu and Johnson) is first simulated using our model in order to permit a direct comparison between our results and Abreu and Johnson's results. The same governing equations and parameters were used here as in the Abreu and Johnson work. As in the approach previously used by our group (23–28) and in other numerical models, Darcy's law was first solved to obtain the pressure and soil gas flow field, and these results were then used to simultaneously solve the transport equations (2) of contaminant and oxygen. Only the boundary conditions at the crack are slightly different between our work and that of Abreu and Johnson. In our model, a negative in-house pressure of -5 Pa was assumed at a 0.005 m wide perimeter crack whereas a 0.001 m crack width was assumed and a soil gas flux equation was applied in

Abreu and Johnson's 3-D model. For the convection and diffusion part of our model, the equation describing mass flux through the crack was used for both the oxygen and contaminant, and an atmospheric oxygen concentration is assumed as the indoor air oxygen concentration.

Figure 2 shows the concentration profiles calculated using the two different models, and indicates that there is no significant difference in the results when the same form of biodegradation rate equation is employed. This is expected since the two models use the same governing equations of transport and reaction.

3.2 The influence of rate law and other environmental factors on chemical concentration profile

The results using the second order rate law are now examined, using the same 3-D model as above. Selected simulation results are shown in Figure 3 – 6.

In Figure 3, the influence of using the two different reaction rate laws was explored for a basement scenario. The results compare the piecewise first order rate approach used by Abreu and Johnson (16) to the second order reaction approach using equation (1). The main difference in results between the two rate laws is that seen in the contaminant concentration profile in the top section of the domain, i.e., the aerobic zone, where oxygen concentration is higher than 5% of that in the atmosphere. The contaminant subslab perimeter crack concentration in the case assuming the second order biodegradation rate law is a bit higher (0.01–0.1) than that in the case using the first order reaction model (0.001–0.01). This is despite the fact that oxygen concentration profiles in both cases look almost the same. It may be argued that by defining λ_2 in terms of λ_1/c_o^{atm} , the second order rate was significantly diminished relative to using the constant λ_1 , and that this is a reason for the difference between the results.

Figure 4 shows the influence of the reaction rate constant (using the second order rate law) on the contaminant and oxygen concentration profiles for basement scenarios, respectively. For both scenarios, the main difference in the contaminant concentration profile occurs in the zone of higher oxygen concentration, and the contaminant subslab perimeter crack concentration decreases as the reaction rate constant increases, as expected. The oxygen concentration profiles in all scenarios are qualitatively similar. Thus examination of oxygen subsurface profiles alone may not distinguish between biodegradation rates under this assumed scenario.

Figure 5 shows the influence of contaminant source concentration on the contaminant and oxygen concentration profiles for basement scenarios, respectively. As the vapor source concentration decreases, the oxygen can penetrate more deeply into the soil. The variation in the zone of oxygen availability causes the significant observed change of normalized contaminant concentration profiles and contaminant subslab perimeter crack concentration. Note that because the contaminant profiles are normalized to source concentration, the left hand panels cannot be directly compared, one to the other.

The above results all confirmed the critical need to properly account for oxygen transport and consumption effects in modeling vapor intrusion with biodegradation. While not directly related to the question of what form of rate law needs to be used, it is interesting to consider the influence of other site-specific parameters, in the context of the assumed second order rate law.

Figures 6 show the influence of assumed contaminant source depth. Making different assumptions regarding source depth, the profiles of both contaminant and oxygen soil gas concentration can be spread out over lesser or greater depth. As the relative depth from the base of the foundation to the source becomes greater, the predicted contaminant subslab perimeter crack concentration increases, and the predicted indoor air concentration also increases sharply. A key point is whether oxygen can penetrate to below the crack area. If it can, the near-crack concentration drops quickly.

Generally, the predicted oxygen concentration profiles are relatively insensitive to the form of the kinetic expression; in most cases simulated and shown here, the contaminant source vapor concentration/ oxygen atmospheric concentration is large enough to produce an aerobic/anoxic interface, where the oxygen concentration is 5% of that in atmosphere. In that case most of the oxygen seems to be consumed at the interface or in a thin reaction zone, as first illustrated and introduced in vapor intrusion modeling by Roggemans et al. (22) and simulated in a previous study by Hers et al. (3). On the other hand, the contaminant concentration profile is very dependent on the rate law of the aerobic biodegradation, and the contaminant concentration attenuation in the aerobic zone plays an important role in the whole soil vapor transport process. The contaminant concentration decays linearly in the anoxic zone, but roughly exponentially in the aerobic zone.

4. Conclusion

In summary, this paper presents a 3-D numerical vapor intrusion model including a second order biodegradation term, reflecting oxygen concentration-dependent reaction kinetics. Scenarios involving different source depth, source concentration and reaction rate constants are simulated. These results show a greater than heretofore discussed sensitivity to oxygen concentration, and thus, to the assumed form of biodegradation rate laws. The simulated soil gas concentration profiles provide an understanding of the influences of site characteristics on contaminant vapor concentration attenuation factors when reaction rate is also determined by oxygen concentration. Generally, compared to the simulations of piecewise first order reaction kinetics, the main difference is seen in the contaminant vapor concentration profile, or attenuation, in the aerobic zone. The aerobic/anoxic interface position is roughly determined by the ratio of contaminant source vapor concentration to atmospheric oxygen concentration, which is in agreement with the conclusion in Roggemans et al. (22). The form of the reaction rate law is thus shown to be of concern in predicting indoor air contaminant concentration attenuation factors.

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FIGURE 1.
Selected measured benzene and oxygen soil vapor concentration profile (3).

FIGURE 2.

Comparison of normalized predicted soil vapor contaminant and oxygen concentration profiles from the Abreu & Johnson (a) and our group's model (b) 3-D models ($d_f = 2 \text{ m}$, $d_s = 8 \text{ m}$, contaminant source concentration $c_c^s = 200 \text{ mg/L}$, first order biodegradation reaction rate constant in water phase $\lambda_1 = 0.18 \text{ h}^{-1}$) (17). The basement of the structure is shown as the rectangular cutout on the left side of the drawings, and results are shown only for half of the domain, because symmetry exists about the y-axis (the unit of the scale is meter, and so is it in the following figures). Reprinted with permission from (17).

FIGURE 3.

Influence of assumption regarding reaction rate law on normalized contaminant and oxygen concentration (a) first order reaction and (b) second order reaction ($d_f = 2$ m, $d_s = 8$ m, $c_c^s = 200$ mg/L, $\lambda_1 = 0.18$ h⁻¹ in (a), $\lambda_2 = 1.79 \times 10^{-6}$ L/mg/s in (b))) (The values of α shown in the “basement” portion of the domain are the contaminant attenuation factor relative to source, i.e. $\alpha = \frac{c_c^{in}}{c_c^s}$, where c_c^{in} is the indoor air contaminant concentration [M/L³]). In this case, the basement is represented by the cutout rectangle on the right side of the figures (and the solutions are symmetrical to the right of the figure).

FIGURE 4.

Influence of second order reaction rate constant on normalized contaminant and oxygen concentration profiles ($c_c^s=200 \text{ mg/L}$, $d_s = 8 \text{ m}$ and $d_f = 2 \text{ m}$)

FIGURE 5.

Influence of contaminant source concentration on normalized contaminant and oxygen concentration profiles, assuming second order biodegradation ($\lambda_2 = 1.79 \times 10^{-6} \text{ L/mg/s}$, $d_s = 8 \text{ m}$ and $d_f = 2 \text{ m}$) for a basement scenario.

FIGURE 6.

Influence of contaminant source depth on normalized contaminant and oxygen concentration profiles, assuming second order biodegradation ($\lambda_2 = 1.79 \times 10^{-6} \text{ L/mg/s}$, $c_c^s = 200 \text{ mg/L}$ and $d_f = 2 \text{ m}$) basement scenario, in which the basement depth is constant at 2 m.

TABLE 1

Input parameters used in 3-D simulation including a second order biodegradation (unless otherwise noted) (17)

Building/foundation parameters
Foundation foot print length: 10 m, width: 10 m
Depth of foundation (d_f): 0.1 and 2 m
Crack/foundation slab thickness(d_{ck}): 0.152 m
Crack width(w_{ck}): 0.005 m
Crack area (A_{ck}): 0.199 m ²
Volume of intruded area (V_b): 3.66×10^2 m ³
Air exchange rate in intruded volume (A_e) 0.25 h ⁻¹
Depth to groundwater/source (d_{source}) 3, 5, 8, 11, 14, 18 m bgs
Pressure difference at the crack (p): -5 Pa
Soil vapor flow properties
Viscosity of air/soil vapor (μ_g): 1.8648×10^{-5} kg/m/s
Density of air/soil vapor (ρ_g): 1.1614 kg/m ³
Soil permeability (k): 10^{-11} m ²
Total soil porosity (ϕ): 0.35
Soil porosity filled with gas (ϕ_g): 0.296
Contaminant vapor source properties
Contaminant: Benzene
Diffusivity of benzene in crack (D_c^{ck}): 8.81×10^{-6} m ² /s
Effective diffusivity of benzene in soil (D_e): 1.04×10^{-6} m ² /s
Diffusivity of oxygen in crack (D_o^{ck}): 2×10^{-5} m ² /s
Effective diffusivity of oxygen in soil (D_o): 2.36×10^{-6} m ² /s
Contaminant source concentration (c_c^s): 20, 100, 200 mg/L
Oxygen concentration in atmosphere (c_o^{atm}): 279 mg/L
Henry's Law constant (H_c): $0.228 \text{ m}^3_{\text{water}}/\text{m}^3_{\text{vapor}}$
Biodegradation constants
second order reaction rate constant [$\text{L}^3_{\text{gas}}/\text{M}/\text{T}$] to the contaminant concentration in water in unit volume of water $\lambda_2 = 1.79 \times 10^{-8}$, 1.79×10^{-7} , 1.79×10^{-6} L/mg/s
3-D Finite Element Analysis Parameters
Size of the grid elements: 0.001 m – 1 m
Number of elements: 200k – 600k