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Estimation of SVE closure time

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Abstract

The ability to predict the time when to stop a SVE system is critical when designing and operating a SVE remediation system. Completed research on the tailing performance of SVE, allowed the development of the closure time index (CTI) concept. CTI is based on breakthrough curves for both lab-scale experiments and a field-scale application of SVE. Application of the CTI concept allows estimation of the time when the SVE system could be shutdown. Shutting down a SVE system at the appropriate time minimizes operational time and reduces clean-up costs as demonstrated by the field case data that was tested.

Keywords: Soil vapour extraction; Three-dimensional mathematical model; Mass transfer limitations; Tailing effect; Closure time index

1. Introduction

Soil vapour extraction (SVE) is a widely accepted and cost-effective technique that is used to remediate unsaturated soils contaminated with volatile organic compounds (VOCs). One of the challenges with SVE remediation is the occurrence of tailing, which causes a decrease in treatment efficiency as a result of mass transfer limitations [1–3]. Tailing occurs when further treatment only minimally reduces the soil contamination (asymptotic part of the breakthrough curve), resulting in the continued treatment being ineffective and expensive. In many situations the soil contamination in the tail still exceeds the required clean-up level. Consequently, it is important to explore the tailing portion of the breakthrough curve to determine if the time to stop SVE can be estimated. Doing so would allow consultants to consider and start more effective remediation methods like bioventing to reach clean-up targets.

Significant development has been made in SVE remediation technologies [4,5] through theoretical and laboratory studies on the governing physical and chemical processes [6]. However, there is still limited understanding of the controlling processes existing in field settings [7]. Accordingly, significant efforts have been placed on modeling work [8]. Unfortunately, very few models have been developed that can predict the response of a real SVE system in three dimensions, making it difficult to predict closure time.

Predicting closure time has always been difficult for SVE remediation operation [9]. Kaleris and Croise [10] utilized dimensionless parameters to estimate clean-up time. Many have used a one-dimensional advective–dispersion transport model to obtain the most direct relationship between parameters of SVE and the removal rate of contaminants. Sawyer and Kamakoti [4] directly used air flow rates to estimate closure time of SVE. Barnes and David [11] coupled an air flow model with further optimization methods to propose a procedure where the length of SVE operation time should be estimated by incorporating principles of uncertainty analysis, soil gas flow with contaminant vapour transport and decision theory. Ng and Mei [12] proposed that the stopping time should be set equal to the elapsed time when vapour concentration is reduced to a mass that is 1% of the initial value. However, lab results and field SVE operation data show that tailing occurs before the 1% threshold is reached [9,13]. This was also seen in field data provided by Conestoga, Rovers and Associates for this work.

Kaleris and Croise [14] estimated the clean-up time for SVE operations using the mixed petroleum engineering reservoir model with local equilibrium mass transfer. This numerical model was based on the advection–dispersion differential equations for Darcian isothermal airflow, local equilibrium contaminant mass transfer between gas phase and soil water, and first-order kinetics for mass transfer between soil water and solid phase [10,14]. However, recent studies have shown that SVE is

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governed by non-equilibrium processes, hence the tailing effect may last several days, months and even several years. A proper decision-making process must include analysis of the tailing phenomenon, since tailing strongly affects the cost effectiveness and the final clean-up level to which the contaminant is removed. Recently, Barnes and White [15] attempted to do this with a simple decision model built on a cost-risk function that was subjected to Monte Carlo analysis. The model works when the mass removal process becomes diffusion limited.

This paper presents a closure time index that analyzes the tailing behaviour of a SVE system. Both laboratory and field data were used in the analysis. First the laboratory data provided by Duggal [13] was used to develop the CTI concept. The developed concept was then tried on field data provided by Conestoga, Rovers and Associates. The development of the CTI concept was supported by a 3D-SVE model that was developed by Zhao and Zytner [18] for another phase of the research.

2. Closure time index

2.1. Model background

The foundation of the proposed closure time index (CTI) is based on the breakthrough curves observed from a typical SVE system. Three types of breakthrough curves were used; lab experimental data, field SVE data and 3D-SVE-L/F numerical model output [3]. The model output provided smooth breakthrough curves which assisted the development of the CTI concept.

The 3D-SVE model developed by Zhao and Zytner [16] represents multiphase flow and multi-component behaviour by applying the basic three phase flow equation [17]:

$$\frac{\partial}{\partial t}(\varphi\rho_\beta S_\beta) = \nabla\left[\frac{\rho_\beta k_{ij} k_{r\beta}}{\mu_\beta}(\nabla p_\beta + \rho_\beta g e_j)\right] + E_\beta + Q_\beta \quad (1)$$

where φ = porosity of porous media; β = phase: aqueous, pure NAPL, gas phases, i.e., $\beta = \alpha$, n, g; ρ_β = density of β phase, kg/m^3; Q_β = source/sink of β phase, mol/m^3 s; S_β = saturation of β phase, k_{ij} = intrinsic permeability of porous medium, m^2; $k_{r\beta}$ = relative permeability of β phase; e_j = components of a unit vector (0,0,1); p_β = pressure of β phase (Pa) and E_β = summation of interphase mass transfer of all components into β phase from other possible phase, mol/m^3 s.

Mass transport in the aqueous, gaseous phase and NAPL phase (if applicable) for each constituent k, is assumed to follow the non-linear advective–dispersive conservation formulation [17]:

$$\frac{\partial(\phi S_\beta C_{\beta,k})}{\partial t} = \nabla(\varphi S_\beta D_{\beta ijk}\nabla C_{\beta,k}) - \nabla(q_\beta C_{\beta,k}) + \gamma_{\beta,\alpha,k} + Q_{\beta,\alpha} \quad (2)$$

where $C_{\beta,k}$ = molar concentration of species k in β phase, mol/m^3 s; $D_{\beta,k}$ = dispersion coefficient tensor, m^2/s; $\gamma_{\beta,\alpha,k}$ = rate of mass transfer between α and β phases, mol/m^3 s; q_β = flow velocity of β phase, m/s; β = phase tackled: aqueous, pure NAPL, gas phases; ρ_β = density of a phase, kg/m^3; Q_β = source/sink of a phase, mol/m^3 s; S_β = saturation of a phase; φ = porosity of porous medium; k_{ij} = intrinsic permeability of porous medium, m^2; $k_{r\beta}$ = relative permeability of β phase and p_β = pressure of a phase, Pa.

Table 1
Mass transfer coefficients applied in 3D-SVE-L model

Non-equilibrium phase pairs	Expressions or values (h^{-1})	Remarks
NAPL to air	$k_{N,g} = a\left(\frac{S_n}{S_{n,i}}\right)^b$	a, b are adjustable parameters
Aqueous to air	$k_{a,g} = 0.001(C_a)^{1.9}$	same as Gidda [2]
Aqueous to solid	3.6	same as Gidda [2]
NAPL to aqueous	36	same as Gidda [2]

Eqs. (1) and (2) are highly non-linear because they account for the various SVE processes that affect the transport of contaminants including advection, dispersion, adsorption, contiguous phase partitioning and rate-limited mass transfer. The rate of mass transfer couples the phase flow and transport equations. Zhao and Zytner [18] outline how this 3D-SVE model was solved using FEMALB by combining the simplifying assumptions related to the real settings of lab and field SVE operations.

For all simulations, the 3D model was calibrated against the lab and field data using the mass transfer expressions in Table 1 as the fitting parameters. Permeability and dispersivity values were constant, with the dispersivity values taken from the work of Gidda et al. [19]. By changing the mass transfer parameters "a" and "b" in Table 1 for NAPL to air, it was possible to fit the model breakthrough curve to the experimental data on a semi-log coordinate system. The log transformation accounts for the bias in the early venting data due to the magnitude of the initial effluent vapour concentrations when compared to the concentrations in the tail portion of the breakthrough curve. The best fit was been obtained when the minimum value of the normalized sum of the squared relative deviations on a log basis was achieved,. More detail on the model and fitting exercise can be found in Zhao [3] as modelling is not the intent of this paper.

Duggal [13] completed 10 cases of experimental SVE runs. Table 2 contains the conditions studied for each case. These completed experiments covered two types of soils under air dried conditions, with flow rates ranging from 2.5 to 30 L/min. The various remediation times lasted from 2.5 to 400 h. Good model fits were obtained, which allowed development of the CTI concept.

Table 2
Cases studied

Case	Soil type	Flow rate (L/min)
1	Elora silt	9.70
2	Elora silt	33.0
3	Elora silt	30.6
4	Elora silt	30.3
5	Elora Silt	20.9
6	Ottawa sand	1.5
7	Ottawa sand	5.4
8	Ottawa sand	10.6
9	Ottawa sand	20.9
10	Ottawa sand	11.1

2.2. Development of CTI

Review of the experimental and model breakthrough curves for each laboratory case suggested that closure time could be related to the slope of the breakthrough curve (off gas concentration versus operation time). Mathematically, relative slope is defined as:

$$R = - = \frac{\Delta C}{\Delta t}\frac{1}{C_{\text{init}}} = -\frac{C_{i+1} - C_i}{t_{i+1} - t_i}\frac{1}{C_{\text{init}}} \times 100\% \quad (3)$$

where R = relative slope of breakthrough curve, h^{-1}; C_{i+1} = concentration of off gas at t_{i+1} elapsed time, mol/m^3; C_i = concentration of off gas at t_{i+1} elapsed time, mol/m^3; C_{init} = initial value of off gas concentration, mol/m^3 and t = time elapsed of SVE operation, h.

Relative slope R indicates the decrease in off gas concentration with respect to the previous time step. Considering the time value of remedial operation, one needs to incorporate a time weighted duration that will consistently work for field SVE situations. Accordingly, elapsed time should be incorporated, giving an effectiveness ratio E, defined by Eq. (4):

$$E = \frac{R}{t} \quad (4)$$

The gradually decreasing E values can be used to show the transition of effectiveness in NAPL removal as shown in Fig. 1, the result of applying Eq. (4) to a typical breakthrough curve exhibiting tailing. Fig. 1, which was obtained from applying Eq. (3) to the data from for Case 1 from Duggal [13], shows that for every magnitude change in "E", there is a corresponding increase in remediation time. Similar shapes can be obtained from any SVE breakthrough curve showing tailing. Hence, there should be a correlation between E and the development of tailing.

Further review of Fig. 1 shows that as the SVE process continues, there are three tailing stages where the process is changing: non-equilibrium sharp decline stage, transition stage and non-zero asymptotic stages. These three sub-stages of tailing can be represented by the *"E"* values and the corresponding time intervals, where ΔE_i is the change in value of the relative slope on the vertical axis:

(1) $\Delta E_1 = 10^{-1}$ to 10^{-2}% (non-equilibrium sharp decline stage) non-equilibrium begins, yet the mass transfer limitations are giving a sharp decline in the breakthrough curve. Tailing is insignificant.
(2) $\Delta E_2 = 10^{-2}$ to 10^{-3}% (transition stage) mass transfer limitations increasing, causing a change in slope of the breakthrough curve towards non-zero asymptotic stage. That is, tailing has started and stop time is approaching.
(3) $\Delta E_3 = 10^{-3}$ to 10^{-4}% (non-zero asymptotic stage) a further 10-fold reduction in the off gas concentration extends the time of operation but has little impact on remediation. During this stage, SVE operation is not cost-effective, and should be shutdown or switched to another more effective remediation technology such as bioventing to reach the clean-up target of the site.

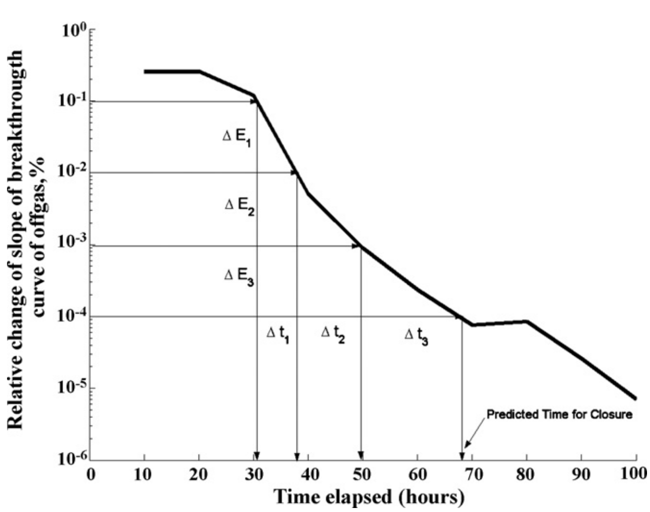

Fig. 1. Typical relative slope breakthrough curve.

The intervals of elapsed time that correspond to each region of "ΔE", which characterize the progress of the tailing stage, are represented by the elapsed time intervals Δt_1, Δt_2 and Δt_3, respectively. Reviewing all cases showed the following tendencies for two contiguous stages:

(i) $\Delta t_1 \le \Delta t_2 < \Delta t_3$ indicates that further SVE operation can improve the level of cleaning;
(ii) $\Delta t_1 > \Delta t_2 < \Delta t_3$ represents typical SVE progression, early slow reduction followed by a sharp decrease then the onset of tailing.

Accordingly, it is proposed that the critical time index (CTI) is related to the ratios of $\Delta t_2/\Delta t_1$ and $\Delta t_3/\Delta t_2$ for two contiguous time stages according to:

$$\text{CTI} = \frac{\Delta t_{i+1}}{\Delta t_i} \quad (5)$$

When CTI reaches the critical value, and "ΔE" falls into the non-zero asymptotic stage, the time to stop the SVE operation has been attained, with $\Delta t_{i-1} < \Delta t_i$. Based on the review of the simulated lab-scale results, it was determined that an average CTI of 2.1 exists, with a standard deviation of 0.5. Further details on the calculation of CTI and how it is implemented will be discussed in the application section.

3. Aplication of CTI

The effectiveness of CTI will be demonstrated by first using the laboratory data to calculate and verify CTI. The results from examining CTI will then be applied to the field case to test the hypothesis.

3.1. CTI for lab-scale SVE experiments

Figs. 2–5Figs. 2a-5a give both the actual experimental data and the fitted model breakthrough curves for a few cases. The breakthrough curves are typical of all the cases studied. These representative curves clearly show that as the SVE process

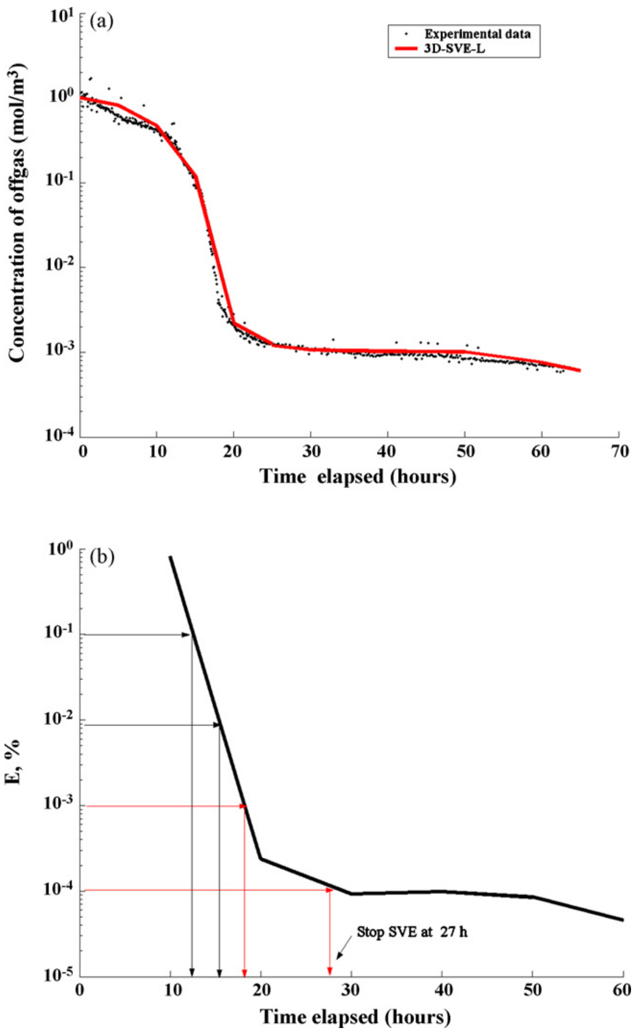

Fig. 2. (a) Breakthrough curves for Case 2 (Elora silt) and (b) CTI analysis of Case 2.

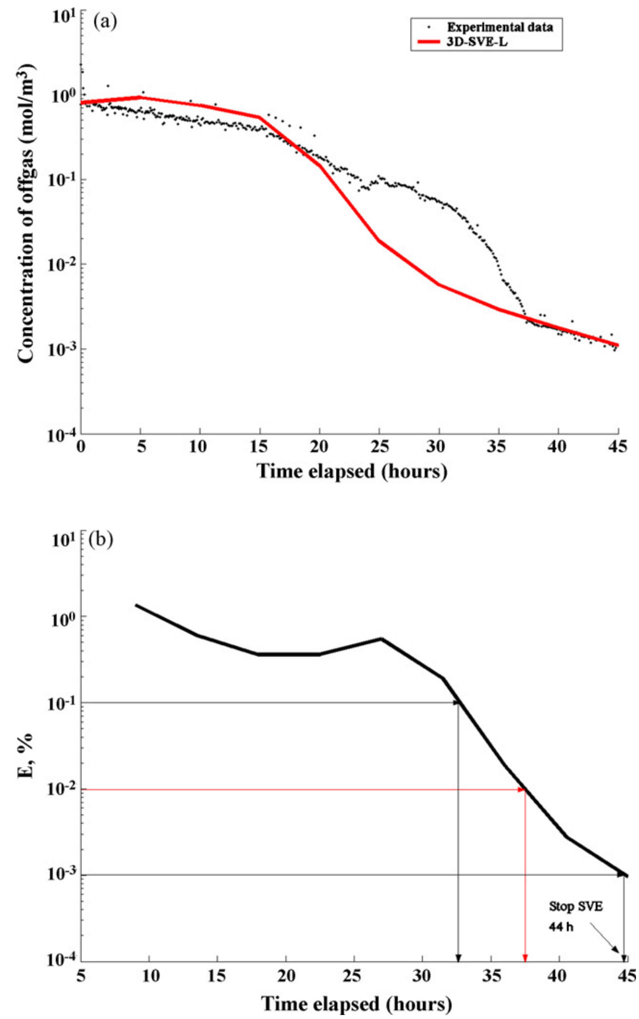

Fig. 3. (a) Breakthrough curves for Case 3 (Elora silt) and (b) CTI analysis of Case 3.

progressed in the lab, tailing became more dominant. This is consistent with mass transfer limitations taking hold and is similar to the patterns seen in field settings. Accordingly, the SVE system should have been shutdown. However, it needs to be stressed that the plots shown are semi-log due to the fitting exercise used, which exaggerates even minor differences. The same data plotted on the normal scale would show very good fits on the tailing portion of the breakthrough curve, including that for Case 3 shown in Fig. 3.

Figs. 2b–5b show the analysis of the breakthrough curves via the proposed CTI concept, and are typical of all the cases analyzed. Table 3 shows that the CTI values range from 1.6 to 3.0, giving an average of 2.1, with a standard deviation of 0.5. Cases 6 and 7 were dropped from the analysis due to very short remediation times, 2.5 and 9 h, respectively. Table 3 also shows that analysis of Case 3 and Case 8 required that the analysis be applied one stage earlier due to the shape of the breakthrough curve, where $\Delta t_1 < \Delta t_2$. This happens when the asymptotic portion of the breakthrough curve starts earlier at an elevated concentration.

Table 3 gives the suggested stop times for the SVE lab experiments. Review of these closure times and the breakthrough curves shows that they are visually realistic. In all cases shown, it would have made sense to shutdown the SVE system due to the occurrence of tailing. The promising part of the concept is that a robust 3D model can be used to estimate how long the site needs to remediated. All that is needed is the relevant site data for the model. However, while these results are encouraging with respect to the average CTI value used, more data and analysis is required to refine the concept. It also suggests that further work should be done on the concept so that upon refinement, CTI can be incorporated directly into the numerical model so that no external analysis is required.

3.2. Field case

The field data for this study was provided by Conestoga, Rovers and Associates (CRA). It was taken from a site undergoing typical SVE remediation. Fig. 6a shows the field data, and while showing the typical SVE shape, it also demonstrates the irregularities typically noticed in field off gas concentra-

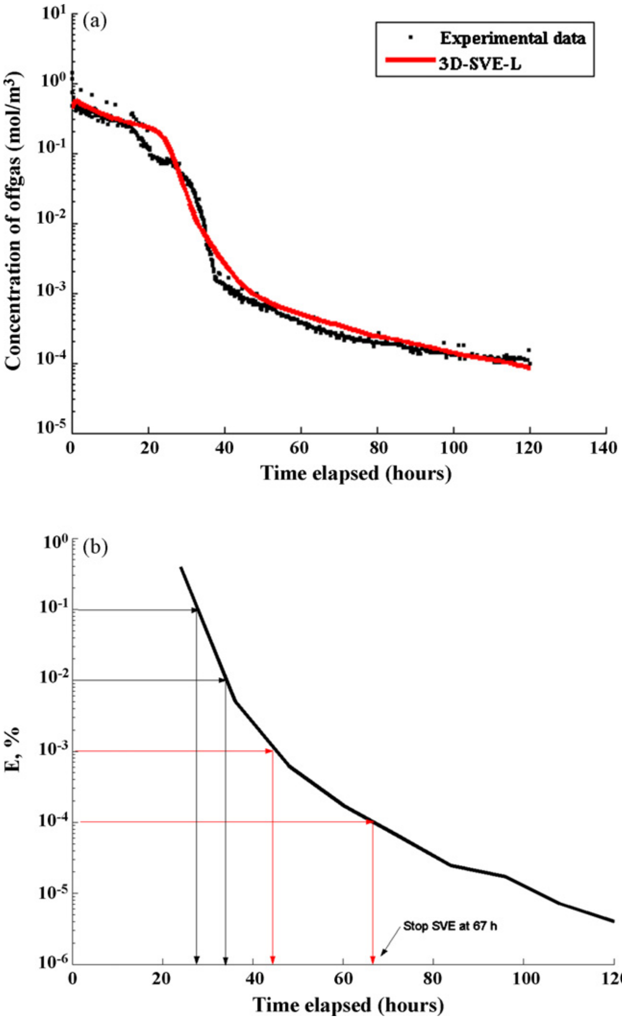

Fig. 4. (a) Breakthrough curves for Case 4 (Elora silt) and (b) CTI Analysis of Case 4.

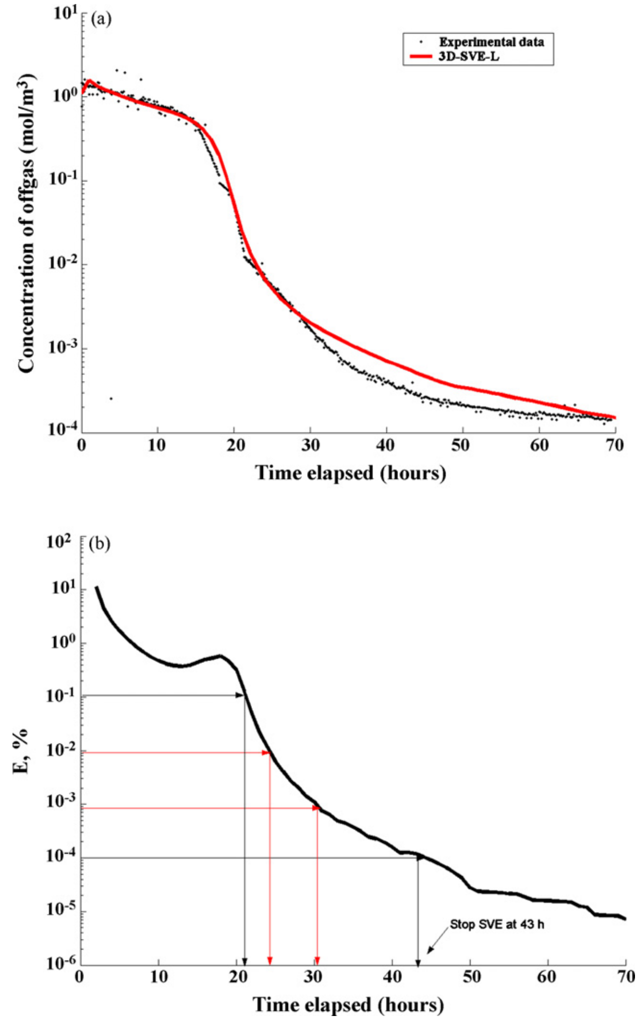

Fig. 5. (a) Breakthrough curves for Case 9 (Ottawa sand) and (b) CTI analysis of Case 9.

tions. The irregularities made model fitting a challenge, so it was decided to fit the three possible tailing curves, low, middle and high as seen in Fig. 6a.

The CTI analysis of the field data is given in Fig. 6b. With three different tailing fits, the CTI analysis was applied to all three breakthrough curves. Fig. 6b shows that despite three possible breakthrough curves, all three CTI curves overlapped nicely, making the analysis easier. For simplification, the middle CTI curve was used for further analysis. At the E value of 10^{-2}% due to the CTI curve being in the non-zero asymptotic stage, the corresponding elapsed run time is 390 d. Applying the lab-scale obtained CTI value of 2.1, the calculated value suggested maximum run time for the field is 390 d × 2.1 = 780 d.

The CTI analysis suggests that after 780 d, the SVE system should have been shutdown and a different remediation process implemented to complete the remediation process. Based on subsequent communication with CRA, it was learned that the system ran for at least 150 d more (950 d in total). No further

Table 3
The predicted time to stop SVE operations

Parameter	Lab-scale							
	Case 1	Case 2	Case 3	Case 4	Case 5	Case 8	Case 9	Case 10
Δt_1 ($E = 1$–0.1‰)	5	3	5	6	6	2.5	3	10
Δt_2 ($E = 0.1$–0.01‰)	9	3	8	10	8	5	6	5
Δt_3 ($E = 0.01$–0.001‰)	18	9	NA	20	13	NA	12	14
CTI = $\Delta t_{i+1}/\Delta t_i$*	2	3	1.6	2.0	1.6	2.0	2	2.8
Time to stop SVE operation (h)	66	27	44	67	71	25	43	64

* The average of CTI for all lab-scale cases is 2.1 with a standard deviation of 0.5 NA—not applicable.

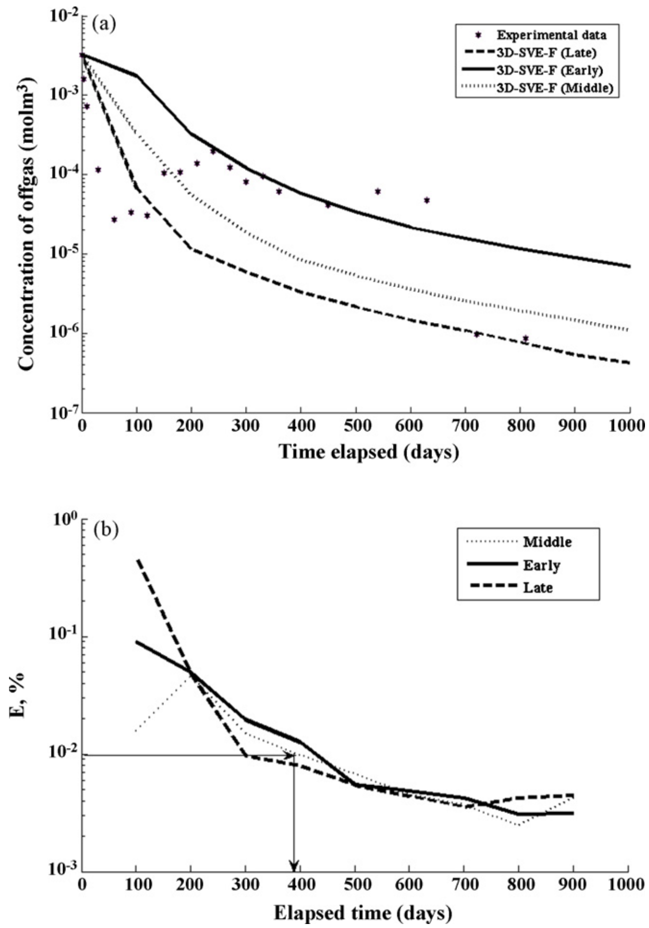

Fig. 6. (a) Breakthrough curves for field data and (b) CTI analysis of field case.

information was provided. With the difference between CTI and run time being 170 d, it shows the importance of having a process by which the operation time of a SVE system could be calculated. Furthermore, analysis of the other two CTI curves also indicated that the SVE could have been shutdown before 950 d.

It is encouraging that the lab data CTI value can be used in a field scenario. The proposed concept worked well, even when three breakthrough curves were generated based on the actual off gas concentration curves. Evaluation of the field data has shown that the site operated longer than necessary due to SVE inefficiency, and if the SVE system was shutdown earlier, money could have been saved on equipment and overhead. Therefore, if the necessary site data is available for a 3D model simulation, consultants can complete a CTI analysis and evaluate how long remediation should take. A question consistently asked by owners of contaminated sites. This information would also be helpful in deciding if the operational equipment needs to be purchased or leased, again saving capital expenditures. However, as noted in the lab case, more field data is required to refine the CTI concept.

4. Summary

The analyses have shown that breakthrough curves for a SVE system can be used to estimate the time when the system should be shutdown. These curves can either be experimental data, field measurements or model simulated results. By analysing the slope characteristics of breakthrough curve of off gas concentration, the time interval "Δt" can be analyzed according to the effectiveness ratio "E".

The prediction process to estimate the closure time can be summarized as follows:

- obtain the breakthrough curve off gas concentrations via measurements or model run,
- calculate the elapsed time weighted relative slope of the breakthrough curve E,
- determine the appropriate time interval according to the E values,
- apply a CTI of 2.1 to determine the corresponding closure time.

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