BioSVE Technical Information - Equations

Chemical Equilibrium Model

Johnson et al. (1990) expressed the mole balance of component *i* during the soil vapor extraction as

$$\frac{dM_i}{dt} = -QC_i^e - B_i \qquad [1]$$

where M_i is the total moles of component *i* in all four phases, C_i^e is the equilibrium gas phase molar concentration, B_i = rate of degradation of species *I, Q* is the air flow rate $\left[L^3T^{-1}\right]$.

The corresponding mole balance equation based on the chemical equilibrium among the gas, water, oil and solid phases was expressed as

$$M_i = \left(\frac{P_i^v \phi_a v}{RT} + M_T^{HC} + \frac{M^w}{\alpha_i} + \frac{K_i M_s}{\alpha_i M_w}\right) x_i \qquad [2]$$

where

x_i = mole fraction of species *i* in free hydrocarbon phase $= \frac{M_i^{HC}}{M_T^{HC}}$

P_i^v = pure component vapor pressure

ϕ_a = air filled porosity

V = volume of contaminated soil

R = gas constant

T = absolute temperature of soil air

M_i^{HC} = moles of species *i* in free hydrocarbon phase

M_T^{HC} = total moles in free hydrocarbon phase

M^w = total moles in soil moisture

k_i = sorption coefficient

α_i = activity coefficient in water

M_w = molecular weight of water

The equilibrium concentration was expressed as:

$$C_i^e = \chi_i \frac{P_i^v}{RT} \qquad [3]$$

The finite difference approximation of equation [1] can be expressed as:

$$M_i^{t+dt} = M_i^t - \frac{Q\chi_i P_i^v}{RT} dt - B_i dt \qquad [4]$$

$$M_i^{t+tdt} = M_i^t - Q\left[\left(\frac{M_i^{Hc}}{M_T^{Hc}}\right)\frac{P_i^v dt}{RT}\right] - B_i dt \qquad [5]$$

Air Pumping Rate

Air flow rate through the contaminated soil is required in soil vapor extraction calculations. It can either be measured directly in the field or calculated directly from the following equation (see Johnson et al. 1990).

$$Q = B\ P_w \left(\frac{\pi\ k_a}{\mu}\right) \frac{1 - \left(\frac{P_r}{P_w}\right)^2}{\ln\left(\frac{r_w}{r}\right)} \qquad [6]$$

where K_a is the average air permeability $\left[L^2\right]$, μ is dynamic viscosity of water $\left[ML^{-1}T^{-1}\right]$, P_r is the absolute gas pressure at radial distance *r* from the well $\left[ML^{-1}T^{-2}\right]$, P_w is the absolute gas pressure at the well, *B* is the contaminated soil thickness, r_w is the radius of the well.

If all of the pumped air is not passing through the contaminated soil, it should be corrected to estimate the air passing through the contaminated zone.

Air permeability may be approximated as

$$K_a = k_i K_{ra} \qquad [7]$$

where

K_i is the intrinsic permeability = $\frac{K_{sw}\mu}{\rho g}$, K_{ra} is the relative permeability and can be approximated equal to the average gas saturation in the unsaturated zone, and ρ = density of water, *g* = acceleration due to gravity, and K_{sw} = saturated hydraulic conductivity $\left(\frac{L}{T}\right)$.

Venting Efficiency

The assumption of chemical equilibrium between the contaminated phases (water, oil, and solid) and the gas phase is often violated. Because of the high fluxes of air and due to the inaccessibility of the contaminant to the flushing air, the kinetics of interphase mass transfer becomes important. BioSVE incorporates the non-equilibrium effects through a venting efficiency η (fraction) that can be estimated through a simple field test explained in the BioSVE document.