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# An Analytical Solution for the Concentration Profile of a Sublation Process

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TECHNICAL NOTE

# An Analytical Solution for the Concentration Profile of a Sublation Process

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## ABSTRACT

The mass balance equations are solved analytically for the solute in the vapor and liquid phases in a batch-type aeration apparatus. The resulting vapor concentration profile can be used to determine the mass of solute trapped by a topping layer of organic liquid. This approach has the potential for favorable comparison with direct numerical analysis both in ease of application and overall problem solving time.

## INTRODUCTION

Lionel, Wilson, and Pearson proposed a mathematical model of an aerator apparatus for removing refractory organics from water (1). The volatile organic to be removed traverses the aqueous column inside air bubbles which are then trapped by a supernatant nonvolatile organic liquid layer (see Fig. 1).

Following Lionel, Wilson, and Pearson, the aqueous column is formally partitioned into $N$ slabs, and the $(N + 1)$ slab is the supernatant layer. The mass balance equations for the solute in the respective vapor and liquid phases in the $i$th slab are:

$$\frac{dC_{\mathrm{w},i}(t)}{dt} = \frac{1}{V_{\mathrm{a}i}}\left\{\frac{4\pi N_{\mathrm{b}}}{3}[r_{i-1}^3 C_{\mathrm{w},i-1}(t) - r_i^3 C_{\mathrm{w},i}(t)] + k_{\mathrm{w}} S_i [c_{\mathrm{w},i}(t) - K_{\mathrm{w}} C_{\mathrm{w},i}(t)]\right\} \quad (1)$$

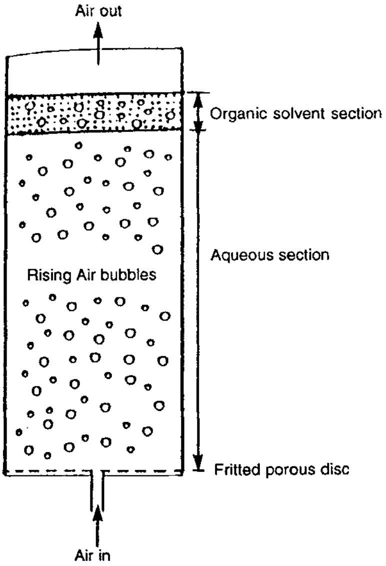

FIG. 1 Schematic diagram of a solvent sublation process.

and

$$\frac{dc_{w,i}(t)}{dt} = \frac{k_w S_i}{V_{wi}} [K_w C_{w,i}(t) - c_{w,i}(t)]; \qquad i = 1, 2, \ldots, N \tag{2}$$

where $C_{w,i}(t)$ is the concentration of solute in the vapor phase in the $i$th slab of the water layer, $c_{w,i}(t)$ is the concentration of solute in the water phase in the $i$th slab, $V_{ai}$ is the volume of air in the $i$th slab, and $N_b$ is the number of bubbles discharged per second and is given by

$$N_b = \frac{3Q_a}{4\pi r_t^3} \tag{3}$$

with $Q_a$ being the air flow rate at 1 atm and $r_t$ the bubble radius at 1 atm. The bubble radius in the $i$th slab is $r_i$, $k_w$ is the mass transfer rate coefficient for vapor–water transfer of solute, and $S_i$ is the total air–water interfacial area in the $i$th slab. $K_w$ is defined as $c_w(\text{eq.})/C_w(\text{eq.})$, that is, Henry's law constant in Ref. 1, and is determined from the equilibrium vapor pressure and water solubility of the solute at the temperature of interest. $V_{wi}$ is the volume of water in the $i$th slab.

Since the total mass ($m_o$) of solute in the supernatant organic liquid is the sum of that in the organic liquid and that in the air bubbles passing through this layer, then

$$m_o = V_o c_{sl} + V_{oa} C_s \tag{4}$$

where $V_o$ is the volume of supernatant organic liquid, $V_{oa}$ is the volume of air in the organic layer, and $c_{sl}$ and $C_s$ represent solute concentration in the liquid (organic) and vapor, respectively (g/mL).

The rate of change in $m_o$ is given by

$$dm_o/dt = Q_{ao}[C_{w,N}(t) - C_s(t)] \tag{5}$$

The usual procedure is to solve Eq. (1), (2), and (5) with the appropriate initial conditions by a suitable numerical scheme. Presented below is an alternative procedure based on solving Eqs. (1) and (2) analytically. The resulting vapor-phase solute concentration profile can then be used to determine $m_o$.

## MATHEMATICAL ANALYSIS

Consider the case where $i$ equals 1, that is, the aqueous column is one slab. Then Eqs. (1) and (2) become

$$\frac{dC_{w,1}(t)}{dt} = \frac{1}{V_{a1}}\left\{\frac{4\pi N_b}{3}[-r_1^3 C_{w,1}(t)] + k_w S_1[c_{w,1}(t) - K_w C_{w,1}(t)]\right\} \tag{6}$$

and

$$\frac{dc_{w,1}(t)}{dt} = \frac{k_w S_1}{V_{w1}}[K_w C_{w,1}(t) - c_{w,1}(t)] \tag{7}$$

respectively, subject to

$$C_{w,1}(0) = 0 \tag{8}$$

and

$$c_{w,1}(0) = \eta \tag{9}$$

Using more familiar variables, we designate the concentration of solute in the vapor phase of slab 1 as $y(t)$ and the solute concentration in the water phase of the same slab as $x(t)$. This results in a system of two linear first-order homogeneous ordinary differential equations:

$$dy/dt = -\phi_3 y + \phi_4 x - \phi_5 y \tag{10}$$

and

$$dx/dt = \phi_2 y - \phi_1 x \tag{11}$$

subject to the conditions

$$x(0) = \eta \tag{12}$$

and

$$y(0) = 0 \tag{13}$$

where the following constants are introduced to simplify the algebra.

$$\phi_1 = \frac{k_w S}{V_w} \tag{14}$$

$$\phi_2 = K_w \phi_1 \tag{15}$$

$$\phi_3 = \frac{4\pi N_b}{3V_a} r_1^3 \tag{16}$$

$$\phi_4 = \frac{k_w S}{V_a} \tag{17}$$

and

$$\phi_5 = \phi_4 K_w \tag{18}$$

This system of differential equations is solvable by the elementary methods discussed in textbooks such as Boyce and DiPrima (2) to give

$$x(t) = A_1 e^{\gamma_1 t/2} + A_2 e^{-\gamma_2 t/2} \tag{19}$$

and

$$y(t) = \frac{1}{\phi_2}\frac{dx}{dt} + \frac{\phi_1}{\phi_2} x \tag{20}$$

where $A_1$ and $A_2$ are integration constants. Then, using the given initial conditions, we get

$$A_1 = \frac{\eta(\phi_1 + \gamma_2/2)}{(2\phi_1 + \gamma_1/2 + \gamma_2/2)} \tag{21}$$

and

$$A_2 = \frac{\eta(\phi_1 + \gamma_1/2)}{(2\phi_1 + \gamma_1/2 + \gamma_2/2)} \tag{22}$$

such that

$$y(t) = C_{w,1}(t) = \frac{\eta(\phi_1 + {}^{\gamma}{}_1/2)\{(\phi_1 + \gamma_2/2)\, e^{\gamma_1 t/2} + (\phi_1 - \gamma_2/2)\, e^{-\gamma_2 t/2}\}}{(2\phi_1 + \gamma_1/2 + \gamma_2/2)\phi_2} \tag{23}$$

and

$$x(t) = c_{w,1}(t) = \left(\frac{\eta}{2\phi_1 + \gamma_1/2 + \gamma_2/2}\right) \times [(\phi_1 + \gamma_2/2)e^{\gamma_1 t/2} + (\phi_1 + \gamma_1/2)e^{-\gamma_2 t/2}] \tag{24}$$

are the necessary concentration profiles, where

$$\gamma_1 = -\alpha\phi_2 + \sqrt{(\alpha^2\phi_2^2 - 4\beta\phi_2)} \tag{25}$$

and

$$\gamma_2 = \alpha\phi_2 + \sqrt{(\alpha^2\phi_2^2 - 4\beta\phi_2)} \tag{26}$$

and $\alpha$ and $\beta$ are given by

$$\alpha = \frac{\phi_1}{\phi_2} + \frac{\phi_3 + \phi_5}{\phi_2} \tag{27}$$

$$\beta = \frac{\phi_1}{\phi_2}(\phi_3 + \phi_5) - \phi_4 \tag{28}$$

This analysis can be extended to processes that subdivide the aqueous column into two or more slabs. The resulting systems will not be homogeneous, however, and the method of variation of parameters as discussed in Ref. 2 will be useful.

Equation (23) can be substituted into Eq. (5), noting that for 1 slab, $i$ and $N$ are both equal to 1. The remainder of the procedure is as given in Ref. 1: That is, determine the mass of solute in the supernatant organic phase at time $t + \Delta t$ by integrating Eq. (5) forward in time. This requires the recasting of Eq. (4) to reflect the most recent value of $m_o$:

$$C_s = \frac{m_o(t + \Delta t) - V_o c_{sl}}{V_{oa}} \tag{4A}$$

The solute concentration $c_{sl}$ is defined as a function of $m_o$ in Ref. 1. In addition, $c_{sl}$ as it appears in Eq. (4A) requires the most recent value of $m_o$ as well. The remainder of the procedure is as given in Ref. 1.

## CONCLUSION

From the above mathematical analysis, a vapor-phase solute concentration profile $C_{w,1}(t)$ is derived. This profile can be used to simplify the procedure for determining the mass of solute in the supernatant liquid in a batch-type aeration process. In addition, the analysis is applicable to multislab processes.

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