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Norman W. Loney[a]
[a] DEPARTMENT OF CHEMICAL ENGINEERING, CHEMISTRY & ENVIRONMENTAL SCIENCE, NEW JERSEY INSTITUTE OF TECHNOLOGY, NEWARK, NEW JERSEY, USA

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TECHNICAL NOTE

Correlating Aqueous Phase Concentration Profile of a Sublation Process

NORMAN W. LONEY
DEPARTMENT OF CHEMICAL ENGINEERING,
CHEMISTRY & ENVIRONMENTAL SCIENCE
NEW JERSEY INSTITUTE OF TECHNOLOGY
NEWARK, NEW JERSEY 07102, USA

ABSTRACT

The aqueous phase priority pollutant concentration profile which was previously derived for a sublation process is further analyzed. This results in an approach that can expedite the determination of the mass of solute trapped by a topping layer of organic liquid. Very favorable results are achieved when compared to experimental data for toluene removal from water.

INTRODUCTION

A mathematical model of an aerator apparatus for the removal of refractory organics from water was proposed by Lionel, Wilson, and Pearson (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.

The mass balance equations were solved analytically (2) to produce vapor and aqueous phase solute concentration profiles. The derived aqueous phase solute concentration profile is:

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

and at $t = 0$:

$$\eta = A_1 + A_2$$

where A_1 and A_2 are integration constants. These integration constants are defined in terms of physical parameters in Ref. 2. However, these parameters are not always readily available in the literature and could become an obstacle in designing a new system.

THEORY

If the initial condition is combined with the aqueous phase concentration profile, we reduce the number of unknowns and introduce a known quantity, η. That is,

$$x(t) = A_1 \left[e^{(\gamma_1/2)t} - e^{(-\gamma_2/2)t}\right] + \eta e^{(-\gamma_2/2)t}$$

Then as a practical matter, if experimental data are available, A_1, γ_1, and γ_2 can be extracted from these data by arbitrarily choosing three distinct times. This can result in a system of three nonlinear equations:

$$x(t_1) = A_1 \left[e^{(\gamma_1/2)t_1} - e^{(-\gamma_2/2)t_1}\right] + \eta e^{(-\gamma_2/2)t_1} \tag{1}$$

$$x(t_2) = A_1 \left[e^{(\gamma_1/2)t_2} - e^{(-\gamma_2/2)t_2}\right] + \eta e^{(-\gamma_2/2)t_2} \tag{2}$$

$$x(t_3) = A_1 \left[e^{(\gamma_1/2)t_3} - e^{(-\gamma_2/2)t_3}\right] + \eta e^{(-\gamma_2/2)t_3} \tag{3}$$

for $0 < t_1 < t_2 < t_3$.

By introducing the variables

$$u_1 = x(t_1) \tag{4}$$

$$u_2 = x(t_2) \tag{5}$$

$$u_3 = x(t_3) \tag{6}$$

and

$$v = e^{(\gamma_1/2)t_1} \tag{7}$$

$$w = e^{(-\gamma_2/2)t_1} \tag{8}$$

Equations (1)–(3) can be recast as

$$u_1 = A_1(v - w) + \eta w \tag{9}$$

$$u_2 = A_1 \left(v^{t_2/t_1} - w^{t_2/t_1}\right) + \eta w^{t_2/t_1} \tag{10}$$

$$u_3 = A_1 \left(v^{t_3/t_1} - w^{t_3/t_1}\right) + \eta w^{t_3/t_1} \tag{11}$$

a system of nonlinear algebraic equations.

Then, given η, u_1, u_2, and u_3, the Mathematica package, NSolve (3), can be used to estimate A_1, v, and w. NSolve (3) is a numerical equation-solving routine that is capable of solving systems of equations (linear or nonlinear) without initial guesses. The values of γ_1 and γ_2 can then be calculated with the aid of Eqs. (7) and (8).

This quasi-analytical approach was used to predict the toluene concentration profile in the aqueous phase of the solvent sublation of toluene (4).

RESULTS AND DISCUSSION

Figures 1, 2, and 3 show a comparison between actual experimental toluene concentration in the aqueous phase and that determined from the quasi-analytical approach. The graphs were developed for the three air flow rates of 32, 60, and 94 mL/min, respectively. These flow rates are the ones used in the toluene sublation experiments carried out by Chen (4). NSolve (3) was then used to solve Eqs. (9)–(11) simultaneously.

Table 1 lists the values of A_1, γ_1, and γ_2 for the respective air flow rates as extracted from the data.

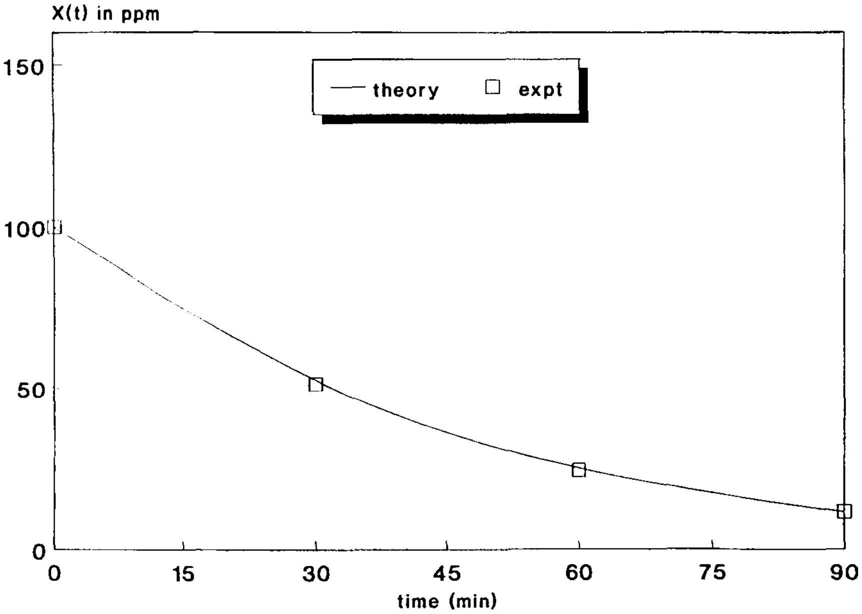

FIG. 1 Toluene aqueous phase concentration as a function of time (32 mL/min air flow rate case).

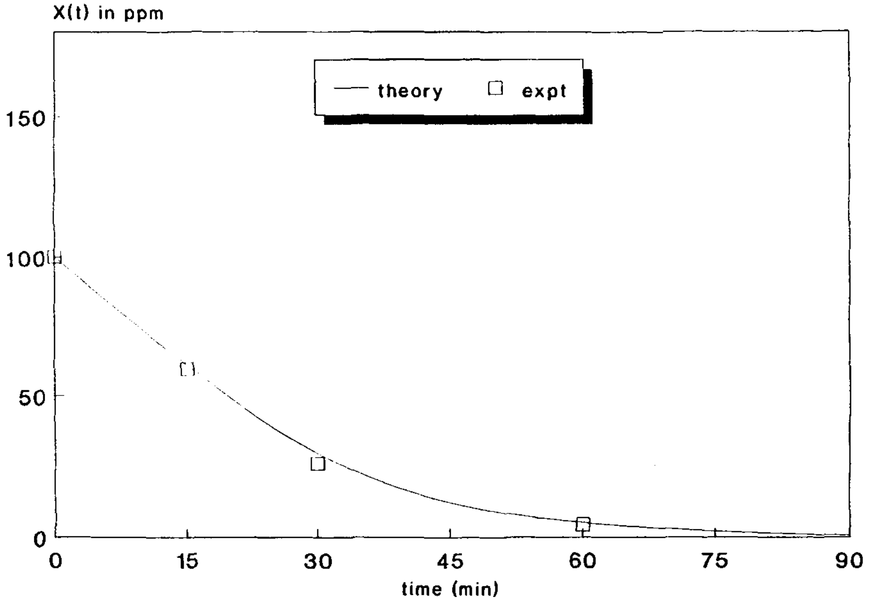

FIG. 2 Toluene aqueous phase concentration as a function of time (60 mL/min air flow rate case).

Since the system of Eqs. (9)–(11) is nonlinear, in the sense of a polynomial with degree > 1, negative or complex results are not unusual. However, if $e^{-m\gamma} < 0$, for m an integer, then we need to examine this type of result as done in Churchill and Brown (5). For example, while analyzing the 32 mL/min air flow rate case, the result

$$e^{-15\gamma_2} = -0.00151569 \tag{12}$$

was achieved. There are at least two paths that one can take to resolve this issue. One path is to assume γ_2 is very large and thus $e^{-15\gamma_2}$ is negligible. However, the calculated initial aqueous phase toluene concentration will be different from the given starting value of η. As a second alternative, our experience tells us that there is no *real number* γ_2 such that Eq. (12) is a true statement. That is, Eq. (12) represents a multiple-valued function of the complex variable γ_2. Then, following Churchill and Brown (5), Eq. (12) can be restated as

$$-15\gamma_2 = \ln(0.00151569) + i(\pi + 2n\pi), \qquad n = 0, \pm 1, \pm 2, \ldots \tag{13}$$

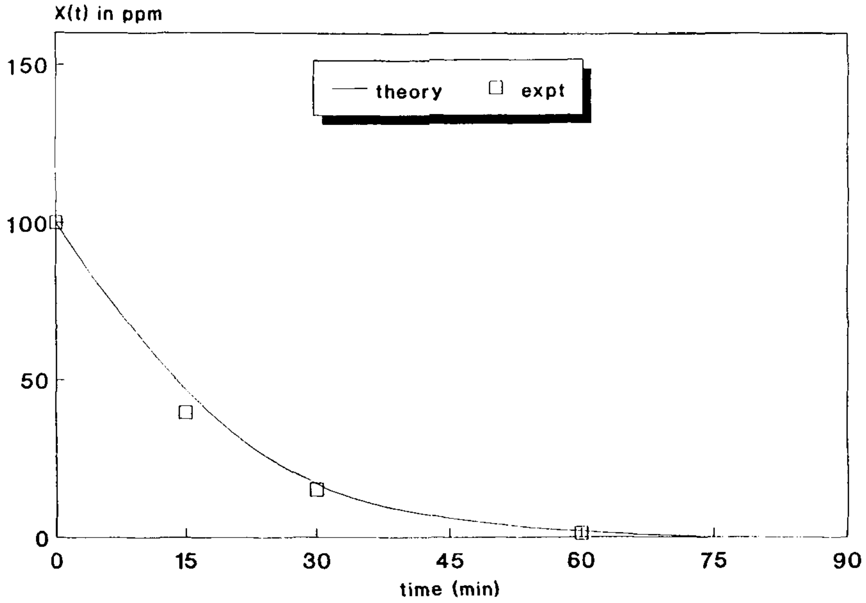

FIG. 3 Toluene aqueous phase concentration as a function of time (94 mL/min air flow rate case).

where $(-1/15)\ln(0.00151569)$ is the real part of γ_2 and $(-1/15)(\pi + 2n\pi)$ is the imaginary part. By considering the principal value of the argument $(n = 0)$,

$$\gamma_2 = 0.4327962 - i\frac{\pi}{15} \tag{14}$$

is a complex number with i being the imaginary unit. Then the modulus (magnitude) of γ_2 is estimated to be 0.4808. That is: $|\gamma_2| = 0.4808$, which is a much improved representation of the physical reality.

TABLE 1

	32 mL/min	60 mL/min	94 mL/min
A_1	108.64	154.95	101.50
γ_1	−0.0500	−0.118	−0.121
γ_2	0.481	0.339	1.88E-03

CONCLUSION

The analytical results as given in Ref. 2 can be used to forecast the mass of solute in the supernatant liquid in a batch-type aeration process. However, one may be working with a priority pollutant whose physical properties (mass transfer coefficient, Henry's law constant, etc.) are not readily available in the literature. If experimental time and aqueous phase concentration data are available, then the alternative approach outlined above can be used. That is, recover key physical parameters (A_1, γ_1, and γ_2) from the data using the outlined quasi-analytical approach discussed. This results in a correlation of the priority pollutant's aqueous phase concentration profile which may be extrapolated beyond the original experimental conditions.

NOMENCLATURE

A_1	$= \dfrac{\eta(\phi_1 + \gamma_2/2)}{(2\phi_1 + \gamma_1/2 + \gamma_2/2)}$
η	initial aqueous solute mass concentration (ppm)
φ_1	$= \dfrac{k_W S}{V_W}$
k_W	mass transfer coefficient for vapor–water transfer of solute
S	air–water interfacial area
V_W	volume of water in the system being analyzed
γ_1	$= -\alpha\phi_2 + \sqrt{\alpha^2\phi_2^2 - 4\beta\phi_2}$
γ_2	$= \alpha\phi_2 + \sqrt{\alpha^2\phi_2^2 - 4\beta\phi_2}$
φ_2	$= H_W \varphi_1$
H_W	Henry's law constant
α	$= \dfrac{\phi_1}{\phi_2} + \dfrac{\phi_3 + \phi_5}{\phi_2}$
β	$= \dfrac{\phi_1}{\phi_2}(\phi_3 + \phi_5) - \phi_4$
ϕ_3	$= \dfrac{4\pi N_b}{3V_a}\eta^3$
N_b	number of bubbles discharged per second
V_a	volume of air in the system under study
ϕ_4	$= V_W\phi_1/V_a$
ϕ_5	$= \phi_4 H_W$

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