

MODELING THE EMISSION AND DISPERSION OF VOLATILE ORGANICS FROM SURFACE AERATION WASTEWATER TREATMENT FACILITIES

CONSTANTINOS V. CHRYSIKOPOULOS¹, LYNN M. HILDEMAN² and PAUL V. ROBERTS²®

¹Department of Civil Engineering, University of California, Irvine, CA 92717 and

²Department of Civil Engineering, Stanford University, Stanford, CA 94305-4020, U.S.A.

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Abstract—A methodology has been developed for predicting volatile organic concentration levels immediately downwind of wastewater treatment facilities, as well as further away, under neutral or stable atmospheric conditions. For the case of a ground-level well-mixed continuous-flow basin with intense mechanical aeration at the surface, the rates of mass transfer of organic pollutants to the atmosphere are obtained by assuming that the entire resistance to mass transfer resides in the stagnant film at the liquid phase interface. The atmospheric transport of the organic emissions downwind are then predicted by a three-dimensional atmospheric dispersion equation, considering dry deposition as a sink mechanism and accounting for variations of wind velocity and vertical diffusivity with height above the ground. The variation of downward concentration levels with Henry's constant is examined for different atmospheric stabilities, deposition velocities, surface roughnesses and basin surface areas.

Key words—surface aeration, organic emissions, atmospheric dispersion

NOMENCLATURE

a = parameter used in the power law wind profile, dependent on q_{z_0} and atmospheric conditions ($L^{1-m} T^{-1}$)
 a_T = interfacial area per unit volume of liquid ($L^2 L^{-3}$)
 b = parameter used in power law vertical eddy diffusivity profile, dependent on q_{z_0} and atmospheric conditions ($L^{2-n} T^{-1}$)
 B = brake power of aerator (P)
 C = contaminant concentration ($M L^{-3}$)
 C_L = bulk average concentration in the liquid ($M L^{-3}$)
 C_L^* = liquid-phase concentration in equilibrium with the bulk gas-phase concentration ($M L^{-3}$)
 C_G^* = gas-phase concentration in equilibrium with the bulk liquid-phase concentration ($M L^{-3}$)
 $C_{O_2}^s$ = oxygen saturation concentration ($M L^{-3}$)
 $\langle C \rangle$ = ensemble average component of concentration ($M L^{-3}$)
 D = molecular diffusion coefficient in water ($L^2 T^{-1}$)
erf = error function
 H_c = Henry's law constant (dimensionless)
 J_a = rate of mass emitted per unit area ($M L^{-2} T^{-1}$)
 J_p = rate of total mass emitted ($M T^{-1}$)
 k = integer
 k_G, k_L = gas- and liquid-phase mass transfer coefficients, respectively ($L T^{-1}$)
 K_L = overall mass transfer coefficient ($L T^{-1}$)
 K_{yy}, K_{zz} = lateral and vertical eddy diffusivities, respectively ($L^2 T^{-1}$)
 l_x = downwind length of the source (L)
 l_y = crosswind width of the source (L)
 l_z = depth of basin (L)
 \bar{L} = Monin-Obukhov stability length (L)
 m = parameter used in power law wind profile, dependent on atmospheric conditions and ground surface roughness
 n = parameter used in power law vertical eddy diffusivity profile, dependent on atmospheric conditions and ground surface roughness

N_{O_2} = oxygen transfer rate ($M P^{-1} T^{-1}$)
 O = order of magnitude
 q_{z_0} = surface roughness length (L)
 q_z^* = some reference height (L)
 \mathbf{q} = vector of Cartesian spatial coordinates:
 $\mathbf{q} = (q_x, q_y, q_z)^T$
 S = source function ($M L^{-3} T^{-1}$)
 t = time (T)
 T = temperature (K)
 \bar{u}_x = downwind deterministic mean fluid velocity ($L T^{-1}$)
 v_d = dry deposition velocity ($L T^{-1}$)
 V = basin volume (L^3)
 \bar{V}_i = molal volume of solute i at its normal boiling point ($L^3 M^{-1}$)
 β = defined in (9b) (dimensionless)
 γ = defined in (9c) (dimensionless)
 Γ = gamma function
 δ = Dirac delta function
 Θ = defined in (9e) (dimensionless)
 Λ = defined in (9g) (L^{-n})
 μ_w = viscosity of water ($M L^{-1} T^{-1}$)
 ν = defined in (9d) (dimensionless)
 ξ = constant
 σ_y^2 = crosswind mean square particle displacement (L^2)
 Ψ = defined in (10) (dimensionless)
 Ω = defined in (9f) (dimensionless)
 $||$ = absolute value

Subscripts

i = refers to volatile solute i
 x, y, z = principal directions of a Cartesian coordinate system: x = downwind, y = crosswind and z = vertical

Superscripts

T = transpose
 $^\circ$ = implies contaminant source location
 $\bar{\bar{}}$ = (overbar) average over time and space

INTRODUCTION

Groundwater and wastewater contaminated by chemicals of anthropogenic origin require treatment to achieve water quality restoration. A variety of methods for treatment of contaminated water are available (Schroeder, 1977; Metcalf & Eddy, 1991; Stenzel and Gupta, 1985). Depending on the effluent discharge requirements, activated sludge, aerated lagoons and oxidation ditches are presently widely used as water treatment facilities. In aerated lagoons and oxidation ditches, the mechanical aeration which is used to increase the purification capacity also promotes volatilization of the organics present. Emissions of these volatile organic contaminants (VOCs) can create potential health risks to on-site workers and to the general public in surrounding communities (Dunovant *et al.*, 1986). To evaluate the potential hazard to the local atmosphere, accurate determination of VOC emission rates and realistic modeling of contaminant transport in the atmosphere are required.

Since the wind velocity and vertical eddy diffusivity vary with height near the surface of the earth, simple Gaussian models for turbulent atmospheric dispersion (Baker and MacKay, 1985; Hinrichsen, 1986; Wolfinger, 1989) are not adequate for ground level sources. Characterizations of wind velocity and vertical diffusivity profiles by power law approximations are a more accurate approach. It has allowed analytical solutions to be derived for several atmospheric dispersion models (Smith, 1957; Huang, 1979; Rao, 1981; Koch, 1989; Chitgopekar *et al.*, 1990; Chrysiopoulos *et al.*, 1992), and has enabled the prediction of evaporation (Brutsaert and Yeh, 1970) and atmospheric dispersion from instantaneous sources (Drivas and Shair, 1974; Dvornik and Vagli-Laurin, 1982). Furthermore, to be realistic, the atmospheric dispersion model should account for potential sink mechanisms for the transported contaminant. Dry deposition can be an important process for the removal of both gaseous and particulate airborne contaminants at the earth's surface layer; particulate matter is removed due to gravitational settling and Brownian motion, whereas uptake of gases at the earth's surface is influenced by reactivity of the chemical as well as seasonal, diurnal and meteorological effects (Seinfeld, 1986). Since deposition velocities of up to 1.0 cm s^{-1} have been estimated for some organic pollutants (Bidleman, 1988), an accurate model of contaminant transport near ground-level should include dry deposition.

In this paper we present a procedure for predicting emissions of VOCs from water and wastewater treatment facilities employing surface aeration, and apply a recently developed analytical three-dimensional atmospheric dispersion model (Chrysiopoulos *et al.*, 1992) which accounts for variations of wind velocity and vertical diffusivity with height above the ground and includes dry deposition as a sink mechanism.

By combining the surface aeration and atmospheric dispersion models, we are able to estimate downwind airborne VOC concentrations based on liquid phase VOC concentrations in the aeration basin. Although only surface aeration treatment facilities have been considered in this work, the same methodology can be applied to bubble aeration treatment units, lagoons, evaporation ponds and hazardous waste sites.

PREDICTION OF VOC EMISSIONS FROM SURFACE AERATION TREATMENT FACILITIES

The VOCs that are present in surface aeration treatment facilities can be transferred to the atmosphere at appreciable rates. Emission of VOCs from an aerated surface of a water body entails mass transport to and from the water-air interface, diffusion through the incompletely-mixed boundary layer commonly present in the near-surface air, followed by turbulent dispersion in the atmosphere. There are several methods available for estimation of VOC emissions from surface aeration basins. Thibodeaux *et al.* (1982) developed a procedure for measuring flux rates of selected volatile organic carbon compounds to the atmosphere from fairly large wastewater treatment facilities of the pulp and paper industry. The method requires average observations of wind velocity, atmospheric temperature and VOC concentrations at a 2 m height above the water surface. Thibodeaux and Parker (1976) presented a model which divides the surface of an aeration basin in turbulent and natural zones. The turbulent zone corresponds to the area of the basin where mechanical surface aeration occurs, whereas the natural zone is the undisturbed area of the basin. In this work, we derive emission rates from a VOC mass balance under steady state flow conditions, assuming that the aeration basin is completely mixed and sorption or biodegradation processes are insignificant.

An adequate rate expression for VOC emissions from a well-mixed continuous-flow basin with intense mechanical aeration at the surface, based on the two-film concept introduced by Lewis and Whitman (1924), is given by

$$J_p = -\frac{dC_L}{dt} V = K_L a_T (C_L - C_L^*) V, \quad (1)$$

where J_p is the rate of total mass emitted, C_L is the bulk average VOC concentration in the liquid, C_L^* is the liquid-phase VOC concentration in equilibrium with the gas-phase concentration, t is the time, K_L is the overall mass transfer coefficient, a_T is the interfacial area per unit volume of liquid and V is the volume of the basin. The product, $K_L a_T$, having units T^{-1} , is the overall mass transfer rate constant. Customarily, in estimating the transfer rate of volatile organic solutes into the atmosphere, it is presumed that sufficient atmospheric turbulence exists such that local saturation in the overlaying air is negligible,

so that C_L^* can be assumed to be zero (Roberts *et al.*, 1984).

The overall rate constant, $K_L a_T$, usually is experimentally determined as a single lumped parameter. Assuming that the entire resistance to mass transfer resides in the stagnant film at the liquid phase interface, $K_L a_T$ is expressed in terms of liquid-phase and gas-phase boundary layer mass transfer resistances as (Liss and Slater, 1974; Thibodeaux, 1979; Roberts and Dändliker, 1983; Roberts *et al.*, 1983)

$$\frac{1}{K_L a_T} = \frac{1}{k_L a_T} + \frac{1}{k_G a_T H_c}, \quad (2)$$

where k_L and k_G are the liquid- and gas-phase mass transfer coefficients, respectively, and H_c is the Henry's law constant expressed as a dimensionless mass concentration partition ratio:

$$H_c = \frac{C_G^*}{C_L}, \quad (3)$$

where C_G^* is the gas-phase VOC concentration in equilibrium with the bulk liquid-phase concentration.

ATMOSPHERIC DISPERSION MODEL

For steady conditions, the transport of an inert contaminant released into atmospheric air may be described by the following stochastic partial differential equation (Seinfeld, 1986)

$$\begin{aligned} \bar{u}_x(\mathbf{q}) \frac{\partial \langle C(\mathbf{q}) \rangle}{\partial q_x} &= \frac{\partial}{\partial q_y} \left(K_{yy}(\mathbf{q}) \frac{\partial \langle C(\mathbf{q}) \rangle}{\partial q_y} \right) \\ &+ \frac{\partial}{\partial q_z} \left(K_{zz}(\mathbf{q}) \frac{\partial \langle C(\mathbf{q}) \rangle}{\partial q_z} \right) + S(\mathbf{q}^\circ), \quad (4) \end{aligned}$$

where $\langle C \rangle$ is the ensemble average contaminant concentration $\mathbf{q} = (q_x, q_y, q_z)^T$ is the vector of spatial coordinates, subscripts x, y, z denote the principal directions of a Cartesian coordinate system, \bar{u}_x is the downwind deterministic mean fluid velocity, K_{yy} and K_{zz} are the lateral and vertical eddy diffusivities, respectively, $S(\mathbf{q}^\circ) = J_p \delta(\mathbf{q} - \mathbf{q}^\circ)$ is a source function located at $\mathbf{q}^\circ = (q_x^\circ, q_y^\circ, q_z^\circ)^T$ and $\delta(\cdot)$ is a Dirac delta function.

For mathematical convenience, \bar{u}_x , K_{yy} and K_{zz} are approximated by the following power functions of q_z , respectively,

$$\bar{u}_x(q_z) = a q_z^m, \quad (5)$$

$$K_{yy}(q_x, q_z) = \frac{1}{2} \bar{u}_x(q_z) \frac{d\sigma_y^2(q_x)}{dq_x}, \quad (6)$$

$$K_{zz}(q_z) = b q_z^n, \quad (7)$$

where the parameters a, b, m and n are not constants, but depend on the atmospheric conditions and on the ground surface roughness; and σ_y^2 is the mean square particle displacement along the q_y coordinate axis (crosswind). Assuming that the contaminant is

initially absent from the atmosphere and the only sink mechanism is dry deposition, the appropriate boundary conditions are

$$\langle C(\infty, q_y, q_z) \rangle = 0, \quad (8a)$$

$$\langle C(q_x, \pm \infty, q_z) \rangle = 0, \quad (8b)$$

$$\langle C(q_x, q_y, \infty) \rangle = 0, \quad (8c)$$

$$K_{zz}(q_z) \frac{\partial \langle C(\mathbf{q}) \rangle}{\partial q_z} = v_d \langle C(\mathbf{q}) \rangle \quad \text{at } q_z = q_{z_0}, \quad (8d)$$

where v_d is the deposition velocity, and q_{z_0} is the surface roughness length. Boundary condition (8d) indicates that the turbulent transport of the contaminant along the vertical concentration gradient is balanced by the net contaminant flux to the earth's surface resulting from an exchange between the atmosphere and the earth's surface.

The solution of equations (4)–(8) for a ground level area source of downwind length l_x and crosswind width l_y is given by Chrysikopoulos *et al.* (1992)

$$\langle C(\mathbf{q}) \rangle = \int_0^{l_x} \frac{J_a \beta \Theta \Omega \exp[-\gamma]}{2a^\nu [\beta^2 b (q_x - q_x^\circ)]^{1-\nu} \Gamma(1-\nu)} dq_x^\circ \quad (q_x > l_x), \quad (9a)$$

where

$$\beta = m - n + 2, \quad (9b)$$

$$\gamma = \frac{a q_z^\beta}{\beta^2 b (q_x - q_x^\circ)}, \quad (9c)$$

$$\nu = \frac{1-n}{\beta}, \quad (9d)$$

$$\begin{aligned} \Theta &= \text{erf} \left[\frac{l_y/2 + q_y}{\sqrt{2\{\sigma_y^2(q_x) - \sigma_y^2(q_x^\circ)\}}} \right] \\ &+ \text{erf} \left[\frac{l_y/2 - q_y}{\sqrt{2\{\sigma_y^2(q_x) - \sigma_y^2(q_x^\circ)\}}} \right], \quad (9e) \end{aligned}$$

$$\begin{aligned} \Omega &= 1 - \sum_{k=0}^{K-1} \frac{[-A(q_x - q_x^\circ)]^{-k} \Gamma(\nu)}{\Gamma(\nu - \nu k)} \\ &+ O(|A(q_x - q_x^\circ)|^{-K}) \quad q_z \ll q_x, \quad (9f) \end{aligned}$$

$$A = -\frac{v_d}{vb} \left(\frac{b}{a}\right)^\nu \frac{\Gamma(1+\nu)}{\Gamma(1-\nu)} \beta^{2\nu-1}, \quad (9g)$$

$\Gamma(z)$ is the gamma function, and $\text{erf}[z]$ is the error function. Since analytical evaluation of the integral in (9a) is not straightforward, numerical integration techniques must be employed.

ESTIMATION OF INPUT PARAMETERS

Surface aeration model parameters

The ratio between the overall mass transfer rate constant of a VOC and that of oxygen is approximately constant for a wide range of volatile solutes, and is proportional to the molecular diffusion

coefficient ratio of the volatile organic and oxygen (Smith *et al.*, 1980; Matter-Müller *et al.*, 1981; Roberts and Dändliker, 1983)

$$\Psi = \frac{(k_L a_T)_i}{(k_L a_T)_{O_2}} = \left(\frac{D_i}{D_{O_2}} \right)^\xi \quad (10)$$

where subscripts *i* and O_2 indicate volatile compound *i* and oxygen, respectively, *D* is the molecular diffusion coefficient in water and ξ is a constant. The value of Ψ for halogenated aliphatic solutes with one or two carbon atoms is in the range $0.5 < \Psi < 0.7$; while the value of ξ is in the range $0.61 < \xi < 0.66$ (Smith *et al.*, 1980; Roberts and Dändliker, 1983; Roberts *et al.*, 1984). The Ψ and ξ values of some representative VOCs are listed in Table 1. The preceding equation enables estimation of $K_L a_T$ for a given compound *i* from that of oxygen. If the diffusivity in water of compound *i* is not available, it can be estimated by the correlation of Wilke and Chang (1955)

$$D_i = 7.4 \times 10^{-15} (18\phi)^{0.5} \frac{T}{\mu_w \bar{V}_i^{0.6}} \quad (\text{m}^2 \text{s}^{-1}), \quad (11)$$

where $\phi = 2.26$ is the association parameter for water (Hayduk and Laudie, 1974; Hayduk and Minhas, 1982), *T* is the temperature (K), μ_w is the viscosity of water ($\text{kg m}^{-1} \text{s}^{-1}$) and \bar{V}_i is the molal volume at the normal boiling point of the solute ($\text{cm}^3 \text{mol}^{-1}$). For typical surface aeration basins, $(K_L a_T)_{O_2}$ can be calculated from agitator manufacturer's oxygenation rate data using the following relationship (Roberts *et al.*, 1984):

$$(K_L a_T)_{O_2} = \frac{N_{O_2} B}{C_{O_2}^s V} \quad (\text{s}^{-1}), \quad (12)$$

where N_{O_2} is the oxygen transfer rate ($\text{kg}_{O_2} \text{kW}^{-1} \text{h}^{-1}$), *B* is the brake power of the aerator (kW) and $C_{O_2}^s$ is the oxygen saturation concentration ($\text{kg}_{O_2} \text{m}^{-3}$).

For sufficiently volatile organics, the liquid-phase resistance controls the rate of interphase mass transfer (Roberts *et al.*, 1984). For instance, in treatment units where mechanical surface aeration is used, a conservative lower limit for the ratio of the gas-phase resistance relative to liquid-phase resistance under treatment plant conditions is given by (Munz and Roberts, 1984)

$$\frac{k_G}{k_L} \geq 20. \quad (13)$$

Under mixing conditions representative of wastewater treatment, the value of the ratio k_G/k_L is approx. 40 (Munz and Roberts, 1989).

Various proposed correlations for liquid- and gas-phase mass transfer coefficients applicable to aerated lagoons and oxidation ditches have been compiled by Thibodeaux (1979) and Hwang (1982). Assuming that C_L^* is approximately zero and combining equations (1), (2), (10) and (13) yields

$$J_p \geq \left(\frac{1}{\Psi (k_L a_T)_{O_2}} + \frac{1}{20 (k_L a_T)_{O_2} H_c} \right)^{-1} C_L V. \quad (14)$$

The preceding equation enables estimation of the rate of mass of compound *i* emitted from an aeration basin with volume *V*, assuming that the values of $(k_L a_T)_{O_2}$, Ψ , H_c and C_L are either known or can be determined experimentally.

Atmospheric dispersion model parameters

In this section we present relationships for estimation of atmospheric dispersion model parameters applicable only for neutral and stable atmospheric conditions. For unstable conditions, refer either to the literature cited or to compilations presented by Chrysikopoulos *et al.* (1992).

The multiplication constant, *a*, and the exponent, *m*, in the power law wind profile can be evaluated based on the Monin-Obukhov similarity theory (Paulson, 1970; Webb, 1970; Dyer, 1974; Huang, 1979):

$$a = \frac{\bar{u}_x(q_z^*)}{(q_z^*)^m} \quad (15)$$

$$m = \frac{1 + 5q_z/L}{\ln[q_z/q_{z_0}] + 5q_z/L}, \quad (16)$$

where q_z^* is a reference height, and *L* is the Monin-Obukhov stability length, that is, the height above the earth's surface where the contributions to the production of turbulence by mechanical and buoyancy forces are equal. The lateral eddy diffusivity, K_{yy} , is obtained from equation (6), where the crosswind mean square particle displacement is commonly treated as an empirical coefficient determined by the relationship developed by Sutton (1932)

$$\sigma_y^2(q_x) = 0.0968 q_x^{1.42}. \quad (17)$$

Similarly, the multiplication constant, *b*, and the exponent, *n*, in the power law expression of the

Table 1. Properties of some VOCs*

Compound	Molecular weight	H_c^\dagger at 293 K	D_i^\ddagger $10^{-9} \text{m}^2 \text{s}^{-1}$	Ψ^\dagger	ξ^\ddagger
CCl_2F_2	120.9	9.3	1.02	0.66	0.65
CCl_4	153.8	0.94	0.85	0.62	0.63
$\text{CCl}_2=\text{CCl}_2$	165.8	0.61	0.79	0.61	0.57
$\text{CHCl}=\text{CCl}_2$	131.4	0.42	0.86	0.62	0.63
CHCl_3	119.4	0.24	0.94	0.56	0.84

*Solvent: deionized water; † from Roberts *et al.* (1984); ‡ from Roberts and Dändliker (1983).

vertical eddy diffusivity [equation (5)] can be determined by (Huang, 1979)

$$b = \frac{K_{zz}(q_z^*)}{(q_z^*)^n}, \quad (18)$$

$$n = \frac{1}{1 + 5q_z/L}. \quad (19)$$

Typical values of the surface roughness, q_{z0} , are 0.01 m for lawn, 0.1 m for fully grown crops and 1 m for tree covered areas (McRae *et al.*, 1982). For these surface roughness lengths at moderately stable conditions, the corresponding values of L^{-1} are 0.107, 0.071 and 0.035 m^{-1} , respectively; whereas for neutral conditions L^{-1} is always zero (Golder, 1972).

APPLICATION AND DISCUSSION

Consider a typical surface aeration basin with volume $V = l_x \times l_y \times l_z = 20 \times 40 \times 4 = 3200 \text{ m}^3$, where oxygen is supplied by a 30 kW surface aerator with oxygen transfer rate of $2.13 \text{ kg}_{\text{O}_2} \text{ kW}^{-1} \text{ h}^{-1}$. Since oxygen saturation at 20°C is $9.17 \times 10^{-3} \text{ kg m}^{-3}$, the value of $(k_L a_T)_{\text{O}_2}$ is approximately $6 \times 10^{-4} \text{ s}^{-1}$. By assigning to Ψ a value of 0.62 and assuming that C_L for compound i is 1 g m^{-3} , the rate of mass emitted as a function of H_c can be evaluated from equation (14).

For dispersion calculations, assume that $q_{z0} = 0.1 \text{ m}$ (for root crops), $\bar{u}_x(q_z^*) = 1.5 \text{ m s}^{-1}$ and $K_{zz}(q_z^*) = 0.025 \text{ m}^2 \text{ s}^{-1}$ at a reference height $q_z^* = 10 \text{ m}$. Then the multiplication constant a , and the exponent m , in the power law wind expression (5) are obtained by equations (15) and (16), respectively. The crosswind mean square particle displacement $\sigma_y^2(q_x)$ in the expression for $K_{yy}(q_x, q_z)$ [equation (10)] is obtained by equation (17). To predict downwind concentrations as a function of H_c , given that $J_a = J_p/(l_x \times l_y)$, equation (9) is employed. The gamma functions in equation (9) are calculated numerically by the approximation derived by Lanczos (1964) [see Chrysikopoulos *et al.* (1992), for further discussion], and the integral over l_x is evaluated numerically by the extended Simpson's rule (Press *et al.*, 1986). For presentation purposes, the calculated concentrations appearing in Figs 1–5 are normalized by the bulk average VOC concentration of the wastewater in the basin. The range of Henry's constant used in the figures is chosen to encompass most of the VOCs commonly encountered in wastewater treatment facilities (see Table 1).

To illustrate the expected VOC distribution in the surrounding atmosphere of the hypothetical aeration basin previously described, normalized concentrations as a function of Henry's constant along the centerline of the plume at a vertical height of 2 m have been calculated for a variety of conditions. In Fig. 1, we have plotted the variation of VOC concentration with Henry's constant at three downwind distances. Concentration levels initially increase with

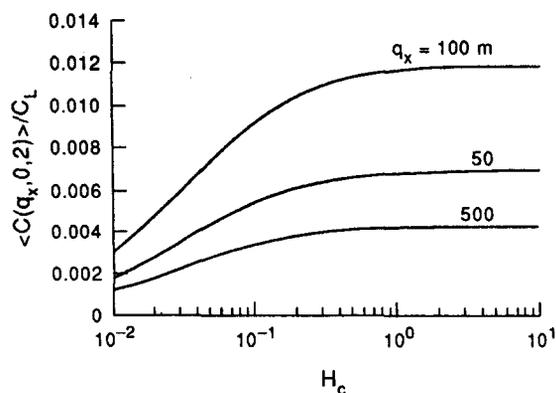


Fig. 1. Variation of normalized concentration with Henry's constant for $q_x = 50, 100, 500 \text{ m}$ and stable atmospheric conditions ($q_z = 2 \text{ m}$, $q_{z0} = 0.1 \text{ m}$, $v_d = 0$).

increasing H_c , and subsequently approach an asymptotic value. From equation (2) it is evident that for low values of H_c , an increase in H_c reduces the overall mass transfer resistance and leads to a higher VOC emission rate [see equation (14)]. For high H_c values, the gas-phase mass transfer resistance becomes insignificant and $K_L a_T \approx k_L a_T$. Therefore, the expected VOC concentration at a specified location in the atmosphere is approximately equal for any compound with $H_c \geq H_c^*$, where H_c^* represents the value of Henry's constant above which J_p is independent of H_c . Figure 1 also shows that the predicted concentrations 100 m downwind are higher than those at 50 and 500 m. Sufficiently close to the source, concentrations at a given height increase with distance downwind as turbulent eddies mix the ground-level emissions upward; at some distance a peak concentration is reached and further downwind the continued dispersive effects of these eddies in the vertical and lateral directions cause the concentrations to decline with distance.

Figure 2 illustrates the effect of surface roughness on VOC concentrations under stable atmospheric conditions. As q_{z0} gets larger, the greater resistance to downwind contaminant transport causes increased VOC accumulation. Hence, predicted concentration

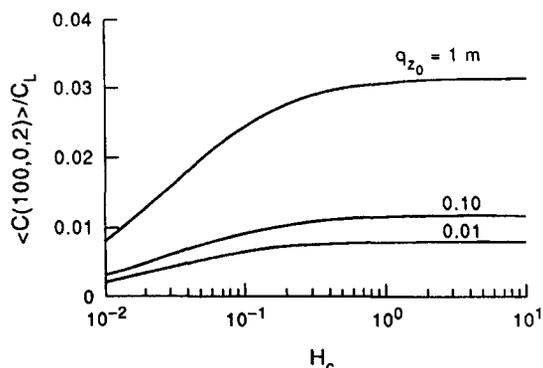


Fig. 2. Variation of normalized concentration with Henry's constant for $q_{z0} = 0.01, 0.1, 1.0 \text{ m}$ and stable atmospheric conditions ($q_x = 100 \text{ m}$, $q_z = 2 \text{ m}$, $v_d = 0$).

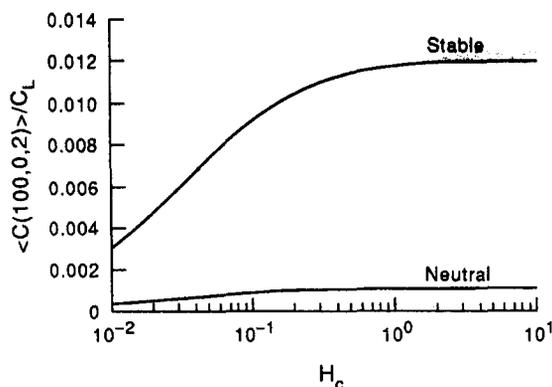


Fig. 3. Variation of normalized concentration with Henry's constant for neutral and stable atmospheric conditions ($q_x = 100$ m, $q_z = 2$ m, $q_{z0} = 0.1$ m, $v_d = 0$).

levels increase with increasing surface roughness length. The 3-fold difference in concentration seen in Fig. 2 for the assumed conditions is predicted to persist for several km downwind (Chrysikopoulos *et al.*, 1992).

The effect of atmospheric stability on VOC concentrations is shown in Fig. 3. The predicted normalized concentrations as a function of H_c at a downwind distance of 100 m are up to 10-fold higher for stable than for neutral atmospheric conditions. This result is attributable to significant differences in vertical mixing for the two stability classes: at neutral stability, vertical movement of an air volume is unimpeded because the air volume adiabatically maintains the same density as the surrounding air, regardless of height; however, for stable atmospheric conditions, a rising air volume will become denser than its surroundings and thus tend to sink back to its initial vertical position (Seinfeld, 1986). Hence, at stable atmospheric conditions, the vertical spreading of a VOC is hindered, leading to higher airborne concentrations near ground level at a given distance downwind.

Figure 4 shows the effect of dry deposition on downwind VOC concentrations. The reduction of VOC concentrations with increasing dry deposition

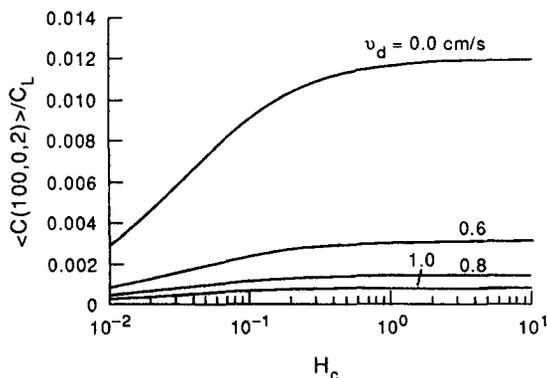


Fig. 4. Variation of normalized concentration with Henry's constant for $v_d = 0.0, 0.6, 0.8, 1.0$ cm s⁻¹ and stable atmospheric conditions ($q_x = 100$ m, $q_z = 2$ m, $q_{z0} = 0.1$ m).

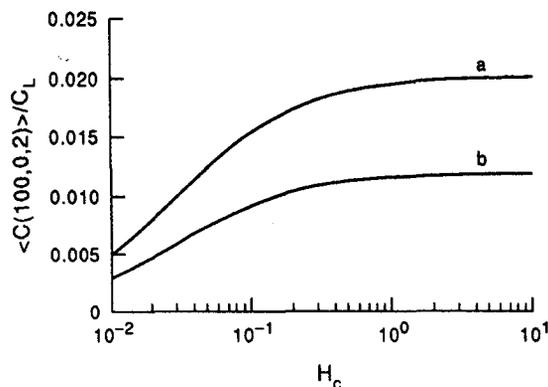


Fig. 5. Variation of normalized concentration with Henry's constant at stable atmospheric conditions for basins of equal volume with dimensions $V = l_x \times l_y \times l_z$: (a) $32 \times 20 \times 5$ m³ and (b) $40 \times 20 \times 4$ m³ ($q_x = 100$ m, $q_z = 2$ m, $q_{z0} = 0.1$ m, $v_d = 0$).

velocity is intuitively expected, since v_d is a mechanism for removing airborne contaminants at the earth's layer. For volatile organics having a deposition velocity of 1 cm s⁻¹, over an order of magnitude decrease in downwind concentration is predicted compared with a compound having no deposition velocity, and this decrease will persist for hundreds of km downwind (Chrysikopoulos *et al.*, 1992).

In Fig. 5, we have presented normalized concentration profiles at $q_x = 100$ m under stable atmospheric conditions assuming zero dry deposition for basins of equivalent total source strengths and volumes, but different dimensions ($V = l_x \times l_y \times l_z$): (a) $32 \times 20 \times 5$ m³ and (b) $40 \times 20 \times 4$ m³, respectively. The atmospheric VOC concentration levels corresponding to the basin with the larger surface area are lower, because the mass emitted from the source is distributed over a larger area. However, at sufficiently large downwind distances ($q_x \rightarrow \infty$) Chrysikopoulos *et al.* (1992) have shown that these VOC concentrations will become approximately equal.

SUMMARY

A methodology has been developed for predicting volatile organic concentration levels downwind of a ground-level surface aeration water treatment unit. Emissions from the basin are calculated based on the aqueous influent concentration of the VOC and a few basic chemical properties, assuming the entire resistance to mass transfer exists in the stagnant film present at the interface. The model then predicts downwind concentration levels with a three-dimensional dispersion model using the prevailing meteorological conditions and assuming the emissions are nonbuoyant. Accurate representation of wind speed and turbulence in the near-surface layer are contained in the model, the roughness of the downwind terrain is included, and dry deposition is accounted for as a sink mechanism.

The effect of various model input parameters on predicted concentrations is examined. Concentration levels markedly increase as atmospheric stability increases, and as the roughness of the terrain increases. Increasing the Henry's constant causes a gradual increase in downwind concentrations under fixed conditions, approaching an asymptotic value as mass transfer resistance becomes negligible. In contrast, increasing the deposition velocity causes a substantial and persistent decrease in downwind concentrations.

This model is able to predict downwind concentrations near ground level based on contaminant levels in the water, the operating conditions of the treatment facility and prevailing local conditions. Hence, it is particularly useful for evaluating the potential risks of organic emissions at a treatment site to workers and nearby communities.

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