Assessing Built-In Wind Friction Parametrisation in WWTP Emission Models for Estimating Compound Volatilisation

Ademir A. Prata[a], Jane M. Santos[b], Neyval C. Reis Jr[b], Richard M. Stuetz[a]

[a] UNSW Australia, School of Civil and Environmental Engineering , Sydney, Australia
[b] UFES, Department of Environmental Engineering, Vitoria, Brazil
r.stuetz@unsw.edu.au

Wind friction is a fundamental parameter in modelling air emissions from passive liquid surfaces at WWTPs. This work assessed preliminary discrepancies associated to the use of an empirical equation to estimate friction velocities for emission modelling, comparing the mass transfer coefficient calculated by different emission models if two distinct approaches are used to address the wind speed range between 1 ms^{-1} and 6 ms^{-1}. Other situations related to the operation of the WWTP, which can affect the volatilisation process are also discussed. In the wind speed range studied, the inclusion of a different expression for the friction velocity can lead to differences of about 20% in the global mass transfer coefficients (assessed here for H$_2$S) and therefore in the emission rate, depending on the model applied.

1. Introduction

Liquid surfaces without active aeration/intense bubbling commonly featured in wastewater treatment plants (WWTP) can be represented by primary and secondary settlement tanks, sequencing batch reactors and stabilisation ponds. These surfaces are important sources of air emissions potentially associated with odour annoyance to local communities, exposure to harmful compounds and greenhouse effect. Emission from passive liquid surfaces is mainly due to the volatilisation of compounds driven by the interaction between the liquid-phase and the sweeping wind and is usually estimated by using Equation (1).

$$J = K_L \left(C_L - \frac{C_G}{K_H} \right) \qquad \text{and} \qquad \frac{1}{K_L} = \frac{1}{k_L} + \frac{1}{k_G K_H} \qquad (1)$$

Where: J is the emission rate (kg m^{-2} s^{-1}) or the compound mass flux per unit area; C_L is the compound concentrations (kg m^{-3}) in the bulk liquid phase which can be easily sampled and measured; C_G is the compound concentrations (kg m^{-3}) in the bulk gas phase which are usually neglected; K_H is the Henry`s law coefficient and depends on the compound and ambient conditions; k_L and k_G are the liquid-film and the gas-film mass transfer coefficients (m s^{-1}), respectively, and K_L is the liquid-phase overall mass transfer coefficient (m s^{-1}). Although very simple for the case of stagnant films, the values of k_L and k_G for the actual field situation, on the other hand, are not necessarily straightforward, since various physical and chemical processes may take place at the air-water interface, for instance: drift currents and sheared boundary layer (Feroni et al., 2012); surface divergence (Jähne and Haußecker, 1998); formation of both capillary and gravity waves, which may be accompanied by micro and macroscale breaking (Mackay and Yeun, 1983; Jähne and Haußecker, 1998); presence of surfactants and surface films (Jähne and Haußecker, 1998); and chemical reactions (Blunden et al., 2008).

k_L and k_G depend on variables representing wind forcing and molecular diffusion. The wind force can be represented by the wind speed at a certain height (U_z) or the friction velocity (u_*). On-site measurements of u_* are not routinely available in most practical applications, but can be calculated based on wind velocity. These variables k_L and k_G are calculated using different expressions involving U_z or u_*.

However, the correlations for u_* were originally developed based on experimental data for wind drag over the ocean where the characteristics of the wave field are expected to significantly affect the wind flow near the

surface and, consequently, the wind drag (Janssen, 1994; Kudryavtsev et al., 2014). The wind-wave field over relatively small liquid surfaces may present differences compared with ocean. Thus, the drag/friction velocity formulations established for the ocean do not necessarily apply to liquid surfaces encountered at WWTP. Therefore, the aim of this work is to discuss and assess preliminary discrepancies associated to the use of empirical equations to estimate friction velocities in order to calculate emission rates associated with passive liquid surfaces at WWTPs.

2. Mass transfer coefficients used in WWTP emissions models

The most common WWTP emission models are WATER9, TOXCHEM+ and Gostelow et al. (2001), among others (Santos et al 2006). The volatilisation removal rates are estimated based on mass transfer coefficient in the liquid and gas phases given by different empirical equation in different emission models (Santos et. al 2012).

2.1 WATER9 model

The WATER9 model has been described by USEPA (1994). This is an emission model applied to different stages of collection and conveyance in sewer networks and treatment for industrial and domestic wastewater. Depending on the treatment stage, some of the removal mechanisms are included, such as: volatilisation from quiescent surfaces, mechanically aerated units, weir or drop structures; stripping from units where aeration is carried out by air injection (bubbled-aerated) and biodegradation. The mass transfer coefficient in the liquid phase (k_L) in quiescent surfaces is calculated in WATER9 model by using the expression proposed by Springer et al. (1994) as described in USEPA (1994) (Equations 2 to 4).

$$k_L = (2.78t10^{-6})\left(\frac{D_L}{D_{L,ether}}\right)^{2/3} \qquad \begin{array}{c} 0 < U_{10} < 3.25 \text{ m s}^{-1} \\ \text{and all } F/D \end{array} \qquad (2)$$

$$k_L = \left[(2.605l10^{-9})\left(\frac{F}{D}\right) + (1.277l10^{-7})\right](U_{10})^2\left(\frac{D_L}{D_{L,ether}}\right)^{2/3} \qquad \begin{array}{c} U_{10} > 3.25 \text{ m s}^{-1} \\ \text{and } 14 < F/D < 51.2 \end{array} \qquad (3)$$

$$k_L = (2.61 \times 10^{-7})(U_{10})^2\left(\frac{D_L}{D_{L,ether}}\right)^{2/3} \qquad \begin{array}{c} U_{10} > 3.25 \text{ m s}^{-1} \\ \text{and } F/D > 51.2 \end{array} \qquad (4)$$

Where: F is the surface length in the wind direction (m), D is the tank depth (m), D_L and $D_{L,ether}$ are the molecular diffusion coefficient (m^2 s^{-1}) of the substance and ether in the water, respectively. U_{10} is the wind speed 10 meters above the liquid surface (m s^{-1}).

If the fetch-to-depth ration is less than 14 ($F/D < 14$), k_L is determined by the expressions proposed by Mackay and Yeun (1983), as described in USEPA (1994) and given by Equations 5 to 6.

$$k_L = 1.0 \times 10^{-6} + 144 \times 10^{-4}(u_*)^{2.2}(Sc_L)^{-0.5} \qquad u_* < 0.3 \text{ m s}^{-1} \ (U_{10} < 3.25 \text{ m s}^{-1}) \qquad (5)$$

$$k_L = 1.0 \times 10^{-6} + 34.1 \times 10^{-4}(u_*)(Sc_L)^{-0.5} \qquad u_* > 0.3 \text{ m s}^{-1} \ (U_{10} > 3.25 \text{ m s}^{-1}) \qquad (6)$$

Where: Sc_L is the Schmidt number ($Sc_L = \mu_L/(\rho_L D_L)$) for the substance in the liquid phase (non-dimensional), μ_L is the dynamic viscosity of water (kg m^{-1} s^{-1}), ρ_L is the water specific mass (kg m^{-3}) and u_* is the friction velocity (m s^{-1}), which, in WATER9, is given by the expression proposed by Smith (1980).

The mass transfer coefficient in the gas phase (k_G) is determined as suggested by Mackay e Matsugu (1973) as presented in Equation (7).

$$k_G = (4.82 \ 10^{-3})(U_{10})^{0.78}(Sc_G)^{-0.67}(d_e)^{-0.11} \qquad (7)$$

Where: Sc_G is the Schmidt number ($Sc_G = \mu_G/(\rho_G D_G)$) for the substance in the gas phase (non-dimensional), μ_G is the air dynamic viscosity (kg m^{-1} s^{-1}), ρ_G is the air specific mass (kg m^{-3}), D_G is the molecular diffusion coefficient of the substance in air (m^2 s^{-1}) and $d_e = (4A/\pi)^{0.5}$ is the effective diameter (m) of the liquid surface and A is the surface area (m^2).

2.2 TOXCHEM+model

TOXCHEM+ model (Environmega, 2003) was proposed by Melcer et al. (1994). This model includes volatilisation from quiescent surfaces, weirs, drop structures and sewer reaches and stripping from mechanically aerated surfaces and bubbled-aerated tanks, adsorption and biodegradation.

These removal mechanisms can be assessed in reactors or units in collection systems and treatment and sludge dewatering processes. The mass transfer coefficients in the liquid phase are calculated by using the

expressions proposed by Mackay and Yeun (1983) in Equations 5 and 6 whereas the mass transfer coefficient in the gas phase is calculated by using the expressions proposed by Mackay and Yeun (1983) in Equation 8.

$$k_G = 1.0 \times 10^{-3} + 46.2 \times 10^{-3}(u_*)(Sc_G)^{-0.67} \tag{8}$$

2.3 Gostelow et (2001) model

Gostelow et al. (2001) presented an emission model including stripping as a removal mechanism in bubble-aerated tanks and mechanically aerated surfaces and volatilisation in quiescent surfaces, channels, weirs, drop structures, and trickling filters (where they suggested the biodegradation mechanism should also be included). Gostelow et al. (2001) fit their own correlation to a compilation of data from the literature, obtaining expressions for the mass transfer coefficients in the liquid (k_L) and gas (k_G) phases as presented in Equations 9 and 10.

$$k_L = 0.0035u_*(Sc_L)^{-0.5} \tag{9}$$
$$k_G = 0.04u_*(Sc_G)^{-0.67} \tag{10}$$

3. Empirical expression in-built in the WATER9 model to estimate friction velocity over liquid surface in WWTPs

Nearly all expressions used to determine k_L and k_G include u_*, therefore a good estimate of this parameter is essential to calculate the emission rate. Equation 11 developed by Smith (1980) is frequently recommended in emission modelling guides (Gostelow et al., 2001; ENVIROMEGA, 2003; US EPA, 1994, 2001) and is included as a built-in component in the US EPA-endorsed modelling code WATER9 (US EPA, 1994, 2001). Smith (1980) presented a correlation for the drag coefficient (air phase over the ocean) as a linear function of wind speed at 10 m height under near neutral atmospheric condition (Equation 11). Smith (1980) used high-frequency wind velocity data measured by an anemometer installed in a floating platform (12.5 m above water level) to estimate values of U_{10} and directly calculate the eddy fluxes of momentum in the surface layer. U_{10} values were found from 6 m s^{-1} to 22 m s^{-1}, with long wind fetch and waves propagating in deep-water regime. Waves are formed in WWTPs unit processes in which the liquid surface is exposed to wind shear (Figure 1), except for very light winds, sheltered surfaces and/or in the presence of surface films and scums. The differences between ocean surface and liquid surfaces in WWTP are the very short fetches (most commonly, between 5 and 100 m) and the absence of free-propagating waves (swell). Therefore, wind drag and wave data obtained for open sea do not necessarily apply for such particular cases. On the other hand, detailed wind and wave measurements are not routinely performed in wastewater treatment tanks.

Table 1: Expression proposed by Smith (1980) to calculate friction velocity based on wind velocity measured at 10m for different ranges of wind speed.

Expression		Wind speed range (m s^{-1})	Conditions
$u_* = 10^{-2}U_{10}(6.1 + 0.63U_{10})^{0.5}$	(11)	$6 \leq U_{10} \leq 22$	neutral atmospheric condition; long wind fetch; deep-water waves.
$u_* = U_{10}\left[\dfrac{1}{k}ln\left(\dfrac{10u_*}{vz_0^+}\right)\right]^{-1}$	(12)	$U_{10} < 6$	neutral atmospheric condition; long wind fetch; deep-water waves; $z_0^+ = 0.11$.

The validity of Smith (1980) expression does not include short fetches and low velocities which commonly occur in WWTP. The experimental work conducted by Smith (1980) found average waves heights from 0.28 m to 1.35 m, which are not verified in short fetch tanks. Furthermore, Smith (1980) also recommend a different approach, based on the turbulent logarithmic wind velocity profile over a smooth flat plate (Equation 12), for velocities lower than 6 m s^{-1}. This is not mentioned in emission models, which means that modellers use Equation 11 for the entire range of wind speed. Figure 2 shows the differences between the calculations obtained with Equation 11 compared to Equation 12 for lower wind speeds ($U_{10} < 6$ m/s). However, the differences in the mass transfer coefficients due to the use of Equation 11 instead of Equation 12 for wind speed lower than 6 m/s will depend on the emission model and the wind velocity. Table 2 shows the maximum relative differences in k_L, k_G, and K_L for H$_2$S, produced by using Equation 11 instead of Equation 12 for the range $1 < U_{10} < 6$ m s^{-1}, comparing three different emission models (the maximum relative differences occur at the extremes of the range, 1 m s^{-1} and 6 m s^{-1}). Considering the global mass transfer coefficient K_L, these differences varied from -21.0% to +18.9% (Table 2). Nevertheless, it is important to highlight that the

expressions proposed are valid only for long fetches and therefore experimental work should be conducted to produce a wind friction equation valid for conditions that apply in WWTP tanks.

(a)   (b)

Figure 1: Near-smooth (a) and wavy conditions (b) for liquid surfaces in an WWTP.

There are several other issues concerning the use of this expression to calculate u_* based on Smith (1980): (i) waves are formed on the liquid surface depending on wind velocity and geometrical aspects of the liquid surface regarding wind direction (Figure 1 (a) and (b)); (ii) scums and foam can occur on the liquid surface altering, the interaction with the wind and the mass transfer process (Figure 3 (a) and (b)) and (iii) aerated or non-passive surface must be treated differently to calculate mass transfer (Figure 4).
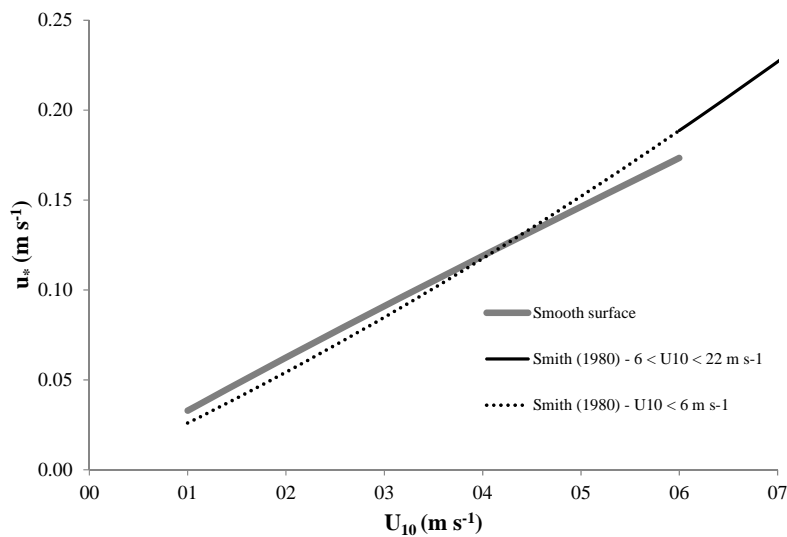

Figure 2: *Friction velocities as a function of wind velocity at reference height (=10 m) proposed for oceans by Smith (1980) for long fetches and neutral atmospheric conditions. The thin solid line indicates the expression used in emission models and produced by Smith (1980) for wind speed between 6 and 22 m s^{-1}, and the dotted line represents the extrapolation of this same expression for the range between 1 m s^{-1} and 6 m s^{-1}; the thick grey solid line represents the expression for a smooth surface, recommended by Smith for wind speed lower than 6 m s^{-1}*

Table 2: Percent differences (%) for the mass transfer coefficients used in different emissions models considering the two formulations proposed by Smith (1980), evaluated at the extremes of the low wind speed range.

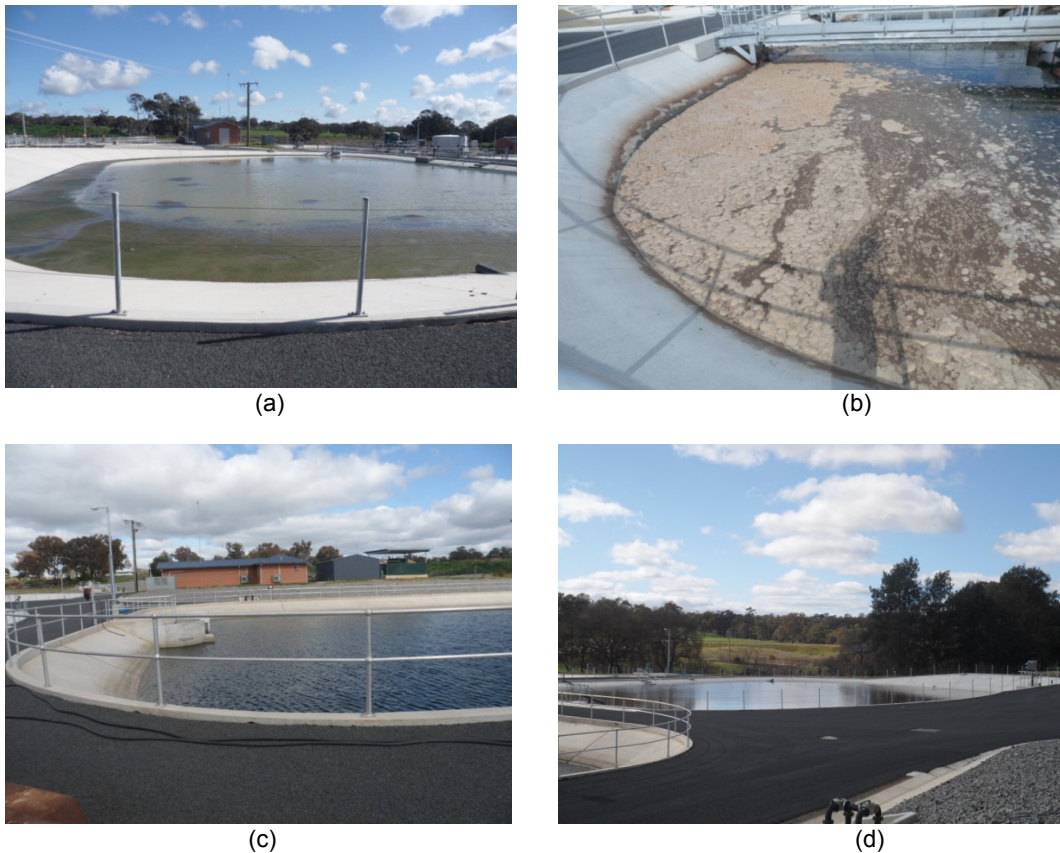| Emission model	U_{10} = 1 m/s			U_{10} = 6 m/s		
	k_G	k_L	K_L	k_G	k_L	K_L
WATER 9	-	-	-	-	18.9	18.9
Toxchem +	-13.1	-10.4	-10.4	7.9	18.9	18.8
Gostelow et al (2001)	-21.0	-21.0	-21.0	8.8	8.8	8.8

Figure 3: Scum (a) and foam (b) covering the liquid surface. Presence of building (c) and trees (d) that modify the wind profile approaching the liquid surface.
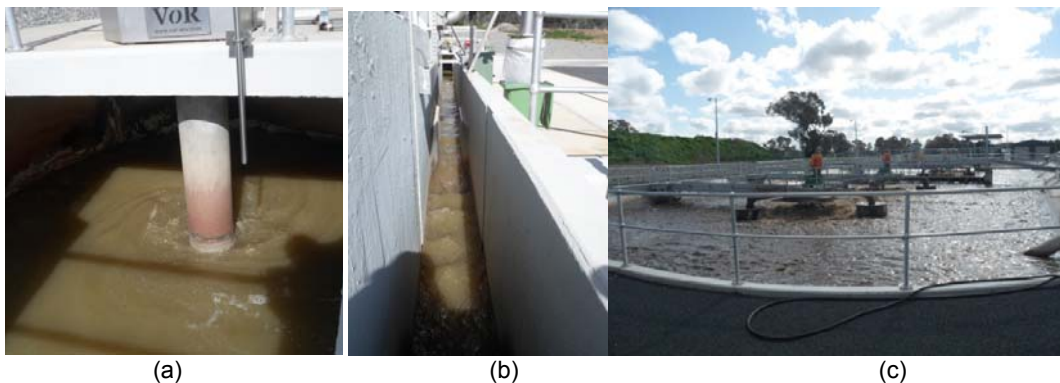

Figure 4: Non passive liquid surfaces: agitation by rotating paddles (a) augment the spiraling flow to create a mechanically induced vortex which settles the grit; inlet channel flow (b) showing a hydraulic jump disrupting the surface and mechanically aerated surface (c).

4. Conclusions

Emission models usually applied to assess the impact of compounds that volatilise from passive liquid surfaces in WWTP tanks are based on two-resistance approach, with a global mass transfer coefficient that depends on the wind flow and surface characteristics. The wind forcing parameter used to calculate the mass transfer coefficients is either wind speed at 10 m or the friction velocity on the surface. The wind speed is easily measured; the friction velocity, on the other hand, is normally calculated using an expression proposed by Smith (1980), which was developed for wind speed higher than 6 m s^{-1} and long fetches over oceans, where large waves are present and can influence significantly the mass transfer process. In WWTP, fetches

are usually lower compared to ocean and winds are weaker. It means that different types of waves driven by wind can be formed and alter the mass transfer process. Nevertheless, the most used emission models do not explain or include the validity of the expression proposed by Smith (1980) into their calculations. Smith (1980) has also recommended the use of a different expression for velocities lower than 6 m s^{-1}, however, it is not included in the models. Depending on the model used, the inclusion of a different expression can lead to differences of about 20% in the global mass transfer coefficients (assessed here for H$_2$S) and therefore in the emission rate. Future experimental work must be carried in order to evaluate the relation between wind speed at 10 m and friction velocity for the conditions found in WWTP. Other problems also arise in the field where buildings and trees around the WWTP can significantly alters the fluid flow and consequently friction velocity over the liquid surface. In this case, only numerical simulations of fluid flow in the real site can estimate more accurately the friction velocity. There are other issues that arise from the operation of the WWTP unities such as accumulation of scum, which avoids emission, and formation of foam after aeration which also covers the liquid surface and limits the volatilisation process.

Acknowledgments

Reference

Blunden J., Aneja V. P., Overton, J. H. (2008). Modeling hydrogen sulfide emissions across the gas– liquid interface of an anaerobic swine waste treatment storage system. Atmospheric Environment, 42, 5602-5611.

ENVIROMEGA (2003). Toxchem+ software for modeling fate of toxics in wastewater. Version 3.21. Enviromega, Inc. Dundas Ontario, Canada.

Feroni R. C., Santos J. M., Reis Jr. N. C. (2012). Volatilization of hydrogen sulfide from a quiescent surface. Water Science and Technology, 66 (9), 1991-1996.

Gostelow P., Parsons S. A., Cobb J. (2001). Development of an odorant emission model for sewage treatment works. Water Science and Technology, 44 (9), 181-188.

Jähne B., Haußecker H. (1998). Air-water gas exchange. *Annu. Rev. Fluid Mech.*, v. 30, p. 444-468.

Janssen P. A. E. M. (1994). Wave growth by wind. In: Dynamics and modelling of ocean waves (Komen G. J., Cavaleri L., Donelan M., Hasselmann K., Hasselmann S, Jansen P. A. E. M.), Cambridge: Cambridge University Press, 71-112.

Kudryavtsev V., Chapron B., Makin V. (2014). Impact of wind waves on the air-sea fluxes: A coupled model. J. Geophys. Res. Oceans, 119, 1-20.

Mackay D., Matsugu R. S. (1973). Evaporation rates of liquid hydrocarbon spills on land and water. Canadian Journal of Chemical Engineering, 51, 434-439.

Mackay D., Yeun A. T. K. (1983). Mass-transfer coefficient correlations for volatilization of organic solutes from water. Environmental Science & Technology, 17 (4), 211-217.

Melcer H., Bell J. P., Thompson D. J., Yendt C. M., Kemp J., Steel P. (1994). Modeling Volatile Organic Contaminants Fate in Wastewater Treatment Plants. Journal of Environmental Engineering-ASCE 120(3), 588-609.

Santos J. M., Sa L. M., Reis Jr N C, Gonçalves R. F., Siqueira R. N. (2006). Modelling hydrogen sulphide emission in a WWTP with UASB reactor followed by aerobic biofilters. Water Science and Technology, v. 54, p. 173-180.

Santos J. M., Kreim V., Guillot J.-M., Reis Jr. N. C., Sá L. M., Horan N. J. (2012). An experimental determination of the H2S overall mass transfer coefficient from quiescent surfaces at wastewater treatment plants. Atmospheric Environment, 60, 18-24.

Smith, S. D. (1980). Wind stress and heat flux over the ocean in gale force winds. J. Phys. Oceanogr., 10, 709-726.

Springer C., P. D. Lunney, and K. T. Valsaraj (1984). Emission of Hazardous Chemicals from Surface and Near Surface Impoundments to Air. U.S. Environmental Protection Agency, Solid and Hazardous Waste Research Division. Cincinnati, OH. Project Number 808161-02.

USEPA (1994). Air Emission Models for Waste and Wastewater. North Carolina, USA. EPA-453/R-94–080A.

USEPA (2001). User's Guide for WATER9 Software. Version 2.0.0. Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina.