Comparative analysis of existing disinfection models.

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Abstract
For a long time Marais's model has been the main tool for disinfection prediction in waste stabilization ponds (WSPs), although various authors have developed other disinfection models. Some ten other empirical models have been listed over the past fifteen years. Unfortunately, their predictions of disinfection in a given pond are very different. The existing models are too empirical to give reliable predictions: often their explanatory variables were chosen arbitrarily. In this work, we try to demonstrate that if influent variables have daily variations, the use of their average values in simulations may overestimate the disinfection effect. New methods are thus needed to provide better fittings of the models. Better knowledge of the mechanisms involved is needed to improve disinfection models.

Keywords Microbial decontamination; modelling; waste stabilisation ponds; kinetic

INTRODUCTION

Efficient bacteria removal is one of the major advantages of waste stabilization ponds (WSPs), a virtue that has been recognized since the beginning of the technology (Thirumurthi, 1974; Marais, 1974). Removal efficiencies (for *E. coli* or the whole faecal coliform group) in the range of 1 to 4 log units have often been reported.

Disinfection in WSPs is essentially due to sunlight, sedimentation and predation. Repeatedly, solar radiation has been shown to be the most influential factor. Nevertheless, the mechanism underlying the solar disinfection is not yet well known. For a long time, a dominant role has been attributed to UVB radiation damage to cellular DNA. Curtis *et al*. (1992) found that wavelengths in the UVB (290-320nm), UVA (320-400nm) and blue-visible (400-500nm) ranges caused damage to micro-organisms. This theory was subsequently proven right by Davies-Colley *et al*. (1997). According to this theory, disinfection by the longer UV and visible wavelengths is due to light absorption by specific molecules, named "photosensitisers" by Davies-Colley *et al*. (1997), which would catalyse the formation of reactive oxygen species that damage both bacteria and viruses by photo-oxidation. Curtis *et al*. (1992) estimated that photosensitisers are principally constituted by humic materials inducing photo-oxidative damage to the external structures of micro-organisms such as cell membranes. Humic substances would absorb a wide range of wavelengths in sunlight. Davies-Colley *et al*. (1997) ascertained that photosensitisers might also be intra-cellular including probably components of cell membranes as menaquinone and constituents of some small RNA such as 4-thiouridine. Different internal structures may be damaged, notably DNA. Endogenous photosensitisers would absorb the very shortest wavelengths in sunlight. The solar disinfection mechanism would be different depending on the specific micro-organism. Davies-Colley *et al*. (1999) found that F-DNA phage solar inactivation was due to the direct action of UVB; F-RNA phage and enterococci sunlight inactivation was caused by photo-oxidation catalysed by exogenous photosensitisers; and *E. coli* sunlight inactivation mechanisms were photo-oxidation reactions catalysed by endogenous photosensitisers at lower pH and by exogenous photosensitisers at higher pH. The impact of environmental factors on sunlight disinfection varies according to the mechanism and micro-organism involved. Sunlight disinfection by direct absorption of UVB is independent of DO (dissolved oxygen) and pH; photo-oxidation catalysed by endogenous photo-sensitisers is influenced by DO but independent of pH; in photo-oxidation catalysed by exogenous photosensitisers, elevated pH acts in synergy with DO. Davies-Colley *et al*.'s (1999) work showed that enterococci disinfection involving photo-oxidation catalysed by exogenous photosensitisers was not affected by pH. The enterococci's capacity to grow in high pH environments would explain this peculiarity. Davies-Colley *et al*. (1997) concluded also that *E. coli* appeared to be more resistant to sunlight inactivation than enterococci in WSPs. Consequently, they suggested the use of *E. coli* rather than enterococci as bacterial indicators in WSPs.

Aiming at predicting and optimizing disinfection in WSPs, models based on first order kinetics have been developed: $\frac{dC}{dt} = -k(t)C$ **(**1)

where C is the indicator bacteria concentration and k the die-off coefficient at time t .

A first pond disinfection kinetics was defined by Marais' (1974) model:

$k = k_{20}\ \theta^{(T-20)}$ (2)

where k_{20} is the die-off coefficient at 20°C, $k_{20} = 2.6$ d^{-1} ; θ a temperature coefficient, $\theta = 1.19$.

As various values had to be attributed to k_{20} and θ to allow the model to fit data, other empirical or semi-empirical formulae of the die-off coefficient have been developed.

The most commonly used equation is: $k = k_d + k_s \cdot I$ (3)

where k_d and k_s are respectively the "dark" and the "irradiance only" disinfection rates; I the total solar irradiance incident upon the pond surface.

Different k_d and k_s expressions were suggested (Table 1).

Some authors estimated that the die-off coefficient would be rather an exponential function of the solar irradiance (Table 1): $k = k_d^{'} . e^{\chi . I}$ **(**4)

where $k_d^{'}$ is the "dark" disinfection rate and χ the irradiance coefficient $k_d^{'}$ and χ expressions are given in Table 1.

This work based on comparative analysis of disinfection models, aims at improving disinfection models for WSP. The effects of explanatory variables on predictions are first studied. Secondly, assuming an important role of sunlight in the disinfection process, the influence of the use of the average of variables such as light, pH, and DO in modelling is investigated. Indeed, the efficiency of disinfection should vary according to diurnal changes. In other words as driving factors such as light but also pH, DO have daily variations, it may be unrealistic to use average values into the kinetic models, especially when the general kinetic model is the first order reaction kinetics (Chick's law) given in Equation 1.

MATERIALS AND METHODS

The comparative analysis of existing disinfection models is based on a simulation process of bacteria concentrations in the effluents of a virtual pond. The predictions of each disinfection model are compared and analysed. The pond characteristics are: 1m depth, a constant volume of 30000 m^3 and influent flow rate of 3000 m^3.d^{-1}.

Taking into account the hydrodynamic conditions, the models predictions are obtained by resolving the differential Equation (1).

Table 1. Die-off coefficients

$k = k_d + k_s \cdot I$				
Authors	k_d	k_s	**Indicator**	**Conditions and remarks**
Mayo (1989)	0.108 (j^{-1})	$\frac{5.79\times10^{-4}\left(1-e^{-KZ}\right)}{Z}$ ($cal^{-1}.cm^2$)	FC	$Z > 0.9m$ or $KZ > 4.6$ $\Rightarrow e^{-KZ} << 1$
Qin *et al*. (1991)	$k_T + k_{pH} + k_{BOD}$ (j^{-1}) where $k_T = 0.0279 + 0.00898T$; $k_{pH} = 0.2207(pH)^2 - 3.5797\,pH + 14.489$; $k_{DBO_5} = 0.46 - 0.184\log(BOD)$	$k_s^{'}(1-B)\frac{1-e^{-KZ}}{KZ}$ ($kLux^{-1}$) with $K = k_Z Z + k_A A + k_{Tur} Tur$	TC	▪ $0.0 \le B \le 0.03$ ▪ $0.154 \le k_s^{'}.\bar{I} \le 2.667$ (d^{-1}) ▪ $0.07 \le K \le 1.69$ mm^{-1}
Curtis *et al*. (1992)	$-6.355 + 0.7437\,pH + 0.163[O_2]$ (h^{-1})	0.001027 ($W^{-1}.m^2$)	FC	
Auer et Niehaus (1993)	$0.73 + \frac{v}{Z}$ (d^{-1})	$\frac{0.00824\left(1-e^{-KZ}\right)}{KZ}$ ($cal^{-1}.cm^2$)	FC	K was measured directly
Mayo (1995)	$0.135\,pH$ (d^{-1})	$\frac{5.67\times10^{-4}}{Z}$ ($cal^{-1}.cm^2$)	FC	▪ Kinetic limitations: $pH \le 9.5$ ▪ Weak temperature fluctuations
Fallowfield *et al*. (1995)	$1.404 - 0.026Z$ (d^{-1})	0.002 ($W^{-1}.m^2$)		Fallowfield_1 model
Fallowfield *et al*. (1995)	$1.67 - 0.02Z$ (d^{-1})	$0.79\times10^{-3}\times e^{\frac{-0.136Z \times Chl\,a + 0.0794}{2.303}}$ ($W^{-1}.m^2$)	*E. Coli*	Fallowfield_2 model
Fallowfield *et al*. (1995)	$0.35\,pH - 1.96$ (d^{-1})	$0.13\times e^{\frac{-0.136Z \times Chl\,a + 0.0794}{2.303}}$ ($W^{-1}.m^2$)	*E. Coli*	Fallowfield_3 model
Juanico and Dor (1999)	$\alpha \cdot \beta^{(T-20)}$ (d^{-1})	$\chi \cdot F_{O2}$ ($J^{-1}.cm^2$)		$F_{O2} = \begin{cases} 1, & [O_2] > 0mg \cdot l^{-1} \\ 0.67, & [O_2] = 0mg \cdot l^{-1}\ during\ more\ than\ 24h \end{cases}$
Craggs *et al*. (2004)	$0.020 - 0.023$ (h^{-1})	$0.056 - 0.114$ ($MJ^{-1}.m^2$)	*E. Coli*	
$k = k_d^{'} . e^{\chi . I}$				
Authors	$k_d^{'}$	χ	**Indicator**	**Conditions and remarks**
Xu *et al*. (2001)	$0.019\times0.915^{(T-20)}$ (d^{-1})	$\frac{0.170\left(1-e^{-KZ}\right)}{KZ}$ ($J^{-1}.cm^2$)	FC	▪ Xu_1 model* ▪ $K = 0.69\,MES + 24.09$
Xu *et al*. (2001)	$0.065\times0.915^{(T-20)}$ (d^{-1})	$\frac{0.191\left(1-e^{-KZ}\right)}{KZ}$ ($J^{-1}.cm^2$)	FC	▪ Xu_2 model*

*Xu_1 and Xu_2 kinetics were based on field monitoring data in first and second tertiary ponds, respectively. Notations are described in Table 2.

Table 2. Notation used in die-off coefficients

Symbol	Parameter	Unit
A	Algal concentration	mg.L^{-1}
B	Surface layer effect coefficient	
Chl a	Chlorophyll a concentration	mg.L^{-1}
I	Total solar irradiance incident upon the pond surface	W.m^{-2} or J.m^{-2} or J.cm^{-2} or cal. cm^{-2} or Lux
K	Irradiance attenuation coefficient	m^{-1} or mm^{-1}
k	Die-off coefficient	d^{-1} or h^{-1}
k_A	Separate die-off coefficient applying to algal concentration	mg.L^{-1}.mm^{-1}
k_d	"dark" disinfection rate	h^{-1} or d^{-1}
$k_d^{'}$	"dark" disinfection rate	d^{-1}
k_s	"irradiance only" disinfection rate	h^{-1} or d^{-1}
k_{Tur}	Separate die-off coefficient applying to turbidity	NTU^{-1}.mm^{-1}
k_Z	Separate die-off coefficient applying to depth	mm^{-2}
$[O_2]$	Dissolved oxygen concentration	mg.L^{-1}
T	Temperature	°C
Tur	Turbidity	NTU
Z	Water depth	m or cm or mm
α	Constant	d^{-1}
β	Temperature coefficient	
ν	Settling velocity	m.d^{-1}
χ	Irradiance coefficient	J^{-1}.cm^{2}.d

*1Lux=1.46x10^{-3}W.m^{-2}; 1Lux=0.35x10^{-3}cal.s^{-1}.m^{-2}

The predictions for a discontinuous Batch Reactor (SBR) are determined as follows, which is the integration of Equation (1)

$$N(t_n) = N(t_0) \cdot e^{-k_1 \cdot (t_1 - t_0) - k_2 \cdot (t_2 - t_1) - \cdots - k_n \cdot (t_n - t_{n-1})} \quad (5)$$

where $N(t_i)$ is the bacteria concentration at time t_i, $i = 0,\ldots,n$; and k_j the disinfection kinetic coefficient at time t_j, $j = 1,\ldots,n$.

The following equation defines the disinfection predictions for a Plug Flow Reactor (PFR):

$$N_E(t_n) = N_I(t_0) \cdot e^{-k_1 \cdot (t_1 - t_0) - k_2 \cdot (t_2 - t_1) - \cdots - k_n \cdot (t_n - t_{n-1})} \quad (6)$$

where $N_E(t_n)$ is the effluent bacteria concentration at time t_n and $N_I(t_0)$ the influent bacteria concentration at time t_0

with $$t_i = t_n - \tau + i \cdot \Delta t\,; \quad i = 0,\ldots,n \quad (7)$$

where τ is the residence time; $\Delta t = \frac{\tau}{n}$.

The disinfection predictions for a Continuously Stirred Reactor (CSR) are expressed as:

$$\frac{N_E(t_n) - N_E(t_{n-1})}{\Delta t} = \frac{Q}{V} N_I(t_n) - \frac{Q}{V} N_E(t_n) - k_n . N_E(t_n) \quad (8)$$

where $N_I(t)$ is the influent bacteria concentration at time t; $N_E(t)$ the effluent bacteria concentration at time t; Q the influent/effluent flow; and V the volume.

All daily models presented in Table 1 were tested except those of Juanico and Dor (1999), Qin *et al.* (1991) and Fallowfield *et al.* (1995) called Fallowfield_1 and Fallowfield_2 models. Indeed, each of these four models has at least one unknown parameter value.
To get the Auer and Niehaus (1993) model to run, the value of 1.38 m.d^{-1} (suggested by these authors) was chosen for the sedimentation velocity ν. The irradiance attenuation coefficient K was calculated with the ratio used by Xu (2001) given in Table 1.

For the simulations the average values chosen for pH, DO, water temperature and solar irradiance were 8.3, 4.6 mg.L^{-1}, 15.0°C and 86 J.cm^{-2}.h^{-1}, respectively.

For the hourly models comparison, to avoid very fastidious simulations, the pH, dissolved oxygen, water temperature and total solar irradiance were preliminarily defined by sinusoidal functions of time t (h) with parameters selected from experimental data (***Table 3***).
The phases in the equations were changed according to observations. These functions are illustrated over a two-day period in ***Figure 1***. We took rather realistic variations, but the equations can easily be changed to simulate greater variations.

Table 3. Theoretical variations in pH, DO, water temperature ***T*** *and solar irradiance* ***I***

$pH(t)$	$DO(t)$	$T(t)$	$I(t)$
$pH_0 \cdot \sin\left(\frac{t}{t_N}+\varphi'\right)+a$	$(DO)_0 \cdot \sin\left(\frac{t}{t_N}+\varphi''\right)+b$	$T_0 \cdot \sin\left(\frac{t}{t_N}+\varphi'''\right)+c$	$\frac{I_0}{2}\cdot\left[\sin\left(\frac{t}{t_N}+\varphi\right)+\left\lvert\sin\left(\frac{t}{t_N}+\varphi\right)\right\rvert\right]$
Parameters description			
$a = 8.384$	$b = 4.574$ mg.L^{-1}	$c = 15.016$ °C	$\bar{I} = 84$ J.cm^{-2}.h^{-1}*
$pH_0 = 1$	$(DO)_0 = 2.363$ mg.L^{-1}	$T_0 = 0.665$ °C	$I_0 = 269.572$ J.cm^{-2}.h^{-1}
$\varphi' = 1.931$ rd	$\varphi'' = 2.064$ rd	$\varphi''' = 2.338$ rd	$\varphi = 4.354$ rd
$t_N = 3.812$ h^{-1}	$t_N = 3.812$ h^{-1}	$t_N = 3.812$ h^{-1}	$t_N = 3.812$ h^{-1}

* $\bar{I}$ is the average value of the total solar irradiance incident upon the pond surface

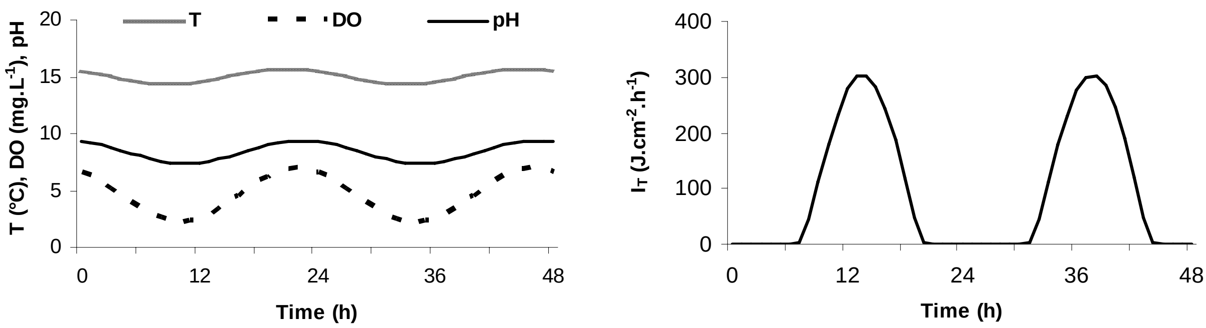

Figure 1.Theoretical variations in temperature, dissolved oxygen, pH and solar irradiance incident upon the pond surface

The study of the effect of using the average values of explanatory variables on models' predictions is based on the previously described simulation process. Only the Curtis *et al*. (1992) and Craggs *et al*. (2004) hourly models (Table 1) were employed for simulations. The respective disinfection predictions obtained using the instantaneous and average values of pH, DO, water temperature and solar irradiance are compared.

RESULTS AND DISCUSSION

The effect of the choice of explanatory variables on model predictions. In the SBR, all models estimated that the bacteria concentration would diminish with time (Figure 2). In the CSR or PFR under the same environmental conditions (Figure 1) the effluent's bacteria concentration does not change with time, since the influent flow rate and bacteria content are assumed constant (equal to 3000 m^3.d^{-1} and 10^{5}UFC.mL^{-1} respectively),. In Figure 2, "transitory periods" precede these "steady-states". For the CSR, this "transitory period" corresponds to the period during which the model predictions depend on initial conditions (the initial value attributed to the effluent bacteria concentration). For the PFR, the predictions from the initial time to the time τ equal to the residence time are uncertain. Indeed, the effluent bacteria concentration would be that predicted for an SBR at time τ, for a bacteria initial content equal to that of the PFR influent (10^5UFC.mL^{-1}).

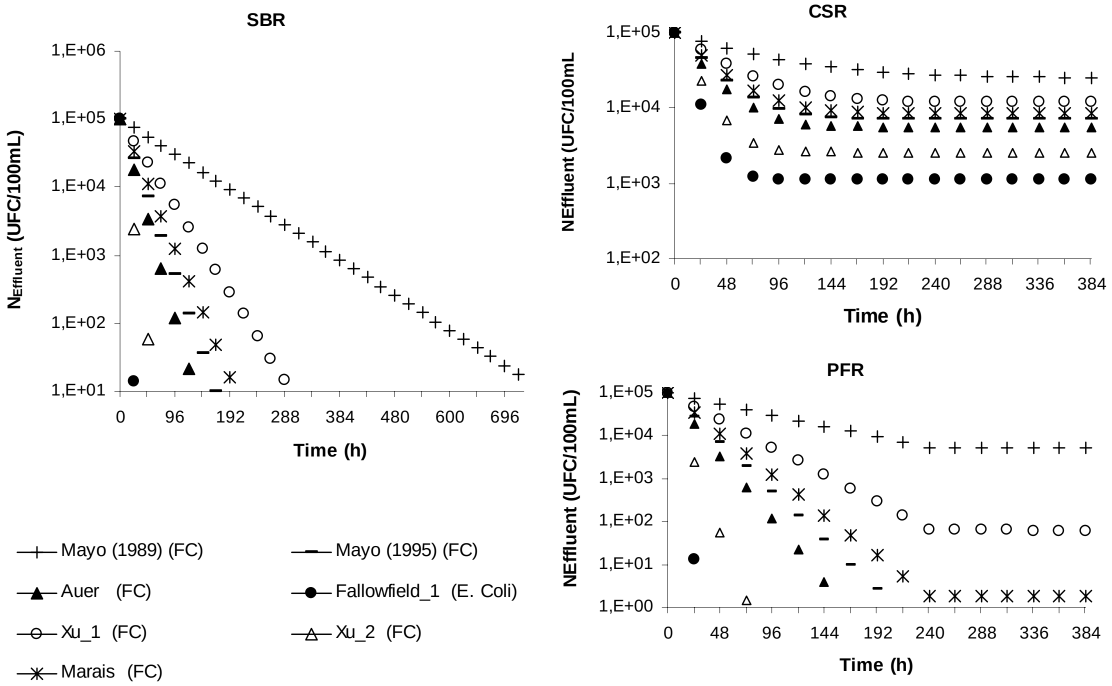

Figure 2. The predictions of pond disinfection for batch, plug flow and continuously stirred regimes by daily models (Table 1) using the average values of pH, DO, water temperature and solar irradiance equal to 8.3, 4.6mg.L^{-1}, 15.0 °C and 86 J.cm^{-2}.h^{-1}, respectively. Initial bacterial concentration in SBR is assumed to be 10^5UFC.mL^{-1}

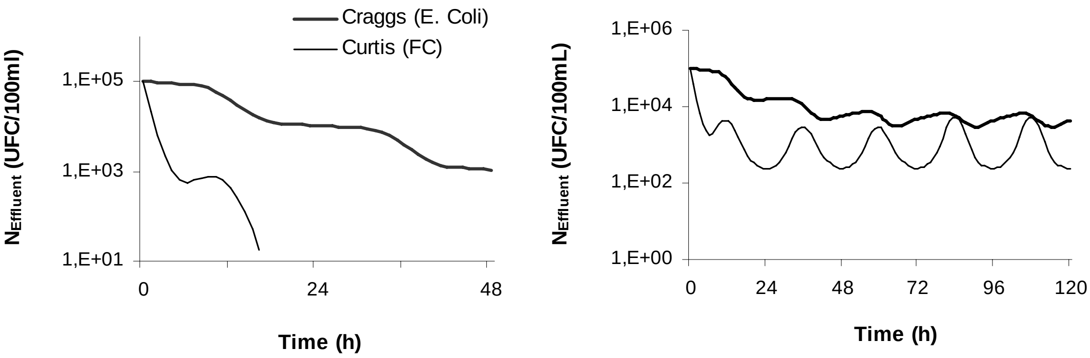

Figure 3. The predictions from Curtis et al. (1992) and Craggs et al.'s models (Table 1) for batch and continuously stirred regimes using instantaneous values of pH, DO, water temperature and solar irradiance (Table 3). Initial bacterial concentrations in SBR and in the influent of CSR were assumed to be 10^5UFC.mL^{-1}. (For plug flow regime, the 2 hourly models predictions tended towards total disinfection, and therefore are not shown.)

Depending on the model, the time needed to achieve a bacterial concentration of 10 UFC.mL^{-1} in a pond operating in batch mode (Figure 2) would vary from 1 day to 1 month while Marais' model estimated this time around 8 days. As expected for a first order kinetic, the best disinfection was predicted in the pond acting as a SBR. The predicted values of effluent bacterial concentration were comprised between 1.1 10^3 and 2.6 10^4 UFC.mL^{-1} and between almost total disinfection and 5.1 10^3 UFC.mL^{-1} for CSR and PFR respectively (***Figure 2***). Marais's model estimations were 8.4 10^3 UFC.mL^{-1} for CSR and 1.8 UFC.mL^{-1} for PFR which are in the middle range. The predictions of the two models developed by Mayo in 1989 and 1995 (Table 1) showed that adding pH to solar irradiance as a driving factor led to a faster disinfection prediction.

The Curtis *et al*. (1992) and Craggs *et al*. (2004) kinetics constituted the only available disinfection models using shorter time-steps. Their predictions are presented in ***Figure 3***. In a perfectly stirred pond, disinfection would undergo daily sinusoidal variations, with differences that should be large enough to be quantified. Generally, the Curtis *et al*. disinfection predictions are higher than those of Craggs *et al*. In the SBR, according to Curtis *et al*., the time needed to reduce bacterial concentration significantly (10 UFC.mL^{-1}) was 10 hours while Craggs *et al*. put it at around 97 hours.

The effect of using the average values of explanatory variables on model predictions.
The effluent bacterial concentrations predicted using the instantaneous and average values of explanatory variables are compared in ***Figure 4***. The virtual pond was successively assimilated to SBR, CSR and PFR flow. Tending towards total disinfection, the predictions for PFR flow are not shown.

Marginal differences can be observed. In the case of the CSR it can be seen that using variables' average values in the models overestimates the disinfection efficiency. The overestimation was about 0.49 and 0.05 log unit according to Curtis *et al*. and Craggs *et al*., respectively.

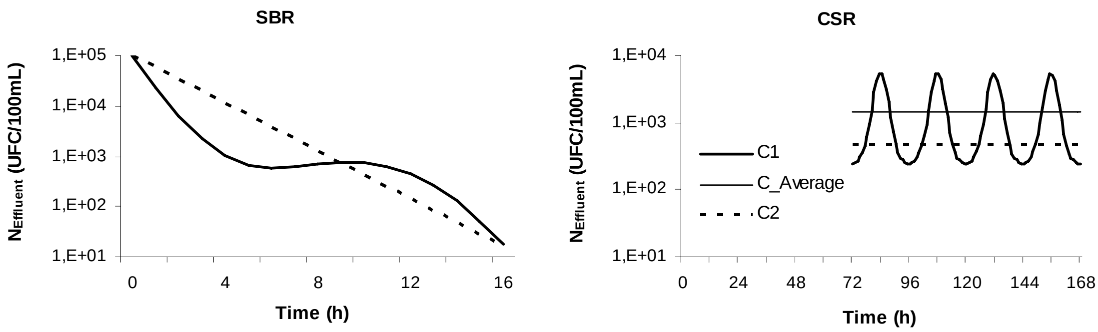

Figure 4. Comparison of Curtis et al. (1992) model's predictions using instantaneous values of pH, DO, water temperature and solar irradiance (Table 3) and the average values of pH, DO, water temperature and solar irradiance equal to 8.3, 4.6 mg.L^{-1} and 15.0 °C and 86 J.cm^{-2}.h^{-1}, noted C1 and C2, respectively. C_Average is the C1 average.
Initial bacterial concentrations in SBR and in the influent of CSR were assumed to be 10^5UFC.mL^{-1}. (The Craggs et al. (2004) model's predictions exhibited similar patterns and therefore are not shown.)

CONCLUSIONS
The disinfection effect is one of the major advantages of a WSP over conventional treatment. But huge differences can be observed between the models describing the process. The existing models are too empirical to provide reliable predictions. While having important effect on simulations, as shown by the significant difference between the predictions of the two Mayo models, explanatory variables were often chosen arbitrarily. Better knowledge of the mechanisms involved is needed to improve disinfection models.

We demonstrated also that if we accept that the driving mechanisms of disinfection are sunlight, pH, O2, which are not constant in the pond, our models should take those variables' variations into account. Moreover, simulations show that models based on average values overestimate the disinfection effect. Simulations also indicate that differences in bacterial concentrations should be observable during the daylight cycles. Thus new methodologies should be developed to take this conclusion into account and to get data that can be used to fit the models. New methods that are faster than conventional methods do exist, making it possible to measure the bacterial (FC, *E coli*, *etc.*) levels in water samples in less than one hour. Such methods could be very useful to fit the parameters of the more realistic models, which would result in improved design methods, especially for maturation ponds.

ACKNOWLEDGEMENTS

The authors wish to acknowledge the support of the National Research Fund (FNR) of Luxembourg for the post-doctoral fellowship granted to the first author.

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