3D-CFD Modelling of *E. coli* Removal in Baffled Primary Facultative Ponds: Classical Design Optimization

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Abstract Three-dimensional computational fluid dynamics (CFD) was used for the first time to assess the improvement in treatment performance of baffled primary facultative ponds operating under both isothermal conditions and thermal stratification. A two-baffle configuration was investigated. Validation of the model was conducted on a pilot-scale baffled primary facultative pond. A scalar transport equation was used to model the decay of *E. coli* using a source term based on first-order kinetics. When the pilot-scale baffled pond developed isothermal conditions during winter, a 2.76-log removal of *E. coli* was observed and the two-baffle CFD model predicted a 2.16-log removal. When thermal stratification developed during the summer season, a 2.25-log removal of *E. coli* was observed and the model predicted a 2.58-log removal. These results show that the CFD model is satisfactory for the prediction of *E. coli* removal in baffled facultative ponds.

Keywords: Computational fluid dynamics; *E. coli* removal; thermal stratification; isothermal conditions; flow pattern, baffles

Introduction

Waste stabilization ponds (WSP) are currently designed based on either modern or classical design methods (Mara, 2004; Banda et al., 2005). However, neither of these design approaches takes into account the improved hydrodynamics and *E. coli* removal that can be achieved by modifying the pond geometry through the installation of baffles.

Mangelson and Watters (1972) showed that WSP hydrodynamics were improved significantly by installing conventional 70%-pond-width baffles along the longitudinal axis of the pond. However, they did not quantify the improved performance of baffled WSP in terms of *E. coli* removal; instead they merely judged increased pond performance by measuring the improvement in actual hydraulic retention time due to the reduction of short-circuiting. Furthermore they did not include any effects due to thermal stratification. These effects were suggested by Pedahzur *et al*. (1993) as the reason why they found that the effluent quality from a full-scale secondary facultative pond did not improve when it was fitted with two and four baffles.

More recently Shilton and Harrison (2003a, 2003b) showed that *E. coli* decay in WSP could be predicted accurately by integrating a first-order reaction model of pollutant decay into a CFD model. These authors and Shilton and Mara (2005) modelled the decay of *E. coli* in primary facultative ponds fitted with 70%-pond-width baffles. Their CFD model assumed isothermal conditions within the ponds.

However, CFD is a very powerful design tool that should make it relatively easy to model *E. coli* removal in a thermally stratified and baffled pond very accurately and so produce a prediction of pond performance that is more precise than that inherent in the classic and modern design methods. Thus, in this paper, we apply an integrated 3D-CFD first-order reaction model of *E. coli* decay to simulate the hydrodynamics and *E. coli* removal in a twin-baffled primary facultative pond both with isothermal conditions and with thermal stratification, and we compare these model results with those obtained from a pilot-scale twin-baffled primary facultative pond.

Methods

CFD model

A 3D-CFD model was set up using the CFD software Fluent, version 6.1.22 (Fluent Inc., Lebanon, NH) such that the flow and transport of a scalar variable representing the concentration of *E. coli* could be used to simulate flow in a pilot-scale twin-baffled primary facultative pond. Derivations of the fundamental conservation equations of mass and momentum on which CFD is based are available in several standard text books (for example, Pantakar, 1980; Versteeg and Malalasekera, 1995). To simulate *E. coli* removal within Fluent accurately, it was necessary to program the desired functionality and incorporate this within Fluent via the 'user defined function' (UDF) facility provided by the software. With the addition of this UDF facility the scalar transport equation was modified to simulate the decay of *E. coli* based on the following equations:

$$\frac{\partial(\rho\phi)}{\partial t} + div\,(\rho\phi U) = div(\Gamma grad\phi) + S_{\phi} \qquad (1)$$

$$S_{\phi} = -\rho k\phi \qquad (2)$$

$$k = 2.6(1.19)^{T-20} \qquad (3)$$

$$k = 4.55(1.19)^{T-20} \qquad (4)$$

where φ is the scalar variable (*E. coli* count per 100 ml); k, the first-order rate constant for *E. coli* removal, day^{-1}; ρ, the density of wastewater, kg/m^3; S_{φ}, a source term, kg m^{-3} s^{-1}; Γ, coefficient of diffusivity, kg m^{-1} s^{-1}; U, the vector form of wastewater velocity [u, v, w], m s^{-1}; and T, temperature, °C.

Equation 3 (Marais, 1974) for the first-order rate constant of *E. coli* removal was used in the unbaffled pond model, and equation 4 was used in the two- and four-baffled pond models. The latter was adopted because baffled ponds have enhanced hydrodynamics that result in faster decay rates than that which occurs in unbaffled ponds.

Isothermal conditions and thermal stratification

In order to simulate *E. coli* decay under isothermal conditions in winter, the temperature profile in the pilot-scale pond was monitored using iButtons (Abis and Mara, 2006). The observed temperature profile had a minimal variation and was taken to be constant at 5°C. The wastewater density at this temperature was 1000 kg m^{-3} (Perry and Green, 1984). Equations 1, 2 and 3 were used to solve the momentum and scalar-transport equations to obtain the flow patterns and effluent *E. coli* count from the pilot-scale pond under isothermal conditions.

Thermal stratification developed in the pilot-scale baffled pond during summer (see Abis, 2002) . The temperature profile varied from 17°C at the pond surface to 8°C at the base. Twenty iButtons were installed in the three baffle compartments; each position comprised five iButtons at 0.25-m intervals. The following density-temperature polynomial equation, developed from the data reported by Perry and Green (1984) over the temperature range 0−40°C, was incorporated in Fluent:

$$\rho = -6\times10^{-7}T^{4} + 9\times10^{-5}T^{3} - 0.0095T^{2} + 0.0817T + 999.82 \qquad (5)$$

where ρ is the density (kg/m^3) and T the temperature (°C) [$r^2 = 1$].

The CFD model simulated thermal stratification by using the following average temperature profile: 8°C, 10°C, 12°C, 14°C, 16°C and 17°C at 0.25 m, 0.5 m, 0.75 m, 1.00 m, 1.25m and 1.5 m above the bottom level of the pond, respectively. *E. coli* decay was modelled by solving equations 1−4.

Boundary conditions

In order to simulate a 'free slip' surface on a pond surface, a zero shear stress was applied at the top boundary wall of the model. The other boundary conditions of the model were based on the inlet velocities of 0.05 m/s for wastewater and 0.046 m/s for fresh water and a pressure value of zero at the pond outlet. Influent *E. coli* counts of 5.38×10^6 per 100 ml and 1.50×10^7 per 100 ml were used for isothermal conditions in winter and for thermal stratification in summer, respectively. The diffusivity of *E. coli* (Γ) was assumed to be zero because it was considered to be have a negligible influence on the results due to the circulation pattern in the pond (Shilton and Harrison, 2003a). A 3-D laminar steady-state solution of the flow equations was calculated with a second-order discretization scheme. A grid-dependence test was carried out to determine the optimum mesh size that provided grid-independent solutions. A grid of this density was then used for all further simulations undertaken.

Pilot-scale facultative pond

The CFD model was used to simulate *E. coli* removal in a pilot-scale twin-baffled primary facultative pond, located at Esholt, Bradford, with top surface dimensions of 10.2 × 3.9 m and a depth of 1.5 m. The pond was loaded at 80 kg BOD/ha d (Abis, 2002). Two baffles were installed equally along the longitudinal axis of the pond (Figure 1). The length of these baffles was 2.7 m, corresponding to 70% of the pond width. The pond had a theoretical (i.e., V/Q) hydraulic retention time of 30 d.

Figure 1. Plan view of the twin baffles in the pilot-scale primary facultative pond.

Influent and effluent samples were taken weekly and analysed for BOD, SS, ammonia-N, TKN, chlorophyll *a* and *E. coli*, using the techniques described in *Standard Methods* (APHA, 1998).

Results and discussion

The pilot-scale baffled pond was operated during winter and summer seasons in order to assess the effects of isothermal conditions and thermal stratification on pond performance. The results of the routine monitoring programme are given in Table 1.

To quantify the efficiency of the pond in the CFD model, a monitoring value is required. Rather than using a single point value, it is more appropriate to select a surface where the effluent wastewater leaves the pond. In this case, the outlet surface of the pond was chosen for which the mean value of *E. coli* count can be monitored. The results of the predicted effluent *E. coli* counts, based on the mass average weight method (Fluent Inc., 2003), are also given in Table 1.

The results in Table 1 show that the CFD two-baffle model has satisfactory predicted the effluent *E. coli* counts and the log removals of *E. coli* in the pilot-scale twin-baffled pond under both isothermal conditions and thermal stratification. When the pilot-scale pond experienced isothermal conditions in winter, the observed effluent *E. coli* counts and the CFD-predicted effluent counts were of the same order of magnitude (1.4×10^4 per 100 ml for the pilot-scale pond and 4.2×10^4 per 100 ml for the twin-baffle model).

Table 1. Results from the pilot-scale twin-baffled primary facultative pond and the CFD models during isothermal conditions (5°C) and thermal stratification (8–17°C)

Parameter (mg/l)	Isothermal conditions			Thermal stratification		
	Influent	Effluent	Removal	Influent	Effluent	Removal
SS	258	45	82%	299	54	82%
BOD	286	6 (34)[a]	98% (88%)	458	5 (31)	99% (93%)
Ammonia-N	45	2.9 (4.1)	94 (91)	34	3.0 (3.5)	91 (89)
Total Kjeldahl N	54.88	3.81 (11)	93 (80)	68	4.6 (14)	93 (80)
E. coli counts per 100 ml and log removals:						
Pilot-scale fac. pond	5.4×10^6	1.4×10^4	2.58	1.5×10^7	3.6×10^4	2.62
CFD model: no baffles	5.4×10^6	3.0×10^5	1.25	1.5×10^7	3.6×10^5	1.62
CFD model: 2 baffles	5.4×10^6	4.2×10^4	2.10	1.5×10^7	1.2×10^4	3.10
CFD model: 4 baffles	5.4×10^6	3.7×10^4	2.16	1.5×10^7	2.9×10^3	3.71

[a] Values in brackets are results for unfiltered effluent concentrations.

However, in terms of log removal, the model underestimated the observed removal by 19% (2.6 log units for the pilot-scale pond *vs* 2.1 log units for the twin-baffle model). During thermal stratification in summer, the observed *E. coli* counts in the pilot-scale pond and twin-baffle model were again the same order of magnitude (3.6×10^4 per 100 ml for the pilot-scale pond and 1.2×10^4 per 100 ml for the twin-baffle model), but the model overestimated the log removal by 15% (2.6 log units for the pilot-scale pond *vs* 3.1 log units for the twin-baffle model).

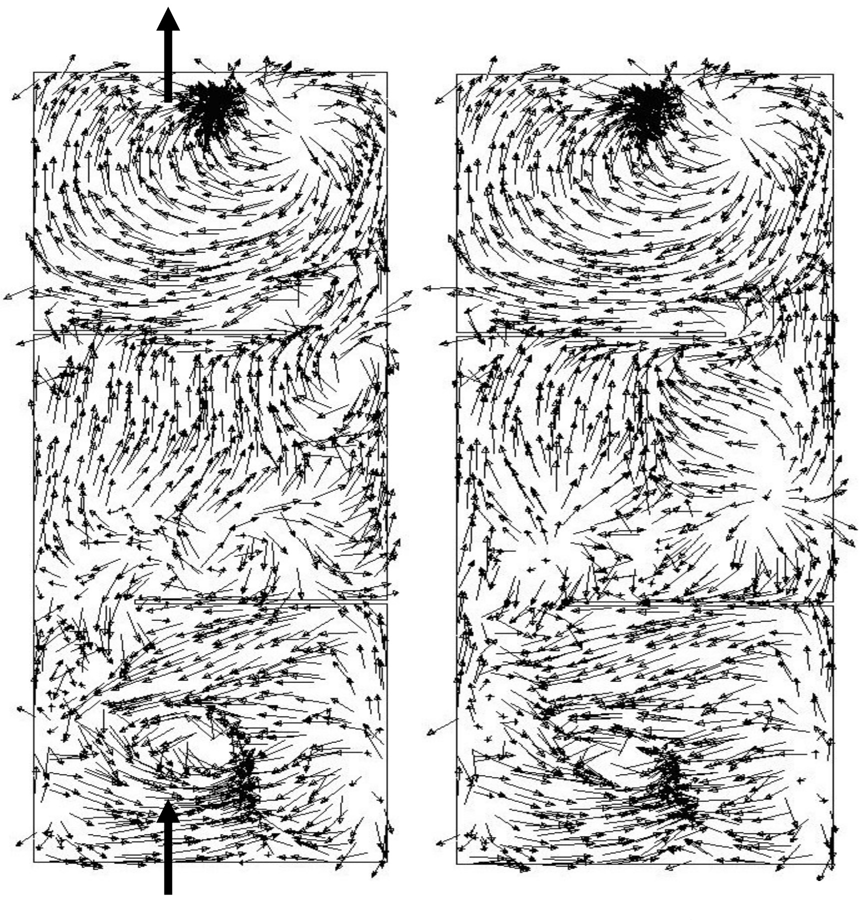
Additional simulation results for a four-baffle model and an unbaffled model are included in Table 1. It can be seen that the effluent *E. coli* count predicted by the four-baffle model under thermal stratification and isothermal conditions are 2.9×10^3 per 100 ml and 3.7×10^4 per 100 ml, respectively. It appears that four baffles reduce the hydraulic short-circuiting associated with thermal stratification, since the four-baffle model results show a potential additional *E. coli* reduction of 3.7 log units in summer, when the pond is stratified, over and above that achieved under isothermal conditions in winter. However, the model results for the unbaffled pond indicate that its winter performance is essentially the same as its summer performance (3.0×10^5 per 100 ml and 3.6×10^5 per 100 ml, respectively).

Abis (2002) observed satisfactory treatment performance of three unbaffled pilot-scale ponds at the same site, which were operated for two years and it was found that the effects of thermal stratification did not diminish the treatment performance of the ponds. Salter (1999) observed improved hydraulic performance of a twin-baffle CFD model that included the effects of thermal stratification. Table 1 shows the satisfactory performance of the pilot-scale twin-baffled pond in removing other pollutants (BOD, SS, TKN, ammonia-N) from the wastewater. During isothermal conditions the removals were 98% for BOD, 82% for SS, 94% for ammonia-N and 93% for TKN; and during periods of thermal stratification they were 98.8% for BOD, 81% for SS, 93% for ammonia-N and 91% for TKN. These results show that the performance of the pilot-scale twin-baffled pond is far above that achieved by the series of five waste stabilization ponds in northeast Brazil studied by Silva (1982), who observed cumulative removals of 93%, 85% and 82% for BOD, SS and ammonia-N, respectively, at a much higher operating temperature (25°C) and a shorter overall retention time (28 d).

The similarity in the treatment performance of the pilot-scale baffled pond when operated during isothermal conditions and thermal stratification indicates that any hydraulic short-circuiting associated with thermal stratification is not significant. This is to be expected as, for a temperature-depth profile of 8^{o}C, 10^{o}C, 12^{o}C, 14^{o}C, 16^{o}C and 17^{o}C, the corresponding wastewater densities are 999.99 kg/m^3, 999.77 kg/m^3, 999.58 kg/m^3, 999.33 kg/m^3, 999.03 kg/m^3 and 998.86 kg/m^3, respectively (equation 4) − thus the density variation is so small that the wastewater layers are capable of mixing, thus preventing any initiation of hydraulic short-circuiting.

Pedahzur et al. (1993) observed significant hydraulic short-circuiting in a four-baffled secondary facultative pond due to the effects of thermal stratification. It was observed that the baffles did not improve the treatment performance of the pond (however, their four-baffled secondary facultative pond was overloaded by 200% and so it not conclusive to suggest that the poor performance of the baffled pond was due to the effects of thermal stratification). Other researchers (Muttamara and Puetpailboon, 1996, 1997; Kilan and Ogunrombi, 1984; von Sperling et al., 2002; Zanotelli et al., 2002) have observed that baffles do improve the treatment performance of waste stabilization ponds that are optimally loaded.

Figures 2 and 3 show the horizontal and vertical flow patterns (in the form of uniformly scaled vectors) at mid-depth plane and along the longitudinal axis of the two-baffle model with effects of thermo-stratification and isothermal conditions. It can be seen that there is no significant difference of flow patterns in the two-baffle models when effects of isothermal and thermo-stratification are included. The vertical flow patterns show that vertical mixing occur in the two-baffle models due to the minimal variation of wastewater density. Examination of flow patterns at the horizontal plane shows that baffles have improved the hydraulic performance of the pilot-



Isothermal conditions Thermal stratification

Figure 2. Horizontal flow patterns in the twin-baffle model at mid-depth

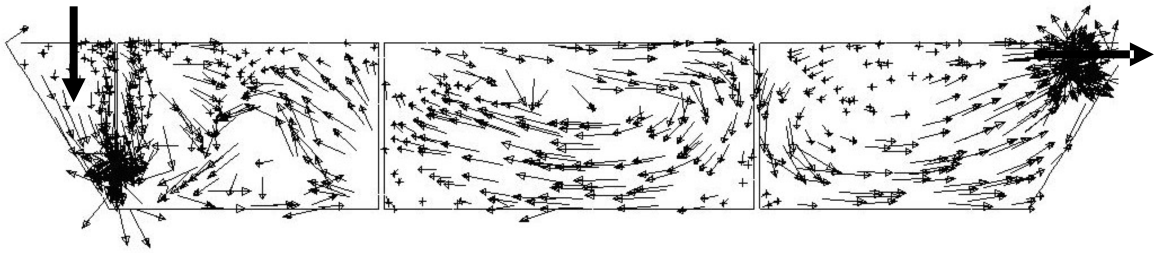


Figure 3 a. Vertical flow pattern in the twin-baffle model during isothermal conditions

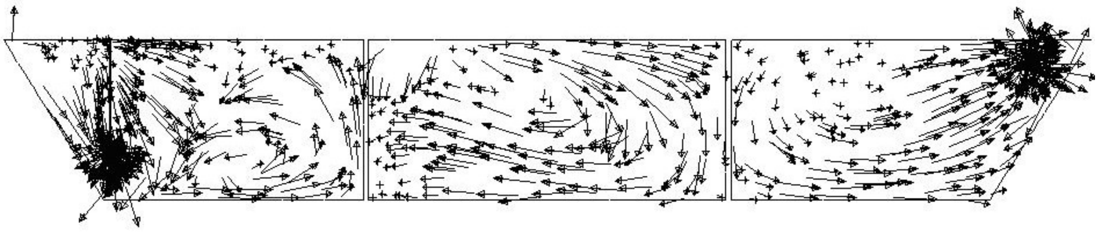


Figure 3 b. Vertical flow pattern in the twin-baffle model during thermal stratification

scale twin baffled pond and that there is no discernable hydraulic short-circuiting. Thus the improvement of the hydraulic performance in the baffled pond resulted in the satisfactory removal of the pollutants in the wastewater.

Conclusions

The 3D-CFD model has satisfactorily predicted the treatment performance of the pilot-scale twin-baffled primary facultative pond. There was no significant difference in the treatment performance of the pilot-scale pond during isothermal conditions and during thermal stratification. Although the CFD-predicted log removals of *E. coli* in the twin-baffle model and the pilot-scale pond are not identical, the predicted effluent *E. coli* counts were the same order of magnitude. The significance of these CFD model results is that regulators and designers can confidently use CFD to assess realistically the treatment efficiency of baffled facultative ponds. The results further show that baffled facultative ponds can reduce significantly *E. coli* concentrations to achieve the required level of pathogen reduction for either restricted or unrestricted crop irrigation, thus obviating the need for maturation ponds and so minimizing the land area requirements of pond systems.

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