Chapter 3

Methodology of the CFD model

3.1 Introduction

A reactor model has been constructed which is based on CFD methodology of solving the time dependent flow and transport equations on a fine three dimensional mesh. The result is a model that can predict precisely the *E. coli* numbers and BOD_5 concentration at all points in the pond and, usually of most interest, in the pond effluent. These particular wastewater parameters were chosen to be simulated because they are reliable and commonly used indicators of effluent quality. They are also convenient from a computational point of view as their decay follows the first-order kinetic theory. This first-order kinetic reaction has been formulated such that it is compatible with the source term function in the scalar transport equation. In addition, the first-order kinetic reaction depends mainly on the temperature of the reaction and this is simple and accurate to measure when designing and evaluating treatment performance of waste stabilization ponds.

Nutrient parameters such as total nitrogen and ammonia were not incorporated into this CFD model because the removal of these parameters depends on various processes such as algae uptake, sedimentation, vaporisation and denitrification, which are more complex to model as several sub-models and empirical measurement would be required. In addition, it would also be difficult to test and verify the results of such complex model.

The use of CFD in this research has enabled the analysis of the spatial residence time distributions in waste stabilization ponds. The model results of these simulated spatial residence time distributions can help design engineers to identify the physical design interventions that can be utilised to minimise the extent of stagnation regions and hydraulic short-circuiting that are inherent in many waste stabilization ponds.

The development of source term functions that represent *E. coli* and BOD_5 removal in the scalar transport equation is the most challenging task that the CFD modeller will encounter when using CFD as the design code. Patankar (1980) and FLUENT manual (2003) present a scalar transport equation in more detail. It is this equation that must be appropriately modified to enable simulation of the transport of pollutants in waste stabilization ponds. The scalar transport equation of the pollutant removal in 3D model was presented in equation 2.29 and is recalled here:

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\phi U) = div(\Gamma grad\phi) + S_{\phi} \qquad 2.29$$

where:

$$div(\rho\phi U) = \frac{\partial(\rho\phi u)}{\partial x} + \frac{\partial(\rho\phi v)}{\partial y} + \frac{\partial(\rho\phi w)}{\partial z}$$

$$grad\phi = \frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y} + \frac{\partial\phi}{\partial z}$$

$$div(\Gamma grad\phi) = \frac{\partial}{\partial x}\left(\frac{\Gamma\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\Gamma\partial\phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{\Gamma\partial\phi}{\partial z}\right)$$

$S_{\phi} = A + B\phi$ = source term of ϕ (kg/m^3/s)

$\phi =$ pollutant concentration (*E. coli* count per 100 ml or BOD_5)

$\Gamma =$ coefficient of diffusivity (kg/m/s)

$\rho =$ density (kg/m^3)

$U =$ velocity vector (m/s) = $[u, v, w]$

3.1.1 Development of the source term function of *E. coli* and BOD_5 removal

In order to simplify the derivation of the source term function to represent *E. coli* or BOD_5 removal, the scalar transport equation presented by equation 2.29 is expressed in one-dimensional form. This one-dimensional scalar transport equation is written as follows:

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\phi u) = div(\Gamma grad\phi) + S_{\phi}$$

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho\phi u)}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\Gamma\partial\phi}{\partial x}\right) + S_\phi \qquad 3.1$$

where:

u = velocity in x direction (m/s)

Using the concept of a steady state plug flow pond, the source term function that represents the *E. coli* and BOD_5 removal can easily be developed. When the steady state flow pattern has developed, temporal derivative terms are zero and equation 3.1 becomes:

$$\frac{\partial(\rho\phi)}{\partial t} = 0$$

$$\frac{\partial(\rho\phi u)}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\Gamma\partial\phi}{\partial x}\right) + S_\phi \qquad 3.2$$

In the plug flow model, fluid elements do not mix with each other; the wastewater flow is carried by convection only, therefore the diffusivity coefficient of the scalar transport equation is zero ($\Gamma = 0$). Thus equation 3.2 can further be simplified to:

$$\frac{\partial(\rho\phi u)}{\partial x} = S_\phi \qquad 3.3$$

Patankar (1980) and FLUENT (2003) define the source term (S_ϕ) as a function that depends on a constant term (A) and a coefficient (B) of the dependent variable, such that the source term function is expressed as:

$$S_\phi = A + B\phi \qquad 3.4$$

The source term function can be changed into a decay (or sink) term by changing the sign of the coefficient of the variable to a negative. The source term function becomes a decay term as follows:

$$S_\phi = A - B\phi \qquad 3.5$$

The scalar transport equation 3.3 can be used to simulate the *E. coli* removal in a plug flow pond by including the source term function ($S_\phi = A - B\phi$) in the solver. Thus equation 3.3 becomes:

$$\frac{\partial(\rho\phi u)}{\partial x} = A - B\phi \qquad 3.6$$

The first-order reaction model of the rate of decay of *E. coli* in waste stabilization ponds is normally expressed as equation 3.7:

$$\frac{\partial\phi}{\partial t} = -k\phi \qquad 3.7$$

where:

ϕ = *E. coli* numbers per 100 ml

k = first-order rate constant of *E. coli* removal (day^{-1})

The first-order reaction model of the rate of decay of *E. coli* (equation 3.7) is equivalent to the scalar transport equation 3.6 when the following simplifications are employed. When isothermal conditions develop in the pond, the wastewater density is constant (Perry and Green, 1985). Therefore, dividing the wastewater density (ρ) to both sides of equation 3.6 and assigning the constant A = 0, equation 3.6 becomes:

$$\frac{\partial(\phi u)}{\partial x} = -\frac{B\phi}{\rho} \qquad 3.8$$

$$\frac{\partial(\phi u)}{\partial x} = -C\phi$$

where:

C = $\frac{B}{\rho}$ = constant

Using dimensional analysis and the classical disinfection kinetic proposed by (Chick, 1908), the term $\frac{\partial(\phi u)}{\partial x}$ in equation 3.8 represents the first-order reaction rate with respect to the *E. coli* numbers being inactivated. Hence equation 3.8 is equivalent to the rate of decay of *E. coli* expressed by equation 3.7. Thus, the source term function of the scalar transport equation can be expressed as the rate of decay of *E. coli* (equation 3.7) by assigning the constant of the source term to zero ($A = 0$) and equation 3.6 becomes:

$$\frac{\partial(\rho\phi u)}{\partial x} = -B\phi \qquad 3.9$$

In order to determine coefficient B that represents the first-order rate of *E. coli* removal, dimensional analysis is applied to equation 3.9. Note that the *E. coli* variable (ϕ) in equation 3.9 represents the scalar variable that is dimensionless. Therefore, the dimensions of coefficient B in equation 3.9 are that of the term $\frac{\partial(\rho u)}{\partial x}$, which are $ML^{-3}T^{-1}$. This implies that the units of the coefficient B in equation 3.9 are $\frac{kg}{m^3 s}$. This can be satisfied if the density of the wastewater is multiplied by the first-order rate constant removal of *E. coli* that is measured in the reciprocal of time to achieve the same dimensions. Equation 3.9 can be rewritten by substituting coefficient B with (ρk) as shown in equation 3.10:

$$\frac{\partial(\rho\phi u)}{\partial x} = -\rho k\phi \qquad 3.10$$

where:

ρ = density of wastewater (kg/m^3)

k = first-order rate constant of *E. coli* removal (s^{-1})

The right hand side of equation 3.10 is the source term function that represents the removal of the pollutants such as the *E. coli* or BOD_5 depending on values of the first-order rate constant and the wastewater density used. The source term function can be included in FLUENT solver to modify the default scalar transport equation when predicting the removal of pollutant in the pond.

Equation 3.10 can further be simplified to derive the classic plug flow equation (2.9) to justify the assumptions used in developing the source term function. The pollutant variable (ϕ) that represents the *E. coli* concentration can be derived using the following mathematical simplification:

$$\frac{\partial(\rho\phi u)}{\partial x} = -\rho k\phi$$

$$\frac{\partial(\phi u)}{\partial x} = -k\phi$$

$$\frac{\partial\phi}{\phi} = \frac{-k\partial x}{u}$$

Integrating both sides of the above equation,

$$\int\frac{\partial\phi}{\phi} = \frac{-k}{u}\int\partial x$$

$$\ell n\phi = \frac{-kx}{u} + D \qquad 3.11$$

where:

D = constant

The inlet boundary condition of waste stabilization pond can be used to determine the constant D. Using the following boundary condition that exists at the pond inlet:

when $x = 0$, $\phi = \phi_0 =$ influent *E. coli* concentration per 100 ml

substituting these values into equation, 3.11 give $\ell n\phi_0 = D$

$$\ell n\phi = \frac{-kx}{u} + \ell n\phi_0$$

$$\ell n\phi - \ell n\phi_0 = \frac{-kx}{u}$$

$$\ell n\left(\frac{\phi}{\phi_0}\right) = \frac{-kx}{u}$$

$$\phi = \phi_0 e^{\frac{-xk}{u}}$$

but $\frac{x}{u} = t =$ residence time of fluid in a plug flow pond

$$\phi = \phi_0 e^{-kt} \qquad 3.12$$

Thus the source term function that represents the removal of *E. coli* and BOD_5 in the CFD model of waste stabilization ponds is given as:

$$S = -\rho k \phi \qquad 3.13$$

It is interesting to note that equation 3.12 is the fundamental equation of the plug flow pond model (equation 2.9). This suggests that the CFD model will predict effluent *E. coli* counts that are close to the plug flow pond solution. Incorporation of equation 3.13 (source term function) into FLUENT solver enables the scalar transport equation to simulate the pollutant removal in models of waste stabilization ponds.

From this demonstration, it can be assumed that the source term function has been developed and incorporated correctly into the basic CFD model equations. It is not necessary to include either the time dependent or advective elements as these do not contribute to the final steady state condition. The diffusive term will, however, need defining with a coefficient of diffusion. Shilton and Harrison (2003a and 2003b) have shown that the diffusive term in CFD model of waste stabilization ponds is negligibly small due to the recirculation flow pattern of wastewater. Plots of velocity vectors in CFD models (Chapter 5) confirm the recommendations of Shilton and Harrison's (2003a and 2003b) that the diffusivity term in the scalar transport equation could be neglected. Although quasi-steady state flow is appropriate for the model of waste stabilization ponds due to the daily variation of influent flow, steady state flow is adopted because the concentration profile of wastewater pollutants in the pond do not vary significantly over time due to the long period of the pond operation.

Inclusion of the source term function within the FLUENT solver is achieved using the *user defined function* facility (UDF) that is provided by the package. The UDF facility allows the user to develop extensions to the basic CFD functionality using the C programming language. In this research the source term function code (equation 3.13) has been added to the 3D scalar transport equation via a UDF. The programming procedures for writing the source term function code are available in Appendix A. In order to check the accuracy and reliability of the developed function, the CFD model was used to predict the effluent *E. coli* numbers in the plug flow pond. The solution of the model is compared with the classic plug flow equation (2.9) in predicting the effluent *E. coli* numbers.

3.1.1.1 A model test for the simulation of *E. coli* decay in plug flow pond

3D plug flow pond with dimensions of 200 m long, 75 m wide and 1.5 m deep was simulated using the CFD model. The dimensions of the inlet and outlet of the pond were 75 m wide and 1.5 m deep (the whole width of the pond). The steady state flow pattern in the model was achieved by treating the walls of the pond and the free surface as *free* slip surfaces to simulate the frictionless boundaries that exist between the walls, free surface and the wastewater. This was achieved by applying zero shear stress to the free surface and wall boundaries. The isothermal condition was assumed to develop in the pond at a temperature of 14^{o}C. Marais' (1974) first-order rate constant removal of *E. coli* ($2.6\times1.19^{(T-20)}$; where T is temperature) was included in the source term function together with the wastewater density. The pond model was meshed with un-structured hexahedral cells and the resulting number of cells was 213,600. The influent *E. coli* count was 1×10^{8} per 100 ml and this was the boundary condition of the scalar transport equation. The hydraulic retention time of the pond was 15 days and this corresponds to a daily flow rate of 1,500 m^3 per day.

Using the Reynolds equation ($Re = \frac{\rho v d}{\mu}$) with ρ = density of wastewater = 1000 kg/ m^3, ν = influent velocity = 1.54×10^{-4} m/s, μ = wastewater viscosity = 1×10^{-3} kg/m/s, d = depth of the pond inlet = 1.5 m, the Reynolds number at the inlet is 231. This suggests that the flow characteristic of the wastewater in the pond is laminar flow regime. The solution of the CFD plug flow model converged very quickly to a steady state after six iterations. The predicted *E. coli* count at the outlet was 108 per 100 ml. Figure 3.1 shows the distribution of *E. coli* concentration and the hydraulic flow patterns in the plug flow pond model.

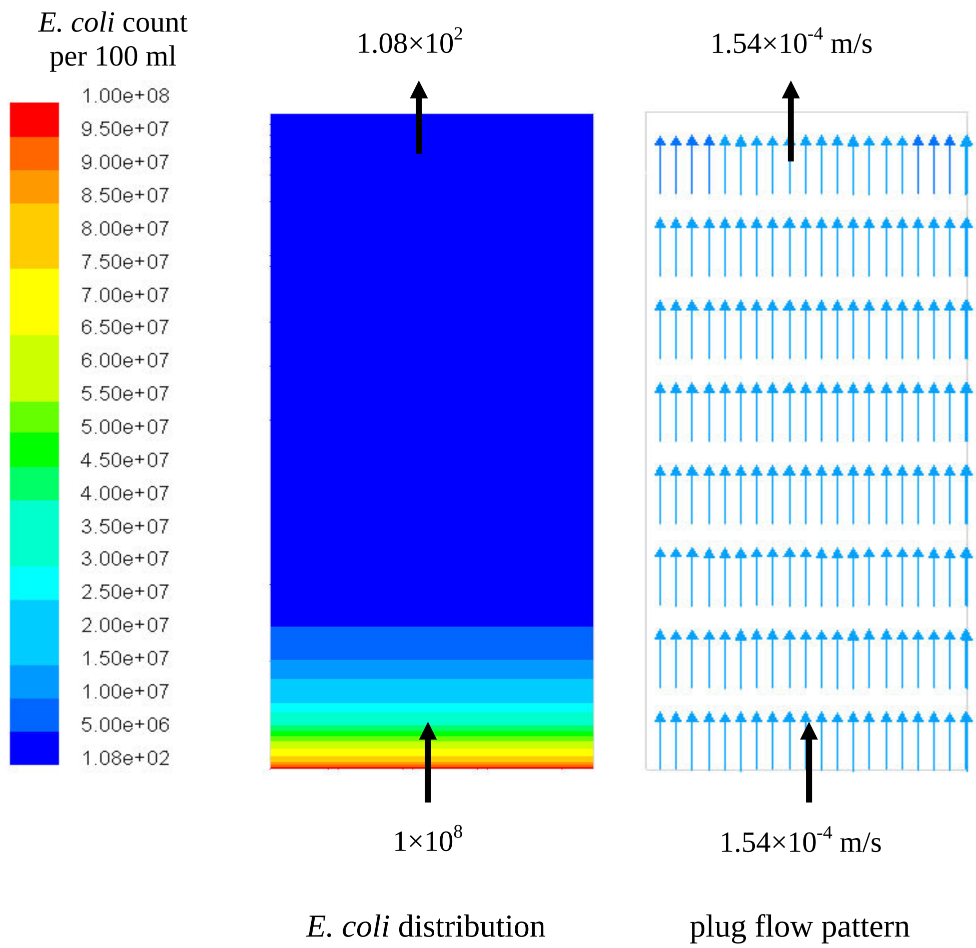

Figure 3.1 *E. coli* distribution and velocity vector in the plug flow pond model

The figure shows that the influent *E. coli* number is 1×10^8 per 100 ml at the pond inlet and 108 per 100 ml at the pond outlet. The velocity vector plot shows a uniform velocity (i.e. plug flow pattern) as the velocity vectors are identical at all points in the pond (0.000154 m/s) and there is no mixing between them. Figure 3.2 presents the longitudinal profile of *E. coli* decay from the CFD model together with the classic plug flow pond model ($N_e = N_o e^{-kt}$) that incorporates the Marais' (1974) first-order rate constant removal of *E. coli* at temperature of 14^{o}C. It can be seen that the exponential decay of *E. coli* in the CFD model and the classic plug flow pond equation are identical along the longitudinal axis of the pond. The predicted effluent *E. coli* count by the plug flow model and the CFD model is 108 per 100 ml. This demonstrates that the modified scalar transport equation with the source term function is developed correctly and can be used in the CFD model simulations of the *E. coli* decay in waste stabilization ponds with more complex flow patterns.

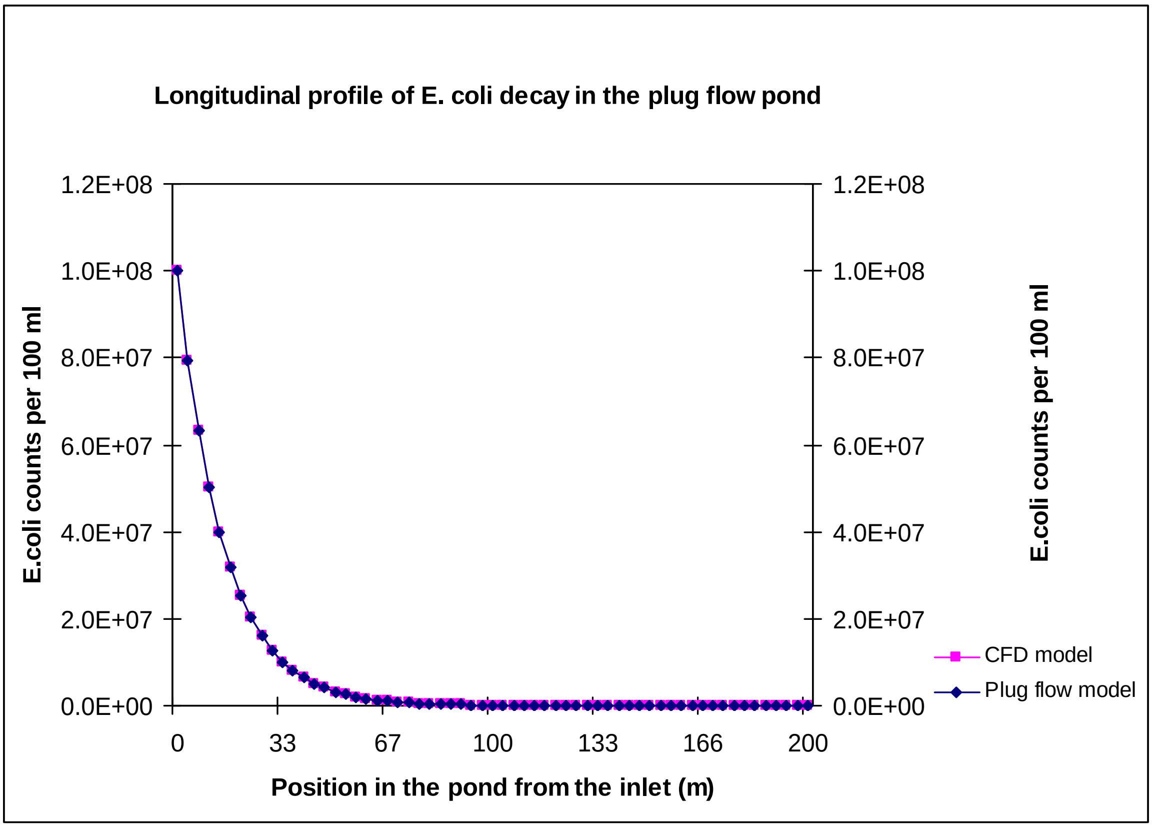

Figure 3.2 Longitudinal profile of *E. coli* decay in the CFD model and plug flow pond model

3.1.2 Development of the source term function of the spatial residence time

The CFD model can be extended to calculate the spatial residence time distributions in the pond by developing a source term function that represents the residence time and incorporated into a second modified scalar transport equation. The spatial residence time is defined as the average time taken by a fluid element to get from the inlet to any point in the pond. The standard 3D scalar transport equation as presented in equation 2.29 can be used as the basis of the derivation. It is recalled here as follows with ϕ replaced by θ to represent residence time:

$$\frac{\partial(\rho\theta)}{\partial t} + div(\rho\theta u) = div(\Gamma grad\theta) + S_\theta$$

In one dimension, this equation becomes:

$$\frac{\partial(\rho\theta)}{\partial t} + \frac{\partial(\rho\theta u)}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\Gamma\partial\theta}{\partial x}\right) + S_\theta \qquad 3.14$$

where:

$u =$ velocity in x direction (m/s)

$\theta =$ residence time (s)

Following similar arguments, considering the steady state plug flow assumption used for the derivation of the source term of the *E. coli* removal (Section 3.1.1), equation 3.15 is derived.

$$\frac{\partial(\rho\theta u)}{\partial x} = S_\theta \qquad 3.15$$

$$\frac{\partial(\rho\theta u)}{\partial x} = A + B\theta$$

The principle of developing the source term function that represents the residence time distributions in CFD model is to understand the physical meaning of the term ($B\theta$) in this equation. The residence time variable (θ) is not the same as the pollutant concentration variable that decays with time. This implies that the value of the ($B\theta$) term should be zero because it is associated with the creation and destruction of the residence time variable. Therefore, equation 3.15 can further be simplified into equation 3.16 as follows:

$$B\theta = 0$$

$$\frac{\partial(\rho\theta u)}{\partial x} = A \qquad 3.16$$

Note that the units of the residence time (θ) in equation 3.16 are seconds (s). Application of dimensional analysis to equation 3.16 shows that the dimensions of the left hand side term $\frac{\partial(\rho\theta u)}{\partial x}$ are ML^{-3}. This implies that the units of constant (A) should be kg/m^3. This can be satisfied if the constant (A) is the product of the wastewater density (ρ) with another constant (C_1). Equation 3.16 is changed with constant (A) being substituted by ($\rho \times C_1$) as shown in equation 3.17.

$$\frac{\partial(\rho\theta u)}{\partial x} = \rho C_1 = A \qquad 3.17$$

However, equation 3.17 represents the mass conservation of wastewater at a particular time in 1D computational cell. Therefore, the constant C_1 should be equal to 1 and equation (3.17) simplifies to:

$$\frac{\partial(\rho\theta u)}{\partial x} = \rho \qquad 3.18$$

The mathematical arguments suggested above can be appreciated when one understands the physical meaning of the integrated equation of the scalar transport equation that includes the source term function of the residence time. Integration of equation 2.29 over the 3D computational cell (cell volume, cv) yields equation 3.19:

$$\frac{\partial}{\partial t}\left(\int_{CV}\rho\theta dv\right) + \int_{CV} div(\rho\theta U)dv = \int_{CV} div(\Gamma grad\theta)dv + \int_{CV}\rho dv \qquad 3.19$$

Gauss's divergence theorem can be used to simplify equation 3.19 such that the face area of the cell volume is used in the CFD computations. The simplified discrete form of the scalar transport equation 3.19 using the steady state flow in the CFD model of the plug flow pond with diffusivity coefficient $\Gamma = 0$ is expressed as follows:

$$\frac{\partial}{\partial t}\left(\int_{CV}\rho\theta dv\right) = 0$$

$$\sum_{f}^{N_{faces}} \Gamma_\theta (\nabla\theta)_n . A_f = 0$$

$$\sum_{f}^{N_{faces}} \rho_f v_f \theta_f . A_f = \rho V \qquad 3.20$$

where:

N_{faces} = number of faces enclosing cell

θ_f = value of θ convected through face f (s)

$\rho_f v_f . A_f$ = mass flux through the cell face (kg/s)

$(\nabla\theta)_n$ = magnitude of $\nabla\theta$ normal to face f (s)

A_f = area of face f (m^2)

V = cell volume (m^3)

dv = differential cell volume (m^3)

The physical meaning of the equation 3.20 is that the generated residence time of wastewater in a cell of mass (ρV) is convected $\left(\sum_{f}^{N_{faces}} \rho_f v_f \theta_f . A_f\right)$ through faces of a cell with similar mass in a given residence time to satisfy the conservation equation of the mass flow rate. This substantiates the value of the constant C_1 that has been evaluated as 1. Simplification of equation 3.18 leads to the development of the equation of the residence time distribution in the plug flow pond as given by equation 3.21, which has been derived using the following procedures:

$$\frac{\partial(\rho\theta u)}{\partial x} = \rho$$

$$\frac{\partial(\theta u)}{\partial x} = 1$$

$$\partial\theta = \frac{\partial x}{u}$$

$$\int \partial\theta = \int \frac{\partial x}{u}$$

$$\theta = \frac{x}{u} + C$$

Substituting the boundary conditions at the inlet of the plug flow pond ($x = 0 ; \theta = 0$) shows that the value of the constant *C* is equal to *0*. Therefore, equation 3.21 is the classic plug flow model that gives the residence time of the wastewater in the pond.

$$\theta = \frac{x}{u} \qquad 3.21$$

where:

θ = residence time (seconds)

x = distance in the pond from the inlet (m)

u = velocity (m/s)

Thus the source term function that represents the spatial residence time distribution in the CFD model of waste stabilization ponds is given as:

$$S = \rho \qquad 3.22$$

Incorporation of the source term equation 3.22 into FLUENT solver as an extra transport equation enables this scalar transport equation to predict the spatial residence time distribution in a waste stabilization pond. The programming procedures for equation 3.22 was carried out in C language and the source term function was added to the solver through the *user defined function* (UDF) facility available in FLUENT software.

3.1.2.1 A model test for the simulation of spatial residence time in plug flow pond

Simulation of the residence time distribution in the plug flow pond was carried out to assess the accuracy and reliability of developed source term function. The same 3D CFD plug flow model as used to test the *E. coli* decay was employed to simulate the residence time distributions (Section 3.1.1.1). All boundary conditions of the model were similar to that of the plug flow pond model described in (Section 3.1.1.1). The procedure to obtain residence time distribution is first to solve the flow equations with no scalar transport or residence time calculation. When the converged flow solution is obtained, the flow equations are not solved and the scalar transport equation for the residence time distribution is solved using the converged flow solution. The residence time distribution in the waste stabilization pond was set to zero at all cells as well as at the pond inlet. The solution converged quickly after three iterations. The predicted residence time of the wastewater was 15 days (1,296,000 seconds) in the CFD simulation. This is equal to the analytical value from equation 3.21 (x = 200 m, u = 1.543×10^{-4} m/s). This demonstrates that the developed source term function (equation 3.22) of the residence time is developed correctly and can be used in further CFD model simulations of waste stabilization ponds with complex flow patterns.

Figure 3.3 shows the longitudinal profile of the residence time in the CFD model together with the plug flow pond model. It can be seen that the profiles of the residence time in the CFD model and the classic plug flow pond model are identical. The CFD simulation solution and the theoretical residence time increase linearly with a value of zero seconds at the pond inlet and 1296000 seconds at the pond outlet. It could be very worrying if the CFD simulation solution did not predict the theoretical residence time correctly.

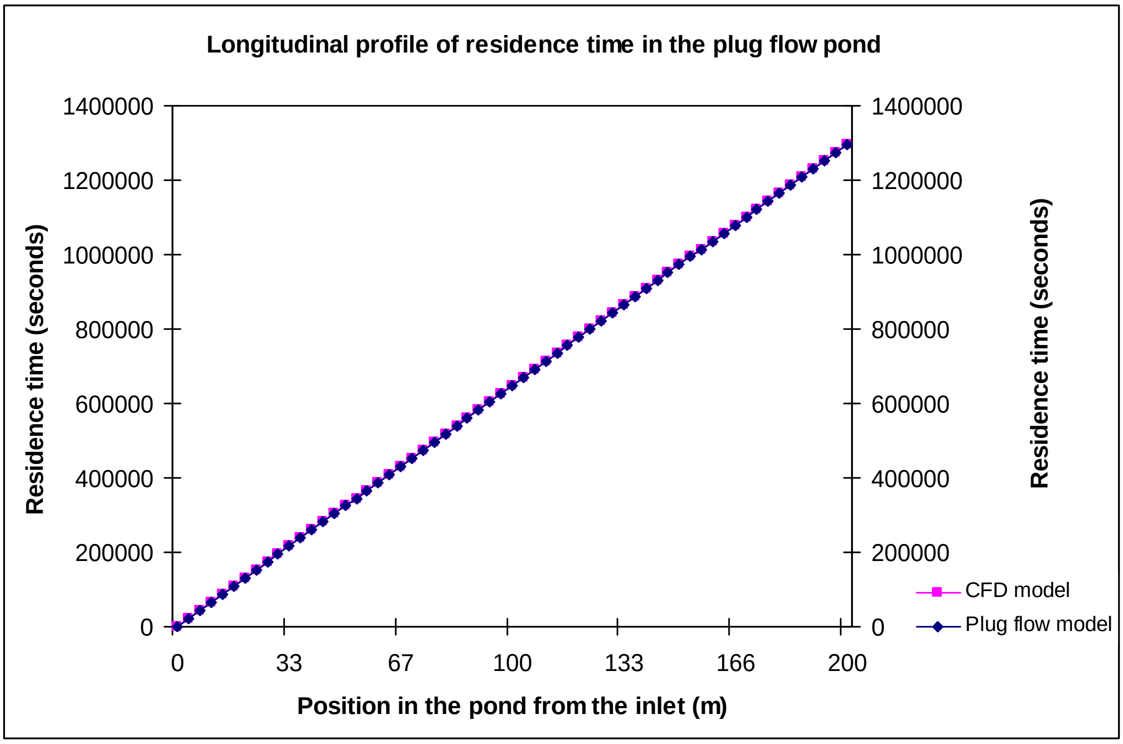

Figure 3.3 Longitudinal profile of residence time distribution in the CFD model and plug flow pond model

3.2 Mesh-independent solution tests for CFD

The accuracy of the CFD solution depends on the quality of the mesh that has been used in the model. Ferziger and Peric (2002) advise that the CFD based solutions must be grid independent – that is the obtained solution does not change if the mesh is refined (made finer or more dense). Patankar (1980) argues that a grid of appropriate structure and fineness should be generated for the geometry of the model. In general it is good practice to have fine grids in areas where rapid variation of flow variables occurs (Versteeg and Malalasekera, 1995) as this minimises the inaccuracy of the CFD solution. The procedure to ensure mesh independent solutions is to start with what appears to be a reasonable mesh for the particular flow and geometry and to obtain a solution for that mesh. The mesh should then be successively refined and the solution obtained at each refinement step. Comparison of the solutions obtained should show a convergence to a constant value. It is usually necessary to select several specific measurements for comparison, in areas where important values are required, or rapidly changing flow variables occur.

In FLUENT, grid refinement is implemented using the adaptation tool that is available. Ferziger and Peric (2002) recommended that the CFD flow solution should be computed on at least three grids until the variation of the solution is not significant. These principles were followed by the author when using CFD to simulate the hydraulic flow patterns and the treatment efficiency of the typical waste stabilization pond and the pilot-scale primary facultative pond that were run with two and four baffle configurations. A typical waste stabilization pond was designed following the modern standard procedures (Shilton and Harrison, 2003a, 2003b; Shilton and Mara, 2005) and was chosen for all simulations that were undertaken.

3.2.1 Mesh-independent solution for unbaffled waste stabilization pond model

Three different grid sizes, each successively more refined than the previous, were investigated to find the optimum grid size that provides grid-independent solution for the unbaffled pond model. Un-structured hexahedral element as shown in Figure 3.4 was used to mesh the geometry of the pond.

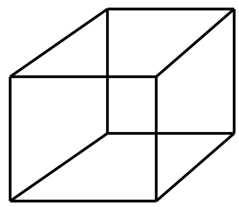

Figure 3.4 The general shape of a hexahedral cell with six rectangular faces

This grid type was chosen because it provided uniform cell shape in the pond thereby reducing potential discretisation error that arises when unstructured grids with different cell shapes (triangular, tetrahedral and pyramid) are used. The size of the primary facultative pond that was simulated was 640 m long, 320 m wide and 1.5 m deep. The inlet and outlet pipes had diameters of 400 mm and were located 10 m from the side edge of the pond. These inlet and outlet structures were located at the diagonal corners of the pond to follow the recommendations of the geometric design procedures (Mara, 2004).

Three un-structured hexahedral meshes of 5 m × 5 m × 0.1875 m (a cuboid cell with square base of 5 m × 5 m and height of 0.1875 m), 2.5 m × 2.5 m × 0.1875 m, 1.25 m × 1.25 m × 0.1875 m respectively were used in meshing the geometry of the pond. Note how the base area dimensions were halved for each mesh in order to increase the number of cells by four times. The generated number of cells for each grid was 66,544, 264,160, and 1,052,624 respectively. For this pond model with height 1.5 m, eight cells were used through the pond depth for each grid. The eight cells in the vertical dimension appeared to be reasonable because the variation of vertical velocity component was not significant as the bulk flow pattern in the pond was due to the horizontal velocity component (the influent momentum was located in the horizontal plane and sustained the flow pattern). The grids were all uniformly distributed (not refined at any region) in the model.

Simulations were performed with the 3D with double precision version of FLUENT as recommended for higher accuracy in the FLUENT manual (2003). The second-order differencing scheme was adopted to simulate more precisely the steeper gradients that capture the recirculation flow pattern that exists in the pond. Initial tests with the default first-order differencing scheme showed that it did not reproduce accurately the recirculation flow patterns in the pond. For this reason, it was not used in further simulations. Other high order scheme such as QUICK was not adopted because the accuracy is not significantly different to that of the second order-differencing scheme. This is generally understood behaviour of CFD simulation (Versteeg and Malalasekera, 1995; Ferziger and Peric 2002).

Although quasi-steady state flow is appropriate in the model of waste stabilization ponds due to the significant variation of the influent during operation, it was decided to use steady state flow because the concentration profile of the wastewater pollutants does not vary significantly over time due to the long period of the pond operation. With this observation, steady state flow was adopted to simulate the hydraulic flow pattern in the pond.

Using the Reynolds number equation ($Re = \frac{\rho v d}{\mu}$) where ρ = density of wastewater = 1000 kg/ m^3, ν = influent velocity = 0.92 m/s, μ = wastewater viscosity = 1×10^{-3} kg/m/s, d = diameter of the inlet pipe = 0.4 m at the pond inlet, the Reynolds number at the inlet was 3.7×10^5. This suggests that the flow characteristic of the wastewater in the pond is turbulent flow regime (Re > 4000).

Shilton (2001) observed that there is negligible difference between the modified turbulence model of the Chen-Kim $k-\varepsilon$ and the standard $k-\varepsilon$ model when simulating tracer experiments using the high order-differencing scheme. Following this, the standard $k-\varepsilon$ model and the second order-differencing scheme were chosen. Tests with other turbulence models showed little difference in the results. The results of the CFD model grid independence tests of the unbaffled waste stabilization pond are presented in Table 3.1.

Table 3.1 Predicted effluent *E. coli* count and log-units removal from the outlet surface of the unbaffled waste stabilization pond model

Mesh No.	Mesh size (m)	Cell number	*E. coli* count per 100 ml	Log-units removal of *E. coli*
1	5 × 5 × 0.1875	66,544	5.00×10^7	0.30
2	2.5 × 2.5 × 0.1875	264,160	1.30×10^7	0.89
3	1.75 ×1.75 × 0.1875	538,720	1.50×10^7	0.82
4	1.25 ×1.25 × 0.1875	1,052,624	1.60×10^7	0.80

The simulations were run on a desktop PC computer (Intel inside Pentium 4) of 512 MB RAM. The solution of the CFD model with the finest grid (mesh 4) took four days to converge while the coarsest grid (mesh 1) and next coarsest grid (mesh 2) took 2 hours and 5 hours respectively to converge. In order to compromise on the computational time required to get a converged flow solution, mesh 3 was tested.

The log-units removal of *E. coli* predicted by the finest mesh 4 and mesh 3 do not differ from each other significantly (0.82 and 0.80). It can also be seen that the predicted *E. coli* counts by mesh 4 and mesh 3 show insignificant difference (1.60×10^7 and 1.50×10^7). Based on these two criteria, the mesh 3 was chosen as the optimum mesh for the simulations because it gave a reasonable solution within the optimum computational time. For all simulations of unbaffled waste stabilization pond (640 m× 320 m× 1.5 m) that were undertaken, mesh size of 1.75 m ×1.75 m × 0.1875 m was used.

3.2.2 Mesh-independent solution for the CFD model for baffled waste stabilization pond

Investigation of the mesh independent test of the CFD model simulations for baffled waste stabilization pond model (640 m × 320 m × 1.5 m) was carried out using similar mesh sizes described in Section 3.2.1. The test was investigated using a two-baffle pond with an inlet and outlet size of 96 m wide by 1.5 m deep. The proposed pond inlet and outlet were adopted to simulate the flow of wastewater through the 30%

pond-width baffle opening. The inlet velocity was assumed by assessing the bulk velocity of wastewater in the unbaffled pond model. The inlet velocity of 0.05 m/s was defined as the boundary condition of the momentum equations. The grids were uniformly distributed in the model. The results of the CFD model grid independence tests of the two-baffle pond model are presented in Table 3.2.

Table 3.2 Predicted effluent *E. coli* count and log-units removal of *E. coli* from the pond outlet surface of the two-baffle pond model

Mesh No.	Mesh size (m)	Cell number	*E. coli* count per 100 ml	Log-units removal
1	5 × 5 × 0.1875	65,008	7.59×10^{7}	0.13
2	2.5 × 2.5 × 0.1875	262,328	7.71×10^{7}	0.11
3	1.75 × 1.75 × 0.1875	534,328	7.80×10^{7}	0.11
4	1.25 ×1.25 × 0.1875	1,046,480	7.83×10^{7}	0.11

It can be seen from Table 3.2 that the predicted *E. coli* count and the log-units removal in the two-baffle model using mesh 2, 3 and 4 are not different from each other. For uniformity with results of the mesh independence test for the unbaffled pond model, mesh size of 1.75 m ×1.75 m × 0.1875 m was used for all subsequent models of baffled waste stabilization pond that were undertaken.

3.2.3 Mesh-independent solution for the CFD model of the pilot-scale baffled primary facultative pond

Investigation of the mesh-independent solution of the CFD model of the pilot-scale baffled primary facultative pond with dimensions of 10.2 m × 3.87 m × 1.5 m was achieved using four different mesh sizes. The tetrahedral mesh as shown in Figure 3.5 was chosen because it was possible to mesh the pilot-scale pond model with sloping sides using this grid type. It was found that un-structured hexahedral mesh (Figure 3.4) could not be fitted into the pond model with trapezoidal volume.

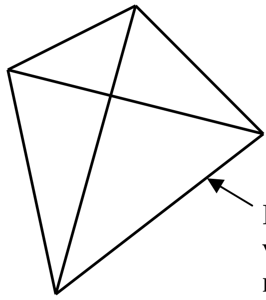

Figure 3.5 The general shape of a tetrahedral cell with four triangular faces

Four unstructured tetrahedral meshes of 0.2 m, 0.1 m, 0.075 m and 0.05 m, each cell with height of 0.1875 m were used to mesh the pilot-scale primary facultative pond. Measurement of a tetrahedral cell refers to the dimensions of the base triangle. Thus a tetrahedral cell of 0.2 m and height of 0.1875 m indicates a cell with equilateral triangle base of 0.2 m and height of 0.1875 m. An approximated eight cells were used in the pond depth

The pilot-scale primary facultative pond model simulated the pond that was operated for 30 days hydraulic retention times and this was achieved using inlet velocities of 0.05 m/s and 0.046 m/s for the wastewater and freshwater respectively. The influent *E. coli* count of 1.0×10^8 per 100 ml was defined as the boundary condition of the scalar transport equation. The grids were refined at the inlet and outlet regions to account for the rapid variation of the velocity. The generated cells in the model were 49,167, 345,591, 673, 861 and 920,480 for mesh size of 0.2 m, 0.1 m, 0.075 m and 0.05 m respectively. The results of the CFD model grid independence tests of the baffled pilot-scale primary facultative pond model are presented in Table 3.3. It can be seen from Table 3.3 that the predicted *E. coli* counts and the log-units removal in the pilot-scale baffled primary facultative pond model with mesh 2, 3 and 4 are not significantly different from each other. Therefore, a tetrahedral mesh of size 0.1 m was used to mesh the volume of the pilot-scale baffled pond because the CFD model provided satisfactory solution at the optimum computational time.

Table 3.3 Predicted effluent *E. coli* count and log-units removal from the outlet surface of the baffled pilot-scale primary facultative pond

Mesh No.	Mesh size (m)	Cell number	*E. coli* count per 100 ml	Log-units removal of *E. coli*
1	0.2	49,167	1.52×10^6	1.82
2	0.1	345,591	2.10×10^6	1.68
3	0.075	673,861	2.20×10^6	1.66
4	0.05	920,480	2.21×10^6	1.66

3.3 Summary of the methodology for the CFD model

The source term functions that represent the *E. coli* removal, BOD_5 removal and the residence time distribution have been developed into a form consistent with a source term function for the scalar transport equation in CFD. Dimensional analysis has been utilised to ensure correct dimensions and units. The chapter has demonstrated through appropriate numerical tests that the source term functions have been developed correctly and can be used in simulating the *E. coli*, BOD_5 removal and spatial residence time distribution in the CFD model of waste stabilization pond with more complex flow patterns and operational conditions.

Tests were performed of three-dimensional simulations on several different grid sizes in order to determine the optimum grid size that provided the grid-independent solution for the unbaffled and baffled waste stabilization ponds. The grid tests results showed that the un-structured hexahedral mesh of 1.75 m × 1.75 m × 0.1875 m was the optimum grid in the 640 m × 320 m ×1.5 m waste stabilization pond model. The tetrahedral mesh of 0.1 m was the optimum grid for the pilot-scale baffled primary facultative pond models that is further discussed in chapter 4.