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Full Length Research Paper

A methodology of finding dispersion coefficient using computational fluid dynamics (CFDs)

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The treatment efficiency of waste stabilization pond is directly related to its hydraulic regime. The hydraulic efficiency of the pond is dependent on parameters such as the pond geometry, the location of inlet and outlet and the inlet flow velocity. Poorly designed or specified hydraulic parameters may lead to short circuiting and dead regions within the pond. This in turn impacts the dispersion coefficient. Drogue and tracer studies are often used to get actual dispersion coefficients; however, tracer studies can be costly and are therefore not practical to do frequently. The objective of this paper is to obtain the actual dispersion coefficient using computational fluid dynamic (CFD) approach (using Fluent). The CFD results are validated using an actual tracer test.

Key words: Stabilization pond, modeling, computational fluid dynamic, residence time distribution, dispersion coefficient

INTRODUCTION

A waste stabilization pond (WSP) is a simple and cost effective method for treating wastewater (Khan and Ahmad, 1992). According to many studies (Arceivala, 1981; Polprasert and Bhattarai, 1985; Chien and Liou, 1995), the dispersed flow model may predict the transport of contaminants more reliably than the idealized con-tinuous stirred tank reactor (CSTR) or plug flow reactor (PFR) models. This model is a strong function of dis-persion coefficient, which is in turn dependent on the hydraulic regime of the pond. Therefore, identifying the hydraulic performance of the pond is required to obtain the actual amount of dispersion coefficient.

Poor hydraulic considerations and design of the WSP reduces the treatment efficiency of this system (Shilton and Harrison, 2003; Shilton and Bailey, 2006). In fact, the treatment efficiency of the WSPs is a function of the numerous physical parameters that may affect fluid movement in a pond (Piondexter and Perrier, 1981; Thackston et al., 1987; Muttamara and Puetpaiboon, 1997; Salter et al., 1999; Torres et al., 1999; Shilton and Harrison, 2003; Aldana et al., 2005; Abbas et al., 2006; Agunwamba., 2006; Fyfe et al., 2007):

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1. Pond geometry (including the influences of baffles)
2. Inlet size and position
3. Outlet position and design
4. Flow rate
5. Temperature/density effects
6. Wind shear stress and its variation over time

Pond geometry is one of the important factors that affect the hydraulic performance of the basins (Marecos et al., 1987; Torres et al., 1999). L/W ratio is the most important factor that affects the hydraulic performance of the basins (Piondexter and Perrier, 1981).

The placement of inlet and outlet impacts the hydraulic efficiency of WSP. Waste water can be discharged at the surface, mid depth and bottom of WSPs. The position of outlet may also be diverse in variety of different ponds.

The effect of inlet and outlet locations on short circuiting was evaluated by Agunwamba (2006). Short circuiting is the phenomena where the retention time of a particle in the pond is shortened due to flow conditions; in essence it decreases the treatment efficiency of the pond. Different inlet/outlet positions showed that short circuiting is highly related to the location of inlet/outlet. Minimum hydraulic efficiency occurs when the inlet and outlet are in front of each other and improves significantly if the inlet and outlet are positioned on the opposite corners of the pond (Persson and Wittgren, 2003). The presence of baffles in the pond reduces short circuiting. When baffles are present, shifting the outlet toward the baffles may reduce short circuiting (Safieddine, 2007). Inflow jet produces short circuiting within the pond depending on the flow velocity (Fyfe et al., 2007). The influence of the inflow jet reduced as the flow heads to the outlet.

Considering the hydraulic behaviors of WSPs, an accurate method of predicting the dispersion coefficient has been sought in a number of research studies. Tracer tests are widely used for tracking the flow motion in WSPs. The determination of the dispersion coefficient of the WSP using tracer studies have been evaluated by many researchers (Marecos et al., 1987; Moreno, 1990; Uluatam and Kurum, 1992; Pedahzur et al., 1993; Salter, 1999; Shilton et al., 2000; Vorkas and Lioyd, 2000). It should be noted that tracer tests are costly in time and finances. The second way for calculating the dispersion coefficient is using empirical equations. The simplest proposed by Arceivala (1981) is based on the pond width. Polprasert and Bhattarai (1985) developed an empirical formula based on the pond geometry and retention time. Other researchers used an empirical formula based on the pond geometry and retention time, but with different correlation factors (e.g. Liu, 1977). Agunwamba et al. (1992) have stated that the shear stress of the wind also affects the hydraulic behavior of the basin and axial dispersion coefficient res-pectively. Some of the empirical equations to obtain the dispersion coefficient can be seen in Table 1.

Empirical equations reduce the cost of actual tracer studies and may be a suitable option for predicting the dispersion coefficient. The empirical equations, unlike actual tracer studies may solve the problem of predicting the dispersion coefficient for the WSPs to be constructed in the future. Although, these equations are themselves defined based on different actual tracer tests, they may not be applicable in all WSPs with diverse hydraulic conditions. Therefore, the fluctuations of hydraulic parameters of the ponds and their effect on dispersion coefficients may not completely evaluated using empirical equations.

Use of CFD is another option to obtain the dispersion coefficient. These programs have the ability to model the various conditions of the pond. For the WSPs that have not been constructed yet, these models give the designer the ability to predict the hydraulic behaviors and dispersion coefficients respectively. Using CFD for finding the dispersion coefficient has the following advantages:

1. Includes the effect of pond's characteristics such as ponds geometry, inlet size and position.
2. Includes parameters such as temperature and viscosity.
3. Includes surrounding environmental parameters such as temperature fluctuations and wind.
4. Considers the effect of hydraulic behavior of the basins.

These programs are case sensitive and the lack of complete description of different parameters in the accurate way would cause uncertainty in the results. Furthermore, the user must be aware of the CFD model limitations, assumptions and working knowledge of actual ponds to prevent misinterpretation results. In this paper, a methodology is discussed using CFD (Fluent) to obtain the dispersion coefficient. The validation of the methodology is done using actual tracer study. The result of this approach is compared with the ones found by using empirical equations.

A METHODOLOGY OF FINDING DISPERSION COEFFICIENT USING CFD

The Fluent CFD model used in this paper is a commercially available computer package which is produced by Fluent Inc. in USA. Fluent solves a finite volume form of the conservation equations for mass and momentum (Fluent, 2003). The methodology is presented to simulate the stimulus response techniques (Levenspiel, 1972) to obtain tracer concentrations in different time steps and to draw residence time distribution (RTD) respectively. As the first step, the model should be meshed using Gambit (A.I.F., 2002). The sensitivity analysis is performed to ensure the mesh-independency of the numerical simulation. For this purpose, the simulation is repeated with different meshes (consecutive smaller meshes) until the differences between solutions become negligible. After meshing the model, two steps are undertaken for the modeling, started by steady state simulation. This work is solved the three momentum components (u,v,w) and the two turbulence components (K and ε) (Fluent, 2003).

After completion of the steady state simulation, particles with the same density and size are injected to the influent. Next, it is possible to carry out a transient simulation of particle movement with respect to the time. For this purpose, the solvers for pressure, momentum and turbulence are turned off and the results of steady state simulation are used. Based on the values stored from the steady state run, the simulation then stimulated through a series of time steps solving for the dispersion of the particles.

For a low surface fraction of dispersed second phase (particle), an Eulerian - Lagrangian approach was used. This allows the effects of turbulence modulation (effect of particles on turbulence) to be neglected. The Lagrangian approach divides the particle phase into a representative set of discrete individual particles and tracks these particles separately through the flow domain by solving the equations of particle movement. Assumptions regarding the particle phase included the following: (i) no particle rebounded off the walls/surfaces (ii) no particle coagulation in the particle deposition process and (iii) all particles are spherical solid shapes. Trajectories of individual particles can be tracked by integrating the force balance equations on the particle (Fluent, 2003):

$$\frac{du_p}{dt} = F_D (u - u_p) + g_x (\rho_p - \rho) / \rho_p + F_x \qquad (1)$$

Where F_D (Drag force) is calculated according to the following equation:

$$F_D = \frac{18 \mu}{\rho_p D^2_p} \frac{C_D \text{ Re}}{24} \qquad (2)$$

Table 1. Empirical equations for determining the Peclet number (UL/D).

Name	Condition	Formula
Liu (1977)	Large width to depth ratio	$d = \frac{0.168 * (\tau .v)^{.25} * (W+2Z)^{3.25}}{(LWZ)^{1.25}}$
Polprasert and Bhattarai, (1985)	Waste stabilization pond	$d = \frac{0.184 *[\tau .v(W+2Z)]^{0.489}\ W^{1.511}}{(LZ)^{1.489}}$
Arceivala (1981)	For pond width greater than 30 m	$D^{**} = 16.7\ W$
Arceivala (1981)	For pond width less than 30 m	$D = 2W^2$
Murphy and Wilson, (1974)	The volume over 300000 m^3	$d = K\tau/L^2$
Nameche and Vasel (1998)	Stabilization pond and lagoon	$\frac{1}{d} = 0.31(\frac{L}{W}) + 0.055(\frac{L}{Z})$
Agunwamba et al. (1992)	Stabilization pond	$d = 0.102(\frac{u^*}{u})^{-0.8196}(\frac{H}{L})(\frac{H}{W})^{-(0.981+1.385\frac{H}{W})}$

*. τ: Retention time, **. The unit of D in Arceivala's equation is m^2/h.

And the Reynolds number is defined as:

$$Re = \frac{\rho D_p |u_p - u|}{\mu} \quad (3)$$

When the flow is turbulent, Fluent uses mean fluid phase velocity in the trajectory equation (Equation 1) in order to predict the dispersion of the particles. The amount of the particles in each time step at the outlet position is monitored until the end of the transient simulation. These concentrations versus time help to draw RTD. The methodology of drawing RTD is demonstrated in Figure 1 Integrating the RTD with Levenspiel formula leads to obtain the dispersion coefficient. The dispersion number, D/UL may be calculated from the dimensional variance which is defined as (Levenspiel, 1972):

$$\sigma^2 = \frac{t_i^2 C_i}{C_i} - \left(\frac{t_i C_i}{C_i}\right)^2 \quad (4)$$

The amount of variance is calculated according to concentrations in each time step (Equation 4). The dispersion number (d) (Levenspiel, 1972) is determined using the following equation:

$$\sigma_i^2 = \frac{\sigma^2}{t^2} = 2d - 2d^2(1 - \exp(\frac{-1}{d})) \quad (5)$$

The variance and t are used to estimate "d" by a process of trial and error using Excel Solver in Microsoft Excel.

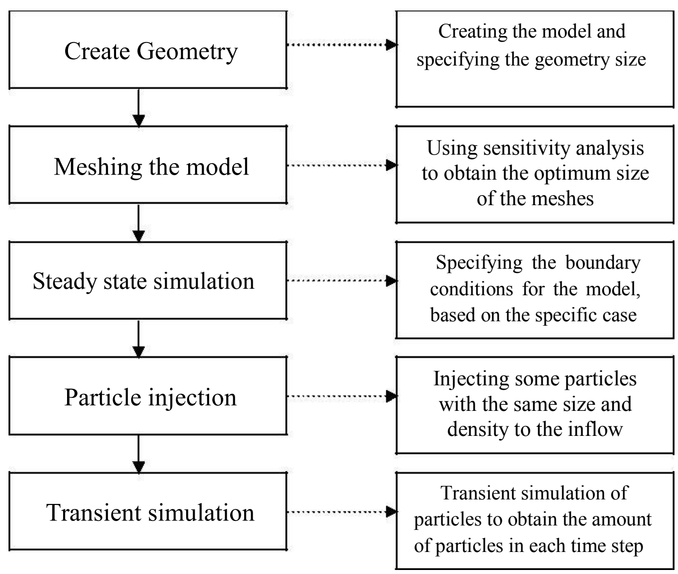

Figure 1. The CFD Simulation methodology to draw RTD.

COMPUTATIONAL FLUID DYNAMIC APPROACH: A CASE STUDY

A methodology for determining the dispersion coefficient is proposed by the combining of CFD approach methodology and Levenspiel's formula (Levenspiel, 1972). Testing and validation of the method is assessed by the field's.data. The name and the place of the basin used as a case study in this paper will not be disclosed herein, due to the confidentiality of the data.

Flow domain and mesh

A two dimensional model was developed for this study. The model created and meshed using Gambit (version 2.4.6). The whole surface was divided to 711819 homogenous quadrilateral cells (0.3

Table 2. Geometry and flow parameters of the basin.

Parameter	Units	Value
Length (L)	m	500
Width (W)	m	100
Inlet width	m	0.45
Inlet velocity in x-direction	m/s	4.63
Inlet velocity in y-direction	m/s	0
Fluid Density	Kg/m^3	998.2
Fluid viscosity	Kg/(m.s)	0.001

Table 3. Inputs to CFD tool (Fluent).

Models	Two dimensional
	Pressure based, Steady state
	Standard k-epsilon turbulence model
Solution Control	Second order upwind discretization
Materials	Liquid water (H2O), Solid particles
Operating conditions	Operating pressure: 101325 Pa
	Gravity: Off
Boundary conditions	Inlet: Velocity inlet (V=4.63m/s)
	Walls: No slip boundaries
	Outlet: Outflow
	Discrete phase condition at walls: reflect,
	normal constant 0.5, tangential constant 0.8
	Discrete phase condition at inlet and outlet: escape
Convergence limit	Scaled residuals: 1.0E-04

x 0.3m). The parameters related to this model are presented in Table 2.

Initial and boundary conditions

The governing equations were solved in combination with the proper initial and boundary constraints. The inlet boundary was specified by inlet velocity (V = 4.63 m/s). The no slip boundary condition was chosen for the walls. For discrete phase boundaries, the outflow was chosen as an escape boundary and the walls as reflective boundaries. The boundary conditions that were picked for this case are presented in Table 3.

Modeling flow and solid phase particles

Fluent solves the equations of turbulent flow in a two-dimensional geometry to obtain the water velocity. The standard K- ε approach is a widely used, robust, economical model, which has the advantages of rapid, stable and reasonable results for many flows (Marshall and Bakker, 2003). In this case study, the standard K- ε model is used. After running the model for 5,000 iterations and obtainning acceptable convergence, the unsteady particle tracking is used for tracking the solid particles within the basin. For this reason, 5,000 spherical particles with the same size are injected at the inlet at the same time. Particle diameters (100 μm) and density (1020 Kg/m^3) is selected based on previous investigation (Gancarski, 2007). This size and density is an acceptable option for modeling the particle as a drogue in the basins. After injection, this model is run for 104 time steps, 1800 s each and the amount of the particles escaped from the basin in each time step is calculated.

RESULTS AND DISCUSSION

The data received from actual tracer studies from the field are plotted, as are illustrated in Figure 2. This is one of the typical RTD for this basin between 12 RTDs that draw during different months of the year, but the final value of ‘d’ is calculated based on the concentrations mean value. Tracer concentration versus time shows the existence of short circuiting in the basin. The maximum concentration of the tracers received approximately four hours after injection which is less than the actual retention time. The existence of short circuiting in the pond was previously reported by other researchers as well (Vorkas et al., 2000; Moreno, 1990). The amount of ‘d’ using actual tracer test is calculated which is 0.6. The process for calculating this coefficient can be seen in Table 4. Concentrations in different time steps are calculated using un-steady particle injection in Fluent, as demonstrated in Figure 2. Integration of this calculation with Levenspiel’s formula as mentioned previously shows the amount of ’d’ is 0.5. The summary of this calculation

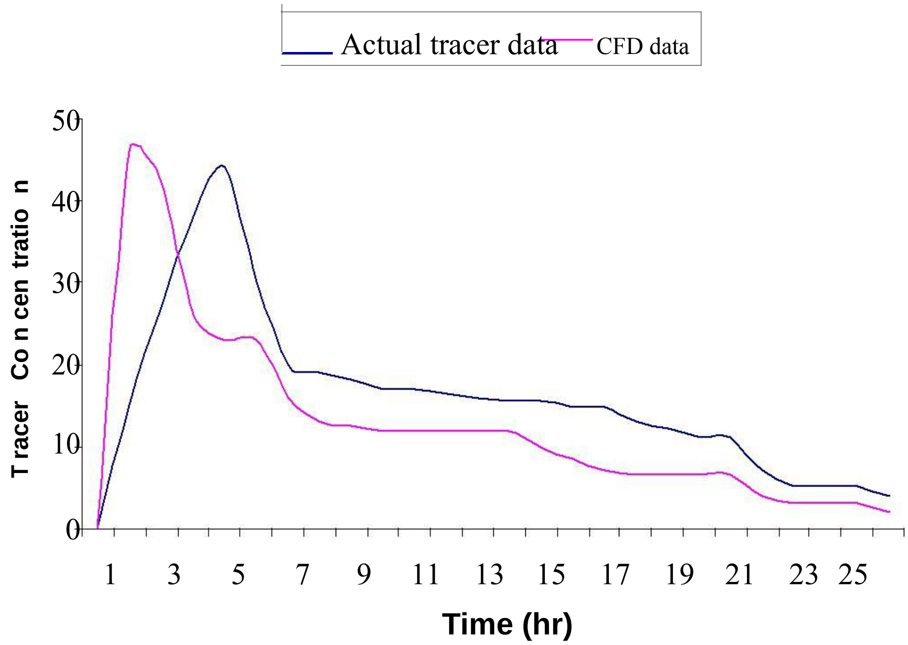

Figure 2. Comparison of CFD versus one typical tracer results.

Table 4. Summary of variables to obtain “d” using actual tracer study.

Function	Value	Function	Value
C_i	712.27	$\frac{t_i^2 C_i}{C_i} - \left(\frac{t_i C_i}{C_i}\right)^2$	2.1E+10
$C_i t_i$	4.9E+7	σ^2	2.1E+10
$t_i^2 C_i$	1.49E+13	σ_i^2	0.61
$\frac{t_i^2 C_i}{C_i}$	2.1E+10	d	0.6

* i = Different time steps.

can be seen in Table 5.

Comparing ‘d’ obtained using actual tracer study and the CFD modeling, it is confirmed CFD is a suitable option for calculating ‘d’. The dispersion coefficient was also calculated using empirical equations outlined previously (Table 6). Although, these empirical equations were a good predictor of dispersion coefficient in their own cases, they are not a comprehensive technique to obtain a dispersion coefficient. Some of these equations (e.g. Agunwamba et al., 1992) was claimed to be simple, accurate and economical in comparison to the use of actual tracer studies, however, there are serious limitations on using these equations for different actual modeling scenario. For the given WSP, the dispersion coefficient found by Arceivala (1981) has a better prediction of actual dispersion coefficient.

The result of finding dispersion coefficient using the CFD, predicts the actual dispersion coefficient better in this case. The use of CFD gives opportunity to consider various hydraulic parameters and their effect on dispersion coefficient. Fluctuations of hydraulic behavior and critical conditions of these fluctuations may be determined by using CFD. The effects of these fluctuations can be seen in obtaining dispersion coefficient as well.

CONCLUSION

The dispersion model is highly dependent on dispersion coefficient which itself is based on hydraulic performance of the WSP. The result of comparing CFD analysis with

Table 5. Summary of variables to obtain “d” using Fluent.

Function	Value	Function	Value
C_i	4457	$\left(\frac{t_i C_i}{C_i}\right)^2$	2.6E+10
$C_i t_i$	2.31E+08	σ^2	2.6E+10
$t_i^2 C_i$	1.27E+14	σ_i^2	0.75
$\frac{t_i^2 C_i}{C_i}$	2.84E+10	d	0.5

* i = Different time steps.

Table 6. Comparing different methods to obtain dispersion coefficient.

Methods	Calculated D	Difference from tracer
Actual tracer test	0.8	---
CFD based approach	0.67	0.13
Liu (1977)	2.18	1.38
Arceivala (1981)	0.58	0.22
Polprasert and Bhattarai (1985)	1.4	0.6
Nameche and Vasel (1998)	0.1	0.7

actual tracer test shows using CFD is a suitable option to determine the dispersion coefficient for use in dispersion model. The value of ’d’ found by using CFD for the WSP used as a case study is 0.5 which is approximately similar to the one found by actual tracer tests which was 0.6. Modeling the tracer using a methodology discussed in this paper (particle injection in CFD) can supplement the actual tracer studies, although, CFD analysis is case sensitive and ignoring the description of hydraulic conditions of the WSP entirely, leads to misleading results. Using CFD in turn reduces the frequency of actual tracer tests. Empirical equations are another option for finding the dispersion coefficient in the design stage. This research shows that the using of these equations for the specific case should be done precisely.

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