BIOKINETIC MODELLING OF A WSP IN COMBINATION WITH A RIGOROUS, YET SIMPLE MIXING MODEL

Andres Alvarado 1,2, Youri Amerlinck 2, Sreepriya Vedantam 2, Peter Goethals 3, Ingmar Nopens 2
1. DIUC, Universidad de Cuenca, Av. 12 de Abril s/n Cuenca, Ecuador, andres.alvarado@ucuenca.edu.ec
2. BIOMATH, Department of Mathematical Modelling, Statistics and Bio-informatics, Ghent University, Coupure links 653, B-9000 Gent, Belgium, Ingmar.Nopens@UGent.be
3. Department of Applied Ecology and Environmental Biology, Ghent University, Gent, Belgium

ABSTRACT
This contribution presents the first results obtained with a combined rigorous hydraulic-biokinetic model of the large scale Ucubamba Waste Stabilization Pond System (WSP) in Cuenca, Ecuador. A Compartmental Model (CM) approach for modelling the pond’s hydrodynamics is compared with tanks-in-series approach for both the RTD analysis and when coupled to ASM3 model extended for algal biomass processes. TIS model does not reproduce the measured mixing behaviour, whereas the CM model does it still at reasonably computational demand. Moreover, the outputs of the hydraulic models superimposed with biokinetics show drastic differences. Hence, a proper hydrodynamic model is required when modelling biokinetics in large WSPs for reliable results and useful for decision support.

INTRODUCTION
Waste Stabilization Ponds (WSPs) are well suited where land availability is not a concern; moreover the low O&M costs make this technology attractive in developing countries. Mathematical models have been used satisfactorily in conventional wastewater systems like activated sludge for a better process understanding and system optimisation. However, the difference in scale between WSP and conventional activated sludge is quite different. Indeed, WSP systems exhibit more complex hydrodynamic behaviour. This might have a huge impact and it can be questioned whether the traditional approach for modelling these systems is valid for WSPs.

Next to solving the advection-dispersion partial differential equation, the mixing behaviour in reactors has been classically modelled with two systemic approaches: the dispersion model and the tanks-in-series (TIS) model. However, the usefulness of dispersion model is questionable in systems where large backmixing occurs (Levenspiel, 1999). On the other hand, the TIS model has the advantage of being simple and not computationally demanding. Therefore, the TIS model has been commonly applied for modelling activated sludge wastewater treatment systems.

The complexity of the hydrodynamics in WSPs, which exhibits multiple recirculation patterns, stagnant zones, etc., cannot be accurately represented with TIS, which describes the fluid flow in only one direction and can only describe some back-mixing behaviour by artificially maintaining the liquid longer in the system through adjusting the backmixing rate (Le Moullec et al., 2010). The major issue with systemic models is that, when combined with a biokinetic model, the flaws in the mixing model will lead to a need to "calibrate" the degrees of freedom present in the biokinetic model. The latter will reduce the predictive power of the model and renders it useless in any subsequent optimization study.

The usefulness of CFD models as a tool for design improvement and hydrodynamics assessment in waste stabilization ponds has already been widely studied and is well reported in literature (Wood et al., 1998; Peterson et al., 2000; Salter et al., 2000; Shilton, 2000; Vega et al., 2003; Shilton and Mara, 2005; Sweeney et al., 2005). However, the number of studies regarding to CFD models validated against experimental data in full-scale systems is still limited (Shilton et al., 2008). It was concluded that the computational resources are the main constraint, especially if the ultimate objective of the modelling is the incorporation of biokinetic reactions.

In light of the above, an intermediate complexity alternative between TIS and full-fledged CFD are so-called compartmental models (CM) (Levenspiel, 1999). The CM generation from CFD turbulence analysis in a chemical reactor was first reported by Alexopoulos et al. (2002) and Alex et al. (2002). Later, several contributions at pilot-scale have been reported (Rigopoulos and Jones, 2003; Bezzo et al., 2004; Kougos and et al., 2005; Guha et al., 2006; Gresch et al., 2009; Vakili and Esfahany, 2009; Le Moullec et al., 2010). In these previous efforts, one can notice the strong influence of the physical system configuration on the respective methodology for deriving the CM. However, for the estimation of the recirculation flow rates between adjacent compartments, the common criterion used is that of the turbulent diffusion coefficient calculated based on the CFD simulation results.

(Alvarado et al., 2011) were the first to apply this methodology to a WSP. In that article the concept is proved on the maturation pond M1 of Ucubamba WSP system analysing the RTD curves from a
The objective of this paper is to assess the impact of using different hydraulic models on the behaviour of the biokinetic model proposed by Alex et al. (2000) with algal kinetics and processes. The latter model incorporates the typical processes occurring in WSPs. CM, TIS model and one Continuous Stirring Tank Reactor (CSTR) were tested in the Maturation M1 pond of the Ucubamba WSP.

METHODS

The Waste Stabilization Pond System

The Ucubamba WSP system, the largest wastewater facility in Ecuador, treats the domestic effluent of Cuenca city (the Ecuadorian third largest city; altitude of 2,560 m a.s.l.), having a population of 400,000 inhabitants (2010). The system is in operation since 1999 by the Municipal Enterprise ETAPA (Empresa Pública Municipal de Telecomunicaciones, Agua Potable, Alcantarillado y Saneamiento de Cuenca, Ecuador). The influent in the WSP system passes through screen bars and a grit chamber before being divided into two parallel lines (Figure 1). Each line includes an aerated lagoon (using mechanical floating aerators), a facultative and a maturation pond. The average discharge influent over 12 years of operation is 1.2 m$^3$ s$^{-1}$. The pond system covers 45 ha, having a total volume of 1 million m$^3$. The maturation pond M1 (Figure 1) where this study is performed is 7 ha large and 1.7 m deep. The inlet/outlet of the pond consists of a submerged pipe of 0.9 m diameter lying at the bottom of the pond and an overflow structure of 10 m length. The location of both structures is shown in Figure 1. Several bathymetries were conducted revealing that in the maturation pond only a thin sludge layer is formed; less than 1% over the total pond volume with a maximum thickness of 10 cm. On the basis of this the authors concluded that the influence of the sludge layer can be neglected for the hydraulic analysis of the pond. Some relevant treatment removal efficiencies are: BOD 79%; TSS 75% F.Colif. 99.92% (Durazno, 2009).

Tracer Study

In 2009, a tracer study was conducted for the maturation pond M1 during the coldest and driest season to prevent the impact of thermal stratification and to minimize the influence of rainfall on the variability of inflow effluent water. The fluorescent tracer Rhodamine WT was used in the stimulus-response technique. The fluorescence concentration in pond samples was measured using an Aquafluor™ Fluorometer (http://www.turnerdesigns.com). The measuring device has a minimum detection limit of 0.4 ppb. Water samples were collected using an ISCO Automatic Sampler model 6712 (http://www.isco.com). Sampling frequency was 15 minutes before the first peak of the tracer was observed, then gradually reduced to 60 minutes until 90% of the tracer was recovered, which was observed approximately after 30 days. The samples were analyzed at a fixed temperature (19°C), using a thermal bath when needed. The influence of natural fluorescence of algal biomass was investigated by measuring the background fluorescence concentration during several hours before the start of the test to prevent erroneous fluorescence readings (Valero and Mara, 2009). A more detailed description of the experimental procedure can be found in (Espinoza and Rengel, 2009).

CFD modelling

Three dimensional CFD simulations were performed on the maturation pond M1 (Figure 1) using the commercial software FLUENT v. 6.3 (ANSYS/FLUENT Inc., http://www.fluent.com). The finite volume method was selected dividing the computational domain into 75,000 quadratic grid elements. In order to account for the flow disturbances near the inlet and outlet structures and in the pond corners, where flow directions require accurate representation, a denser grid was applied in those regions of the maturation pond. Preliminary tests revealed that increasing the grid density in the remainder of the pond did not produce remarkable differences in the accuracy of the modeling results. Hence, in order to keep the computational cost at an acceptable level the grid size of 75,000 elements was maintained throughout all analyses, including the residence time distribution analysis. A detailed approach of the three-dimensional mass and momentum equations is available in (Alvarado et al., 2011).

The fluid in the pond is assumed to be incompressible and exhibiting the Newtonian fluid properties of water with a density of 998.2 kg m$^{-3}$ and a dynamic viscosity of 1.003 E-3 kg m$^{-1}$ s$^{-1}$. These values are realistic considering the concentration of suspended solids in the pond, which are in the order of 30 mg/l, a concentration that should not significantly affect fluid properties.
The turbulence in the pond was modeled using the standard k-ε model. The k-ε model is the most commonly used of all turbulence models and has been shown previously in literature to be functional for free-shear layer flows with relatively small pressure gradients.

A transient inlet velocity profile obtained from the pond system records was applied as an inlet boundary condition, which accordingly calculates the inlet turbulent boundary condition. The effect of wind and temperature gradients has been neglected. Additionally, in order to limit the computational expense, flow fields obtained at various vertical heights were compared, yielding nearly the same pattern. Therefore, it was decided to neglect the vertical diffusion, while building the compartmental model.

The tracer residence time distribution (RTD) analysis (Levenspiel, 1999) was performed by imposing a transient simulation of tracer as a scalar on the velocity and turbulent fields obtained from the flow simulation. The species transport model in FLUENT v. 6.3 was used for the determination of RTD, following the procedure described in Vedantam et al. (2006).

**Compartmental Model Generation**

A compartmental model comprises of a certain number of fully mixed volumes, which can be interconnected by means of exchange fluxes. In comparison with TIS, CM has more freedom to define compartments in more than one dimension. Once a clear picture of the velocity and turbulence pattern is calculated in a certain reactor, the next step is the determination of the exchange fluxes, which depends upon the flow variations and the identification of a number of tanks, approximately behaving as CSTRs, within the reactor. In this study, having the objective to introduce the biokinetics at a later stage into the integrated compartmental model, the decision of the number of fully mixed volumes had to be based upon the flow directions in the pond considering the minimum number of tanks able to represent adequately the flow profile.

From CFD results, and classifying iso-contours of velocities, the location of compartments could be identified based on the velocity fields, and could be connected with exchange fluxes. Since the WSPs behave as continuous flow systems, the flow direction in the compartments is selected based on the dominant spatial dimension, from the inlet to the outlet (Gresch et al., 2009). The exchange fluxes are determined based on the diffusion coefficient \( D_t \) (Guha et al., 2006; Le Moullec et al., 2010) evaluated from the turbulence characteristics of the flow \((k, \varepsilon)\) and the constant of the turbulence model \(C_\mu\). Hence, the exchange flux \( Q_r \) is calculated based on the cross-sectional area \( A \) and the distance between the centres of adjacent compartments \( \Delta x \),

\[
Q_r = \frac{D_t A}{\Delta x}
\]  

A detailed description of the procedure for compartmental model generation for the Maturation pond M1 in Ucubamba WSPs can be found in Alvarado et al. (2011).

**RTD and Coupled Models Assessment**

The hydraulic performance of the TIS model, the CM and the one CSTR was first analysed obtaining the RTD with a pulse of inert solution. For this purpose, the modelling and simulation software WEST (http://www.mikebydhi.com/) was used.

In order to prove the compartmental model concept, the distinct hydraulic models were coupled and tested with the biochemical model proposed by Alex et al. (2010). This was also done in WEST. In order to compare the behaviour of the biochemical parameters in the models under a real wastewater influent, the benchmarking influent composition and diurnal dynamics of BSM1 (Copp, 2002) were used in conjunction with the flow rate measured at the pond system, hereby respecting the incoming load to the system.

---

Figure 2. Velocity vectors and contour plot of velocity magnitude in the maturation pond M1 after 3 days of simulation.
RESULTS AND DISCUSSION

CFD analysis
Figure 2 shows the contour and vector velocities in the middle depth horizontal layer of the pond M1 obtained after 3 days of unsteady CFD simulation. The vectors have a clear dominant direction, illustrating the strong circular pattern of the flow around the pond. According to Figure 2 the flow mixing occurs in the region around the inlet. Despite the difference in depth location of inlet and outlet the variability of the velocity and turbulence horizontal profiles along the depth is minimal. The latter observation allowed the simplification of the model, neglecting the vertical diffusion. It is stressed that no meteorological boundary was accounted for in the model.

Compartmental model layout
As stated before, flow direction has been given utmost importance in order to divide the pond into compartments. This could also be generalized for systems with dominant flow directions. Thus, based on the analysis of the flow field, the computational domain is divided into 3 different zones (depicted in Figure 3).

Each zone depicted in Figure 3 is sub-divided into compartments of specific volume. The selection of zones is based on (1) dominant spatial dimension of flow from inlet to the outlet, leading to the first peak in the RTD curve obtained from CFD simulations and RTD study (Figure 4); (2) backward liquid flow occurring due to the lower velocity magnitudes and turbulent kinetic energy values; (3) recirculation zone, which could further be divided into two internal zones, based on the velocity vectors from flow field analysis (Figure 2).

Each zone was then subdivided in a number of compartments. In zone 1, the number of compartments was obtained from the CFD-RTD curve, assuming a plug flow defined under the first peak (Figure 2), allowing therefore a determination of the number of tanks as a function of the Peclet number:

$$2(n - 1) = Pe = \frac{u_{avg} \Delta x}{D_t}$$ (2)

Where $n$ is the number of tanks connected in series, along the major flow dimension and $u_{avg}$ is the average flow velocity along the zone. The required number of tanks in zone 1 using this approach was calculated to be 13.

In zone 3, the number of tanks remaining as low as possible for ease of computational load. Since each zone comprised of compartments connected as tanks-in-series, the division of compartments in zone 2 and 3 played a crucial role in evaluating the exchange flux. Thus, zones 2 and 3 were divided into compartments such that $\Delta x$ could be determined straightforward. Moreover, reduction in the number of tanks, in zone 2 and 3 did not influence the comparison of RTD curves with the tracer study.

The methodology summarised here, confines the choice of number of compartments to the computational expense that can be handled, since the next step in the modelling involves the inclusion of the biokinetic model in each of the compartments (note that adding 1 tank results in adding more than 100 equations to the overall model). With the aim of establishing the proof of concept, this compartmental model has been developed with 25 compartments (Figure 3).

RTD Analysis
Figure 4 shows the RTD for both the TIS and CM approaches along with the CFD simulation results and the tracer data. The differences among the models are substantial, where the CM yields the best match to both tracer and CFD simulation. The number of tanks in the TIS model ($n=29$) was calculated with equation 2, using the RTD-CFD curve, and adjusting the backmixing rate to 90% (the best adjustment to CFD curve according to Alvarado et al. (2011)). The RTD curve from a
single CSTR is totally out of any match with the previous approaches.

Figure 4. RTD from different hydraulic models in Maturation 1 pond.

**Coupling biological and hydrodynamic models assessment**

The biokinetic model used in this study was borrowed from (Alex et al., 2010). It combines the mixed bacterial ASM3 model and the algal processes, which include algal growth, decay and respiration; nutrient and light limitation on algal growth; and self-shading effects of algal biomass. The model also includes at this stage an artificial CO₂ addition to the influent to prevent process rate limitations (this needs further attention in future, but is not the focus of this paper).

Figure 5 includes the biomass output from CM, TIS and one CSTR over a period of 14 days using the dynamic BSM-based influent. Figure 5 (a) shows a drastic difference in the algal biomass concentration. The CM is able to keep the algae in the system although it seems to decrease over the whole period, but tends to level off towards the end of the dynamic simulation. In contrast, both the TIS and one CSTR models virtually washed out the algal biomass within 7 days. Considering the fact that the symbiotic process between the aerobic bacteria and algae population is the major characteristic of WSPs, this finding confirms the danger to use simple systemic models when modelling large WSP systems.

Figure 5 (b) shows the concentration of autotrophic and heterotrophic organisms. Both TIS and one CSTR behave similar keeping biomass concentrations of about 30% higher than that in CM models. It is noticed however, that in TIS and CSTR, the heterotrophic biomass is very sensitive to the influent changes, which is not the case in the compartmental model.

Figure 5. Biomass output from different hydraulic models in Maturation 1 pond: (a) algal biomass, (b) sludge biomass
Figure 6 shows the soluble substrate (SS) output from the different hydraulic approaches. Considering the average SS influent concentration of 70 g m\(^{-3}\), both systemic models behave very efficient to remove the SS. In practice, when using systemic models, this different behaviour could suggest the modeller to adjust biomass kinetics, and as consequence, to assign possibly erroneous kinetics to the organisms.

![Figure 6. Soluble substrate output from different hydraulic models in Maturation M1 pond](image)

### Computational expense

The fully coupled hydraulic and biokinetic model in the CM approach for 25 tanks, performs 14 days of unsteady simulation in 15 min, using the WEST software v3.7.6 in a Intel core 2 Duo CPU with 4.0 GB of installed RAM memory in 64-bit operation system. In contrast, the CFD simulations performed in Fluent v6.3 in a Intel Core 2 Quad CPU takes few weeks for simulation of the same period. New releases of the WEST software (already available) could certainly even improve the performance reported here. Hence, the CM approach seems promising to further investigate the pond system's performance by using optimisation approaches. Next to curing some flaws in the biokinetic model, this will be the next step in the research along with the full-scale calibration using dynamic data sets collected at the WSP.

### CONCLUSION

- The developed CFD model demonstrates its robustness and accuracy to describe the hydrodynamics of a full-scale WSP but at a high computational cost. The incorporation of biokinetic models would in that case be practically unfeasible.
- It is demonstrated that neither TIS model nor one CSTR are able to describe the mixing behavior in a large scale pond properly. In contrast, the CM is able to reasonably predict the pond’s mixing behavior at a very low computational demand, which makes the inclusion of a biokinetic model feasible.
- The impact of the mixing model on the behavior of a biokinetic model is illustrated. For the maturation M1 pond, both TIS model and one CSTR predicted very different behavior of biomass in comparison to the CM, especially for algal biomass which is washed out in both TIS and CSTR. Conclusions based on those models should not be trusted.

### ACKNOWLEDGMENT

This work has been supported by a grant from the VLIR-UOS (Flemish Inter-University Council-University Development Cooperation) Program and by ETAPA (Empresa Pública Municipal de Telecomunicaciones, Agua Potable, Alcantarillado y Saneamiento de Cuenca, Ecuador). The authors express their gratefulness to the ETAPA-DGA personnel, especially to Galo Durazno, Manager of the Ucubamba WSPs, and to Dr. Peter Aelterman for having contributed to the tracer experiment campaigns.

### REFERENCES


