MODELING AND SIMULATION OF REACTOR- SETTLER SYSTEM FOR WASTEWATER TREATMENT

M. Tarek Sorour
Sanitary Engineering Department, Faculty of Engineering,
Alexandria University, Alexandria, Egypt.

ABSTRACT

In spite of the tremendous effort has been done in the field of wastewater treatment modeling, surprisingly little attention has been given to the evaluation of these models against field data of full-scale plants. In this study a comprehensive model is proposed for wastewater treatment system by linking a biological reactor model to an advanced settler model. Modifications are made to the settler model to give more accurate predictions. The model is calibrated to reflect more closely the actual behavior of a large wastewater treatment plant. Computer simulation is used to investigate the model against the data of this large plant. Computer simulation shows good agreement between the model and the data, which supports the use of the model for both design and control purposes.

Keywords: Wastewater treatment, Modeling, Computer simulation.

INTRODUCTION

The primary objective of wastewater treatment is high quality treatment of large amounts of wastewater at low cost. Wastewater treatment plants consist of an assemblage of interdependent biological, physical, and chemical processes operating under time- varying hydraulic and organic load conditions. This is why the dominant problems of wastewater treatment have shifted from those of design and construction to those of plant operation.

From the standpoint of process operation, a wastewater treatment process has the following characteristics. First, all wastewater flowing into the plant must be treated. In addition, the quantity and quality of wastewater inflow cannot be adjusted. Wastewater treatment processes are subject to large disturbances such as influent flow rate, concentration, and composition. These variations and disturbances should be taken into account. Dynamic modeling, computer simulation, and modern control systems are valuable tools for use in both the design and operation of such dynamic systems.

The activated sludge process is recognized as the most common and major unit process for wastewater treatment. Its dynamical properties have been studied extensively during the last decade and several modeling studies have been presented and documented. The process comprises two units: a reactor basin, in which the degradation of pollutants is mediated by bacteria; and a settler, whose function is both to thicken the biomass for recycle to the reactor, and to clarify the treated effluent.

In fact, most of publications on dynamic models of the process are restricted to the subject of biochemical interactions in the mixed liquor of the reactor unit. Moreover, the potential of mechanistic models of biological wastewater treatment is not widely accepted, this might be due the fact, that the literature on mathematical models is not easy to read, is in many times not well structured and frequently does not provide the background which led to the development of the model.

One more problem is that, relatively little attention has been given to the evaluation of these models against field data. All these factors reduce the potential use of dynamical modeling techniques for design and control wastewater treatment plants.

In this paper an effort is made to represent a realistic example of using a comprehensive dynamical model to simulate an actual full scale treatment plant, aiming to evaluate the model against the actual data of this plant.

ELEMENTS OF THE MODEL

Deterministic mathematical models, as they are used here, describe biological wastewater treatment process based on material balance equations. These equations relate changes of the state of the system (concentrations) to transport and transformation processes, where transport process are characteristic for the design of a system (reactor configuration, distribution of influent, etc.). Transformation processes are governed by the local intensive conditions and involve the change of the components.

A deterministic model of a wastewater treatment system is therefore composed of at least the following elements:

- A list of components of interest
- A characterization of the transformation processes affecting these components
- A characterization of the flowscheme of the system, including final settler
- A characterization of internal transport and mixing.

Reactor Model

The biokinetic expressions are taken from the IAWQ model [1]. The model depicts 7 biochemical processes: aerobic heterotrophic growth, anoxic heterotrophic growth, aerobic autotrophic (nitrifier) growth, decay of heterotrophs, decay of autotrophs, hydrolysis of particulate organics, and ammonification of soluble organic nitrogen. There are a total of 13 process variables, including soluble and particulate inert organics (S_I and X_I), soluble and particulate degradable organics (S_s and X_s), heterotrophic and autotrophic biomass ($X_{B,H}$ and $X_{B,A}$), particulate products from biomass decay (X_p), nitrate plus nitrite nitrogen (S_{NO}), ammonia nitrogen (S_{NH}), soluble and particulate degradable organic nitrogen (S_{ND} and X_{ND}), dissolved oxygen (S_o). The first seven components are expressed in units of COD, the nitrogen species are expressed in terms of their nitrogen content, dissolved oxygen is expressed as negative COD. Detailed descriptions of the model biokinetic rate equations may be found elsewhere [2].

Settler Model

The model used in this study is based on the solid flux theory, as described by Kynch [3]. This theory says that the sedimentation velocity for suspension varies only with the initial concentration in the regime of hindered settling. Based on this postulate, an analysis of continuous sedimentation can be performed [4]. To conclude the mathematical description of sedimentation, it is necessary to propose a functional relationship between Vs and X. Several models can be found in literature, but in practice the exponential model of Vesilind [5] is most used [6].

$$V_s = \alpha \cdot e^{-n \cdot X} \qquad (1)$$

Where α a and n are constants and have to be calibrated for each sludge.

The dynamic approach is based mostly on the flux theory introduced above. The vertical cylinder is divided into horizontal layers. In each of those layers mass conservation has to be fulfilled. In discretized form, the time dependent difference equation for layer i reads:

$$\Delta Xi/\Delta t = 1/\Delta hi.[(Vs,i.Xi - Vs,i-1.Xi-1) + Vu(Xi - Xi-1)] \qquad (2)$$

where the left side represent the change of concentration ΔXi per time step Δt, and Δhi is the height of the respective layer. Special attention has to be paid to the settling flux Vs,i . Xi . Of course, the settling velocity depends not only on the local concentration Xi, but also on the condition given by the sludge below the observed cross section. Without additional conditions a sludge profile over the depth cannot be obtained. Two options can be found in literature:

- The settling flux out of layer i is bounded to the flux out of the lower layer i+1 [7], assuming that layers are numbered from top to bottom. The minimum flux min (Vs,i .Xi ; Vs,i+1 . Xi+1) of the two neighboring layers is to be respected, and consequently leads to the condition that the limiting flux is not exceeded.
- The settling flux is corrected by so-called W-function introduced by Hartel [8]. The W-function includes the effects of the transition

from hindered settling to compression and the zero settling velocity at the bottom.

Takacs et al. [9] aims to predict also the effluent quality. His model is based on a separate settling approach for low concentration regions or for small particles, whose settling velocities are overestimated by Eq 1. He suggested a double exponential function:

$$Vs = K_o.e^{-ca(X-Xi)}-K_o.e^{-cb\ (X-Xi)} \qquad (3)$$

where K_o; Xi; ca; and cb are parameters and must be calibrated for each sludge.

The novelty of this model is the fact that an expression is proposed for Vs which is valid for both the thickening and clarification zone. In the upper layers, Vs can be related to X through a double exponential function due to the operational constraints of the settler.The incoming flux in a certain layer is determined as the minimum of the flux in the layer just above and the flux in the layer itself. This approach is employed in our study.

Some soluble COD utilization occurs in the final settler. To incorporate its effect, each layer of the settler was modeled according to the IAWQ model [1], and was assumed to act as a single continuous stirred tank reactor.

While the reactor model deals with compounds mainly as COD, and the settler model generally based on suspended solids, there is a need to convert the COD compounds of the reactor to suspended solids concentration used in the settler. COD compounds and other compounds which contributes to the suspended solids concentration are converted to suspended solids by calculating the particulate fractions of COD, Hetrotrophic, and Autotrophic concentrations at every layer in the settler according to the IAWQ model. The summation gives the total suspended solids concentration which used in the mass balance equations to calculate the change in the suspended solids concentration in the layer.

For the soluble compounds which are coming from the reactor, the settler model is modified to predicted their concentration in each layer. Aerobic and anoxic growth of Hetrotrophs results in soluble COD removal, while hydrolysis of particulate COD produces soluble COD. The difference is the soluble COD removed in each layer. Aerobic growth of biomass also depends on the dissolved oxygen concentration, which is assumed to act as a complementary limiting nutrient through the adoption of a double Monod expression.

SIMULATION PROGRAM

Having described the individual model components in the previous sections (Reactor - Settler), now it is possible to put the pieces together for the development of the overall process model. For each unit of a wastewater treatment plant a mass balance is written for the concentration of each of the constituents (Xs, Ss, etc.) as follows:

$$V\ \frac{d}{dt}.C_{i,r}=S(Q_{in}.C_{i,in})-S(Q_{out}.C_{i,r})+V.R_i \qquad (4)$$

where

V = reactor volume (L^3)
$C_{i,r}$ = concentration of constituent i in the reactor (M/L^3)
Q_{in} = input flow rate into reactor (L^3/d)
$C_{i,in}$ = concentration of constituent i in the input flow to reactor (M/L^3)
Q_{out} = output flow rate from reactor (L^3/d)

This general model equation, which relates the biokinetic model and the system (transport) model is the mass balance equation written for any compound of interest. For the reactor model introduced above, the mass balance equations are a set of ordinary differential equations, which due to the process or transformation rates, are coupled and non linear.

A simulation program requires, that the stoichiometry, the kinetic, and the settling parameters are identified (model calibration). Moreover, the reactor system and the feed concentrations can be specified. Then the mass balances must be set up and means to solve these equations must be provided. For time varying conditions (dynamic) solutions may be obtained by numerical integration of the mass balances, for steady state the mass balances degenerate into non linear algebraic equations which may be solved, or alternatively the differential equations may be solved by relaxation. Integration or relaxation requires the choice of initial conditions.

The initial conditions can be obtained using one of the following methods:

- For many experiments, it is possible to obtain measured values for the initial values of all state variables, then it is possible to introduce these values directly into the simulation.
- Since the mass balance equations for steady state are algebraic equations, algebraic techniques may be used to obtain steady state solutions for the state variables, which can be introduced as initial conditions.
- For more complex reactor schemes it may be useful to find a steady state values for a simplified reactor scheme first and then to use this first steady state as initial condition for the differential mass balance equations, which may be solved with integration procedures in order to yield the steady state for complex flow schemes.

For this study the third method was applied. The overall model (Reactor - Settler) proposed in this study was simulated using the simulation language Simnon [10]. Simnon is a command driven simulation package that allows a high degree of interaction. Once a number of systems are connected to a plant configuration the system is ready for execution.

Parameters can be changed by commands, and the suitable initial conditions can be added. It also gives an option to read input variable values directly from a measurement file, which gives the user a powerful tool for model verification. Specific parameters for a given plant can be added in a separate file, that is called by a simple command before execution.

MODEL EVALUATION

In spite of the tremendous effort has been done in the field of wastewater treatment modeling , surprisingly little attention has been given to the evaluation of these models against field data.

In this study an attempt is made to evaluate the proposed comprehensive model against field data of a large full scale treatment plant.

Plant Case Study

In order to investigate the qualitative validity of the proposed model, it has been tested against full scale data from the Hamilton Water Pollution Control Plant(WPCP), this data is published and can be found in [11].

The Hamilton Water Pollution Control Plant is a major wastewater treatment plant with a technological line containing primary, biological, advanced and anaerobic processes. Figure (1) gives some details on the layout of the plant.

The Hamilton WPCP is designed to treat an average combined sewer flow of 410 000 m^3/d. The plant is also able to cope with an approximately 600 000 m^3/d short term stormwater flow which occurs quite frequently.

In order to keep the model executable within reasonable simulation time, the following 2 simplifications were applied to the complex layout:

- Simulating parallel technological units as one unit, with the combined volume and surface of the individual units.
- Omitting all technological processes not directly associated with the performance of the Reactor - Settler system (anaerobic digestion, incineration, etc.)

The data from three dynamic events were selected. The second one will be used to identify the model, while first and third events will serve as model verification tests:

Event#1: a small storm on with peak load of 409 000 m^3/d;

Event#2: a peak flow rate of 600 000 m^3/d;

Event#3: a hurricane "Hugo" downgraded to a tropical storm that hit Hamilton. The hydraulic load of the plant increased to 727000 m^3/d and bypassing had to be activated in order to prevent flooding of the plant. The maximum influent load to the plant was kept around 600 000 m^3/d.

Parameters Identification (Calibration)

The calibration of models can be done at various levels with various resources. A calibration is always based on results from experiment performed with the actual wastewater or the process layout to be studied. There is not a general method of calibration, which can be used in all cases. Calibration of models can be made at different complexity, based on the amount of data available and the planned use of the simulation results.

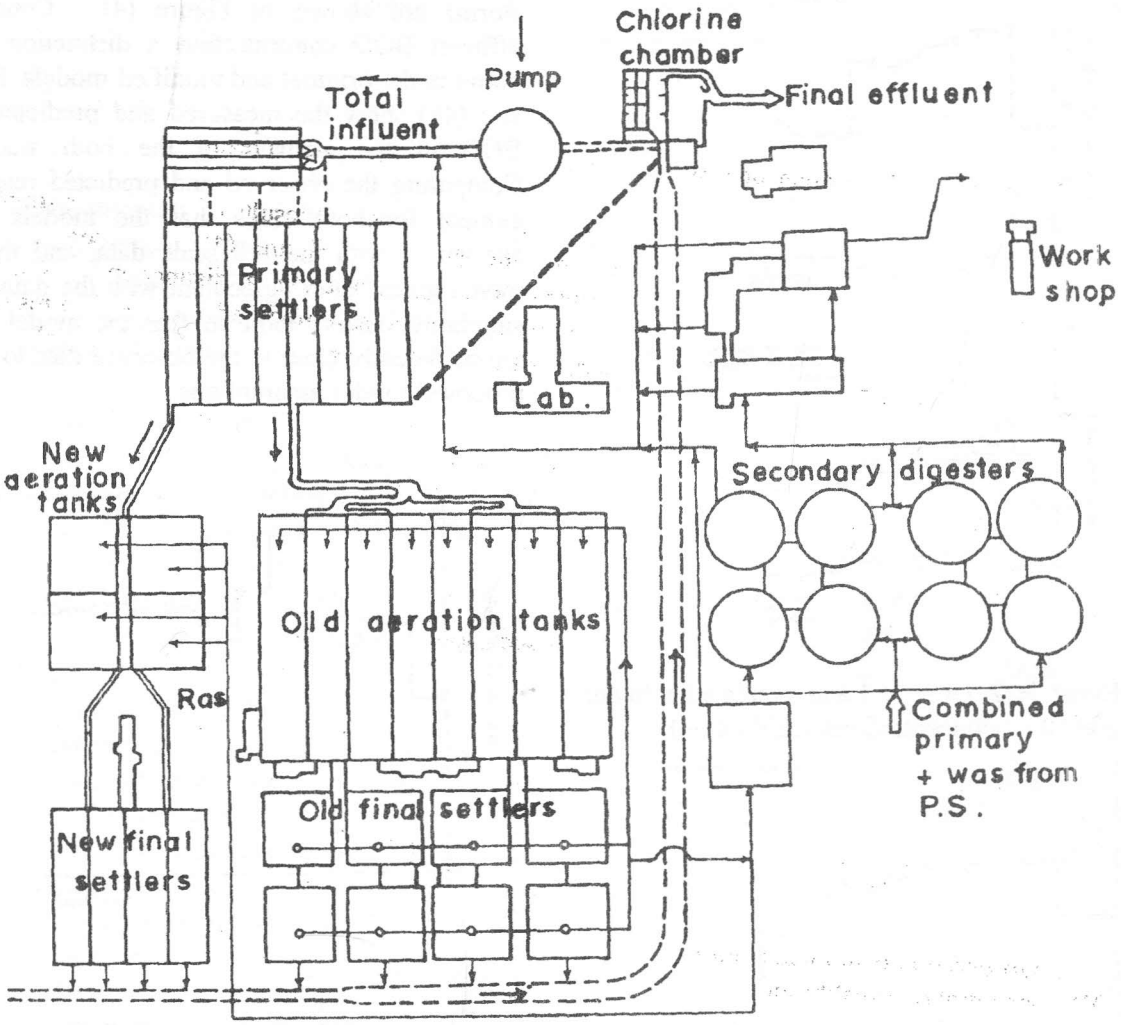

Figure 1. The layout of hamilton WPCP.

In this study where the model is dealing with biological activities, and therefore being confronted with the problem of limited and uncertain data, sophisticated numerical calibration methods may not be too well placed. The model was calibrated by varying some of the parameters to give the best fit with the data of event #2 which was selected as a database for dynamic calibration.

Default stoichiometric, kinetic and settling parameters available in the literature were incorporated. Table presents the final model key parameters. After having identified the parameters all simulation were performed without changing any of them for the same plant.

Figure (2a) shows the influent flow during event #2 and Figure (2b) the actual data points with the calibrated simulations of influent and effluent BOD. The model fit to the effluent BOD concentration is not accurate. This is natural, since the measurement inaccuracy is related to the absolute value of the concentration.

Model Verification

The comprehensive model (Reactor - Settler) was verified against the data of events #1 and #3. The analysis was focused on the effluent BOD concentration both before the final settler (original model) and after the settler (modified model). Results from event #1 are shown in Figure (3) and compared with the recorded observations. This event was a small and steady storm with peak flow of 409 000 m^3/day.

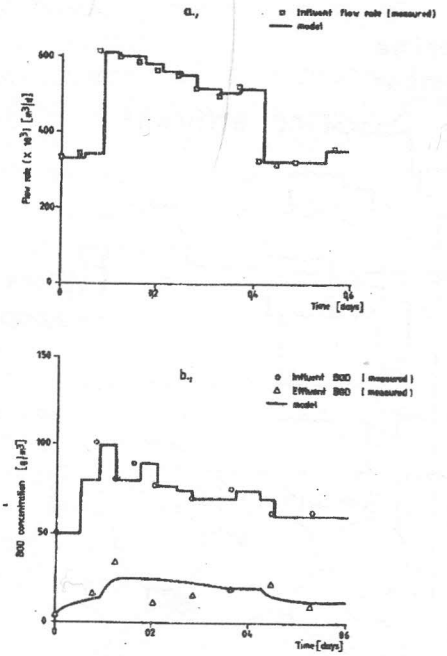

Figure 2. Event ≠ 2. Observed and simulated influent flow rate, and BOD concentrations (calibration).

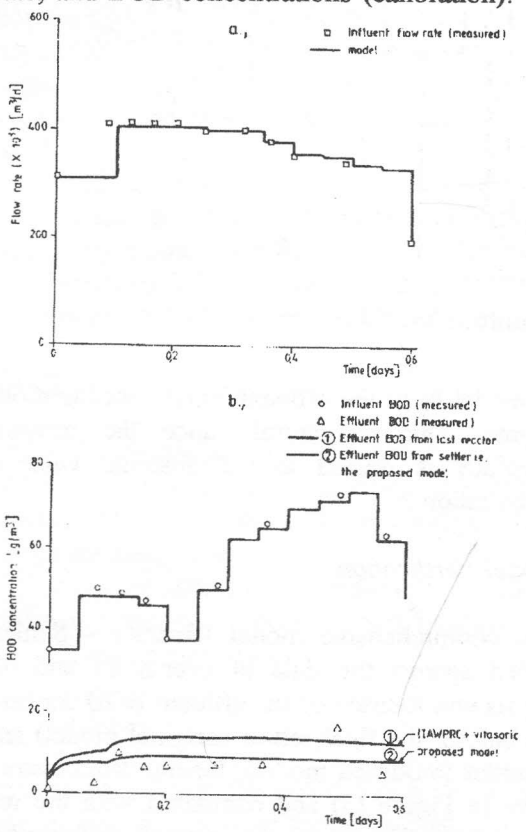

Figure 3. Event ≠ 1. Observed and simulated influent flow rate, and BOD concentrations.

Simulated and measured results of event #3 (a tropical storm) are shown in Figure (4). Concerning the effluent BOD concentration a distinction was made between the original and modified models. Figures (3b) and (4b) show the measured and predicted values of BOD in the effluent of the both studied cases. Comparing the observed and predicted responses it is evident for both cases that the models give good agreement with the full scale data, and the modified model gives better agreement with the data.In general, simulation results indicate that the model predictions are sufficiently close to the observed data to support the proposed model assumptions.

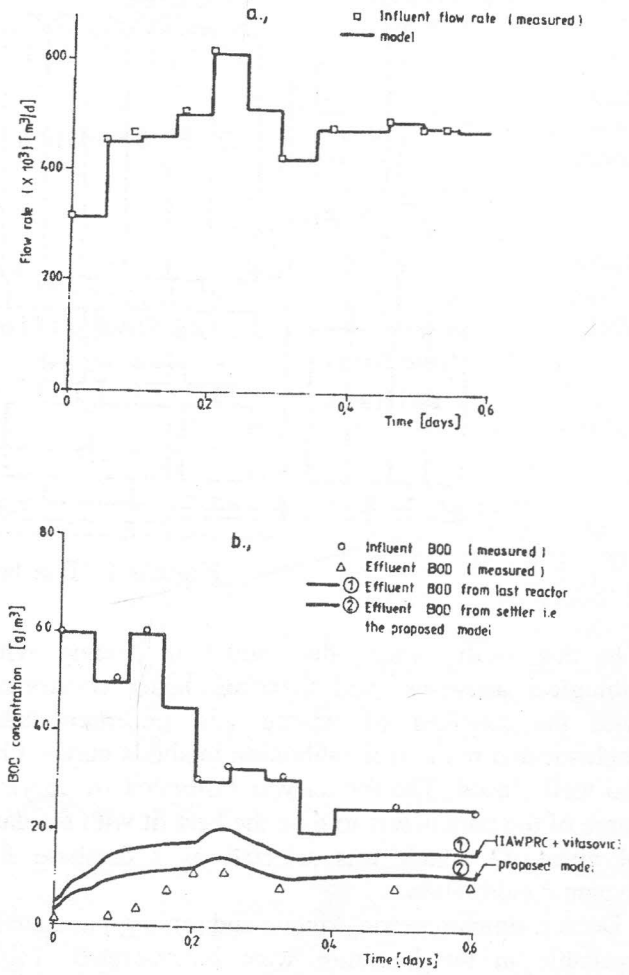

Figure 4. Event ≠ 3. Observed and simulated influent flow rate, and BOD concentrations.

Table 1. Model Calibrated Parameters.

Parameter	Symbol	Value	Unit
Stochiometric constants			
heterotrophic yield	Y_h	0.67	
autotrophic yield	Y_a	0.24	
unbiodegradable fraction of biomass	f_u	0.08	
COD/VSS ratio	icv	1.48	
VSS/TSS ratio	ivt	0.68	
Kinetic constants			
max. heterotrophic growth rate	μ_h	3.10	d^{-1}
saturation coefficient for S_s	k_s	20.00	$gCOD/m^3$
heterotrophic oxygen half saturation	k_{oh}	0.20	gO_2/m^3
nitrate half saturation	k_{no}	0.50	gN/m^3
anoxic growth factor	η_g	0.80	
max. autotrophic growth rate	μ_a	0.43	d^{-1}
autotrophic half saturation	k_{oa}	0.40	gO_2/m^3
heterotrophic decay	b_h	0.62	d^{-1}
autotrophic decay	b_a	0.12	d^{-1}
ammonification rate	k_a	0.08	$m^3(gCODd)^{-1}$
max. hydrolysis rate	k_h	3.00	d^{-1}
hydrolysis half saturation	k_x	0.03	
anoxic hydrolysis factor	η_h	0.40	
Settler parameters			
sludge blanket conc.	x_t	3000	g/m^3
floc settling parameter	c_a	0.00035	m^3/g
colloids settling parameter	c_b	0.0024	m^3/g
non- settleable fraction of susp. solids	f_{ns}	0.0015	
max. settling velocity	K_o	256	$m\ d^{-1}$

SUMMERY AND CONCLUSIONS

Generally, after a dynamic mathematical model has been developed for a process, the equations which comprise the model must be solved in order to predict the behavior of the process with respect to time. This procedure is known as simulation. Simulation is used to explore the effects of changing conditions on real system.

The major advantage of simulation is that time can be compressed on the computer in seconds or minutes. This is very important for the biological processes involved in wastewater treatment systems where rates are relatively slow and experiments may require weeks and even months.

As a matter of fact, a huge number of model are available for describing wastewater treatment systems.

However, little effort has been done in order to investigate the validity of these models against full scale data. In this study, a comprehensive model of Reactor - Settler system was adapted and verified against full scale data. Computer simulation has shown good agreement of the model with the data. For the investigated situations the model was able to predict the dynamic behavior of the plant.

According to the results of this study, the proposed

model is recommended to be used by engineers who are dealing with wastewater treatment plants. Simulation with the model would allow them to investigate several modifications and control strategies without jeopardizing the actual treatment plant. Consequently, the selected modification could be implemented safely.

REFERENCES

[1] IAWQ Task Group on Mathematical Modeling for Design and Operation of Biological Wastewater Treatment, "Activated Sludge Model No. 1", Scientific and Technical Report No. 1, London, 1987.

[2] W.W. Gujer and M. Henze,"Activated Sludge Modeling and Simulation", *Wat. Sci. Tech.*, vol. 23, pp. 1011-1023, 1991.

[3] G.J.Kynch,"A Theory on Sedimentation", *Trans., Faraday Society*, vol. 48, pp. 166-176, London, 1952.

[4] S. Marsili-Libelli,"Dynamic Modeling of the Sedimentation Process", *Civil Eng. Syst.*, vol. 10, pp.207-224, 1993.

[5] P.A. Vesilind,"The Influence of Stirring in the Thickening of Biological Sludge", Diss., University of North Carolina at Chapel Hill., 1968.

[6] M. Smollen and G. A. Ekama, "Comparison of Empirical Settling Velocity Equations in Flux Theory for Secondary Settling Tanks", *Wat. SA,* vol. 10, pp.175-184, 1984.

[7] G.G. Patry and I. Takacs,"Settling of Flocculent Suspension in Secondary Clarifiers", *Wat. Res.*, vol. 26(4), pp. 473-479, 1992.

[8] L. Hartel and H.J.Popel,"A Dynamic Secondary Clarifier Model Including Processes of Sludge Thickening", *Wat. Sci. Tech.*, vol.25(6), pp.267-284, 1992.

[9] I. Takacs, G.G. Patry and D. Nolasco,"A Dynamic Model of the Thicknening-Clarification Process", *Wat. Res.*, vol.25, pp.1263-1271, 1991.

[10] H. Elmqvist, K.J. Astrom, T. Schonthal and B. Wittenmark,"SIMNON User's Guide for M.S.DOS Computers", Dept. of Automatic Control, Lund Inst. of Technology, Lund, Sweden, 1990.

[11] I. Takacs, G.G. Patry and W.J. Snodgrass,"Hamilton Water Pollution Control Plant, Analysis of Plant Performance", Dept. of Civil Engineering and Engineering Mechanics, McMaster University, Hamilton, Ontario, Canada, 1991.