BioSys: software for wastewater treatment simulation

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Abstract

Modeling wastewater treatment parameters such as concentrations of components and particle size distribution of solid particles, viable biomass and dead biomass requires the simulation of several processes within various wastewater plant layouts. Although the software is not a specialized tool for the simulation of the UV disinfection unit, it predicts parameters critical for such purpose. Multi-purpose flexible software was thus developed with the ability to simulate several key processes used in the municipal and industrial wastewater treatment processes. A special feature is the ability of the software to predict particle size distribution at the clarifier–thickener unit outputs. A presented case study showed a simulation of the typical biological and settler processes usually located upstream of the UV disinfection unit.
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1. Introduction

Wastewater treatment is a widely used process for both residential and industrial purposes. Several wastewater and water treatment software tools are present in the market such as the ones by Hydromantics® Inc., Aspetech® Technology and many other companies. Such software tools provide vast capabilities for the modelling and optimization of batch and continuous processes. Some of them provide costing and sizing tools for engineers and workers in the field of water and wastewater treatments. Nevertheless, several important parameters critical for realistic simulation of different unit operations are sometimes simplified or neglected. An example is the simulation of critical parameters at the feed to the UV disinfection unit. It should be noted that the presented software is extremely limited when compared to the capabilities of the simulation platform of the above-mentioned commercial software and is not an equal alternative to them.

The objective behind developing the software is to accurately simulate *input* characteristics to the UV disinfection unit by simulating key upstream process without necessarily simulating the UV disinfection process itself. Simulating the biological reactor and the settler is the main focus of the software since they are the processes that control parameters such as concentration and particle size distribution of components usually present in waste-water treatment plants. The reader is advised not to assume that the work presented is concerned about simulating the UV disinfection unit.

2. Applications

BioSys is multi-purpose personal computer-based software for the simulation and modelling of municipal and industrial wastewater treatment plants. The software is useful for optimizing and improving new facilities and existing plants using simulation. Also, special capabilities are provided by BioSys for the simulation of UV disinfection unit.

Several factors affect UV disinfection operation including the particle size distribution and concentrations of microorganisms and solid particles, the ultraviolet transmittance (UVT) of water, the concentration of soluble material and the input flow rate. Predicting the sensitivity of these factors to changes in flow rate and substrate concentration (COD and BOD) at the plant feed is not an easy task. The conditions of the feed of wastewater treatment plants continuously change within the day and

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Nomenclature

a	ratio of cell surface area to cell volume (length^{-1})
A	cross sectional area (length^2)
C	concentration (mass/length^3)
F	flux function (mass length^{-2} time^{-1})
I	UV intensity (power/length^2)
I_{eff}	UV effective intensity (power/length^2)
j	jth reactant.
K	constant
k	inactivation rate coefficient (length^2 power^{-1} time^{-1})
k_d	the death rate (time^{-1})
K_i	inhibition constant
k_L	mass transfer coefficient (length/time)
K_s	monod constant (mass/length^3)
k_p	product inhibition constant
l	dead biomass concentration (mass/length^3)
l_i	input dead biomass concentration (mass/ lenght^3)
l_o	output dead biomass concentration, (mass/lenght^3)
m	number of substrates consuming a microorganism type (unitless)
M	maintenance coefficient (time^{-1})
n	number of microoganisms types consuming a substrate (unitless)
N	number of microorganisms (unitless)
N_D	initial number of non-shielded microorganisms (unitless)
$N_{D,t}$	current number of non-shielded microorganisms (unitless)
N_p	initial number of shielded microorganisms (unitless)
$N_{p,t}$	current number of shielded microorganisms (unitless)
P	parameter with different definitions (unitless)
Q	flow rate (length^3/time)
r	reaction rate (mass/time)
s	source (feed) function
S_i	input substrate concentration (mass/length^3)
S_o	output substrate concentration (mass/length^3)
t	time (time)
V	volume (length^3)
$Y_{x/y}$	yield of biomass to substrate (unitless)
X	viable biomass concentration (mass/length^3)
X_i	input viable biomass concentration (mass/length^3)
X_o	output viable biomass concentration, (mass/length^3)
z	depth or length (length)
μ	specific growth rate (time^{-1})
μ_{max}	maximum growth rate (time^{-1})
μ'	specific growth rate (time^{-1})
δ	delta function
Δt	small time step change (time)
ρ_{cell}	cell density (mass/length^3)

from one day to another. In addition, wet weather has a tremendous unpredicted effect on the feed conditions. The problem is further exacerbated by the presence of different plant layouts, control strategies, waste feed quality and high load handling strategies.

Due to the complexity presented above, it is a wide practice by UV disinfection industry to over-design the UV disinfection unit to ensure efficient UV kill dose at any case scenario. BioSys prediction of the factors mentioned above would provide a significant tool for the design and optimization of the UV disinfection units.

BioSys is also useful for selecting the best plant layouts and design alternatives, evaluating several feed scenarios, predicting the effect of adding or removing a unit for maintenance, predicting the effect of rainfall conditions, controlling mass balances and evaluating new designs.

3. Software design

The software is built on hierarchical classes. Classes of properties, reactions, settling velocity models and processes embody the basic code segments on which the software performs the calculations. Collection classes were developed as holders for these basic classes. Such design allows greater extendibility of the software to include more

reactions, processes and properties with less load and time in programming.

4. Flow sheet

It was part of our strategy to develop an easy to use user interface that would allow flexibility in setting up the process layout. But in order to start using the flow sheet, a property package that includes the selected components, their properties and the reactions sets should be created.

4.1. Property package

The first dialog that appears when BioSys is launched is the property package dialog in which the user creates and selects components that will be used in the simulation. If the user intends to use operations that require solid particles density and particle size information such as in the case of the settler, then the user should define the values of these properties. If the user wants to simulate certain reactions, then reaction sets should be created. After defining all necessary information, one can enter the simulation environment. It is also possible to go back any time to the property package dialog to change, remove, or add any compounds, properties, or reaction sets.
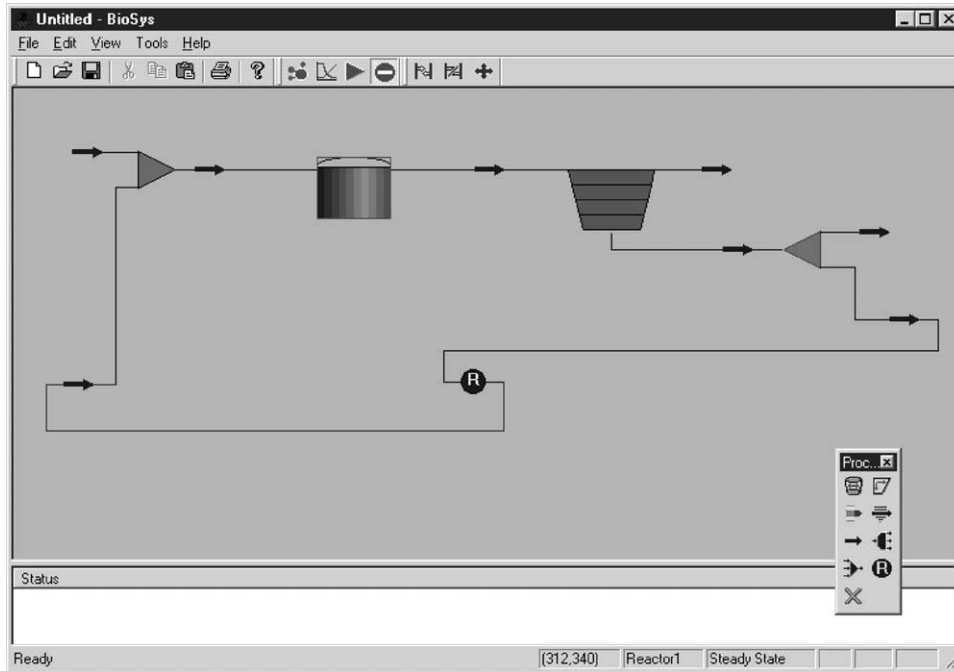
Fig. 1. Typical activated sludge layout simulated in BioSys.

When creating components from the property package dialog, the user is asked to select a phase. Inert and particulate solids could be defined in BioSys by creating a component and selecting 'solid' as the phase. Solid phase is also used to represent dead biomass. Viable biomass is defined using the 'viable' phase. Soluble material including soluble substrate is declared using the 'soluble' phase. Particulate substrate is not supported in BioSys, but would be considered for future development of the software.

Conversion of typical biological units such as COD and BOD to regular mass per volume units is not supported by BioSys. The user has to convert such values to regular mass per volume units before inputting them to BioSys. Future development of the software would include using default conversion factors to automate the calculations and allowing the user to overwrite them.

4.2. Process flow sheet

BioSys provides a flexible flow sheet where the user simply adds graphical icons that represent the processes at any location and with any frequency. A flexible simulation tool is necessary because of the different unit operations and

plant layouts used across the world. The process icons are connected through material streams as shown in Fig. 1. The software can handle simulation of multi-inputs to the plant and multi-parallel processes.

Fig. 2 shows currently supported processes in BioSys. Selecting a process from the shown Process toolbar and clicking on the flow sheet would add the process at the clicked location. Also, selecting a process from the flow sheet and clicking the delete command in the Process toolbar would delete the process and disconnect any attached streams. Connecting, disconnecting, or moving processes around are done easily using the process flow diagram (PFD) toolbar shown in Fig. 3. Double clicking any of the process icons on the flow sheet launches a dialog that represents the unit operation clicked such as the one shown in Fig. 4. The user can easily add specifications and observe calculated properties using that dialog.

4.3. Simulation environment

BioSys provides three simulation modes: steady state, dynamic and batch modes. Steady state and dynamic modes are fully supported for all process. Batch mode is limited to
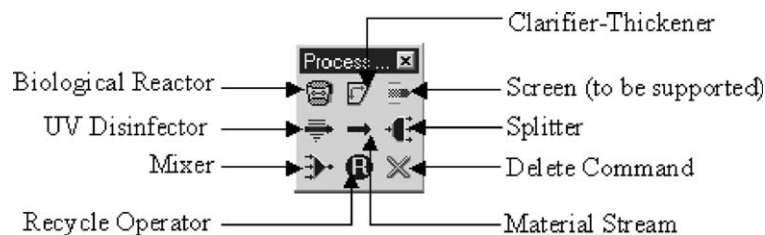

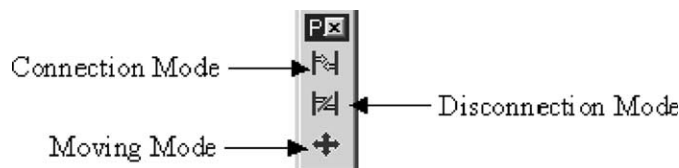Fig. 2. Process toolbar: currently supported unit operations.
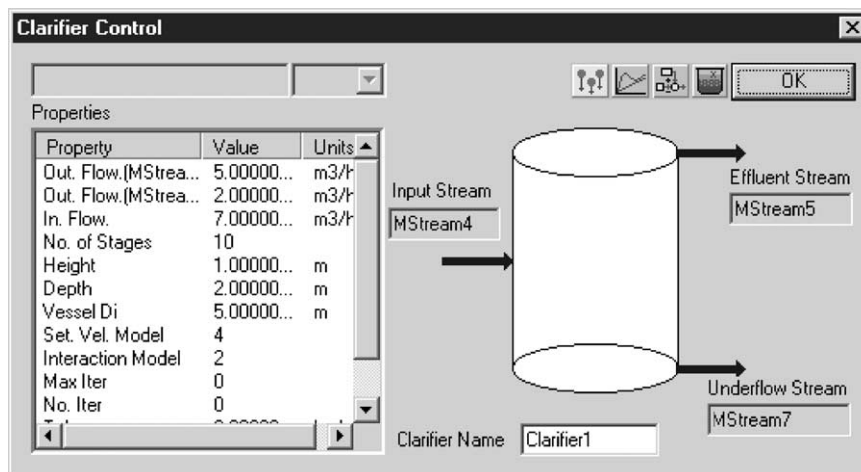
Fig. 3. PFD toolbar.

Fig. 4. Clarifier dialog launched when the clarifier graphical icon is double clicked.

the reactor, clarifier–thickener, and mixer units. In addition, BioSys allows the user to simulate dynamic and batch modes in real time or 'run and observe' mode. Real time mode makes the whole simulation interactive, enables fast feedback, and allows the user to change conditions and see their impact on the process directly. On the other hand, run and observe mode is faster and useful when the user wants to collect detailed data for later analysis.

The change of calculated values with time could be observed and saved through three means provided by the Results Dialog. In the dialog box, the user can specify which properties are to be observed. Then, the user can create a text file, a Microsoft Excel sheet or a Microsoft Excel chart.

To use the last two options, the user should have the corresponding Microsoft Excel COM objects, which is usually supplied with the Microsoft Office package, registered on the computer. Fig. 5 shows an example of the use of COM objects result charts. It should be also noted, as described earlier, that double clicking any process graphical icon launches a dialog related to the selected (clicked) process. In that dialog, all necessary information should be added and all calculated properties could be observed.

The simulation starts from the material stream that is not connected to a source and is connected to a target. An exception is when the source of the stream is a recycle
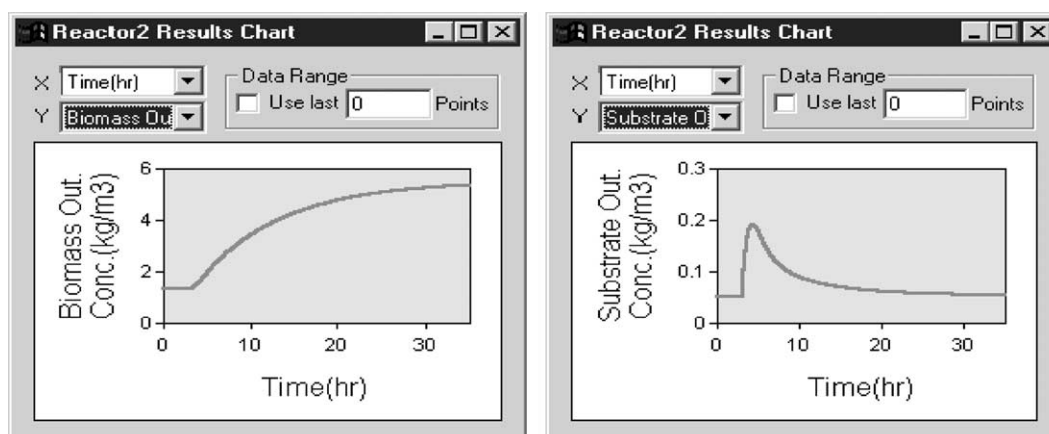

Fig. 5. Example of microsoft chart COM objects: the impact of a step change of BOD substrate input to a biological reactor. Left, change of viable biomass output concentration with time. Right, change of BOD substrate output concentration with time.

logical operator, where the simulation starts from there as well. The simulation does not start from an intermediate stream between two processes. An example is shown in Fig. 1, which illustrates the activated sludge process. The simulation starts from the feed at the top-left corner of the flow sheet. Note that the feed is connected to a target but is not connected to a source, thus it will be the first to be activated/solved. The simulation then proceeds to the mixer (combiner) symbolized by a triangle with many inputs and one output. The mixer will not solve until all input streams have been activated. Only one input stream to the mixer has been activated up to this point, which is the feed stream. The software then looks for other feeds or starting points. The software resumes the simulation from the left-bottom corner stream, for which the source is a recycle operator symbolized by a blue circle with an 'R' inside it. The two inputs to the mixer are now activated allowing it to solve and continue to the reactor then the clarifier and finally the splitter. The recycle operator checks if the source and the target streams connected to it have the same flows and compositions. If not it will copy the source information to the target and restart the simulation through the mixer until equality is achieved. The recycle operator is not a real process but a logical one required by necessities of simulation.

5. Theoretical background

BioSys supports several processes used in standard municipal wastewater treatment plants. Also, processes and calculations related to industrial applications could be added in the future. The unit operations currently supported by BioSys are biological reactors, UV disinfection units, settlers, mixers, splitters, material streams, and recycle logical operators.

5.1. Biological reactors

Biological reactors are currently simulated assuming an excess availability of oxygen and a well-mixed culture. The general mass balances on substrate and biomass components are used in the simulation along with the regular biological reaction models mentioned in Section 5.2. It should be mentioned that applying other sophisticated biological models like the ASM1 [1] and ASM2 [2] are considered for future development of the software. The models provide sophisticated modelling of the activated sludge process including the quality of the materials classified into biological components. On the other hand, the simplified models used in BioSys are still widely known and used for their ability to model a biological system. The simplified models might not predict the product quality accurately and do not have capabilities of simulating extremely non-ideal processes, but they can model typical biological systems with satisfactory or even accurate results.

The choice of the model depends on the user's desired degree of sophistication, simulation objectives and the suitability of the model to the system investigated, which would be determined by the user on a system-by-system basis. An example is the well-known Monod equation that its simplicity does not undermine its capability to simulate the biological reactor. The terms of the Monod equation, which are determined experimentally, make the model fit the system investigated.

The user is allowed to have multiple reactions in one vessel, though caution should be exercised for the validity of the reaction rate equations in the investigated system. Regardless of the applicability or limitations of these reaction rates, the user can declare that a substrate is consumed by more than one type of microorganisms. On the other hand, the user can specify that a single microorganism would consume more than one type of substrate. Different reaction rates and reaction equations could be used simultaneously. All these capabilities are allowed to provide a wide range of applications. This is achieved by using additive non-competent kinetics for the calculations [3]. The following are the substrate, viable biomass and dead biomass material balances for a well-mixed system with excess oxygen.

$$V\frac{dS_o}{dt} = QS_i - QS_o + V\sum_{j=1}^{n} \frac{X_{o,j}}{Y_{s/x,j}^m} \mu_j \tag{1}$$

$$V\frac{dX_o}{dt} = QX_i - QX_o + VX_o\left(\sum_{j=1}^{m} \mu_j - \frac{1}{m}\sum_{j=1}^{m} k_{d,j}\right) \tag{2}$$

$$V\frac{dl_o}{dt} = Ql_i - Ql_o + VX_o\frac{1}{m}\sum_{j=1}^{m} k_{d,j} \tag{3}$$

where V is volume of the reactor, Q is the flow rate, S_o is the output substrate concentration, S_i is the input substrate concentration, X_o is the output viable biomass concentration, X_i is the input viable biomass concentration, l_o is the output dead biomass concentration, l_i is the input dead biomass concentration, μ is the specific growth rate, $Y_{x/y}$ is the yield, k_d is the death rate constant, j is the jth reactant, n is the number of microorganism types that consume a certain substrate and m is the number of substrates consumed by a certain microorganism. Mass balance equations are simulated simultaneously to describe the dynamic behaviour of the aeration tank using the fourth order Runge–Kutta numerical method. The user is allowed to choose between two methods to obtain the steady state solutions: the Newton–Raphson method for non-linear set of equations or the Runge–Kutta fifth order method with adaptive step size determined using error criteria. As the error increases, the step size decreases and the opposite is true. The error is determined by taking the difference between the fourth order and the fifth order Runge–Kutta methods.

5.2. Biological reaction equations

Several models can be used to describe the specific growth rate μ, which is a function of substrate concentration. Currently BioSys supports several models described by Blanch and Clark [3] such as the Monod equation, Moser model, Konak relationship, Tiessier equation, and several inhibition models. Fig. 6 shows the reaction control dialog box, where the user can create reaction sets and specify their parameters and reactants.

BioSys also supports substrate inhibition models of the Monod equation reported by Blanch and Clark [3] including competitive inhibition, uncompetitive inhibition and the allosteric inhibition. Product inhibition is also supported for all growth equations through the common exponential inhibition and the non-competitive inhibition models, which are usually used for such purposes. The exponential product inhibition model is described as follows

$$\mu = \mu' e^{-k_p X} \tag{4}$$

where k_p is the product inhibition constant and μ' is the specific growth rate calculated using one of the above equations. The non-competitive product inhibition equation is described as follows

$$\mu = \mu' \frac{k_p}{k_p + X} \tag{5}$$

Another model supported by BioSys is the combination of the Monod equation with mass transfer calculations of substrate from the bulk medium to the surface of cell. The model is useful in the case when diffusion rate limits the reaction rate or mixing imperfection should be considered.

$$\mu = \mu_{max} \frac{S}{K_s + S + \frac{\mu_{max} \rho_{cell}}{k_L a Y_{x/s}}} \tag{6}$$

where ρ_{cell} is the cell density, a is the ratio of cell surface area to cell volume and k_L is the mass transfer coefficient.

5.3. Settler and settling velocity

Modelling a settler is one of the most challenging mathematical problems in the wastewater treatment simulation. In general, two and three-dimensional models are available in literature, but it was difficult to verify these models experimentally. Such models are time-consuming and require several days of simulation time.

One-dimensional models have proven to provide a better alternative in terms of reasonable output predictions and relatively faster computation. One-dimensional models assume a one-dimensional behaviour along the height of the clarifier–thickener unit. They are described by the following partial differential equation [4].

$$\frac{\partial C(z,t)}{\partial t} + \frac{\partial}{\partial z}[F(C(z,t),z)] = s(t)\delta(z) \tag{7}$$

where z denotes the settler depth, t is the time, F is the flux function, s is the source (feed) function, and δ is the Delta function and C is the concentration. The flux is a function of concentration, fluid velocity and settling velocity. Eq. (7) is solved using specialized finite difference methods that divide the thickener into equal distance intervals. The main challenge that these methods resolve is the discontinuities
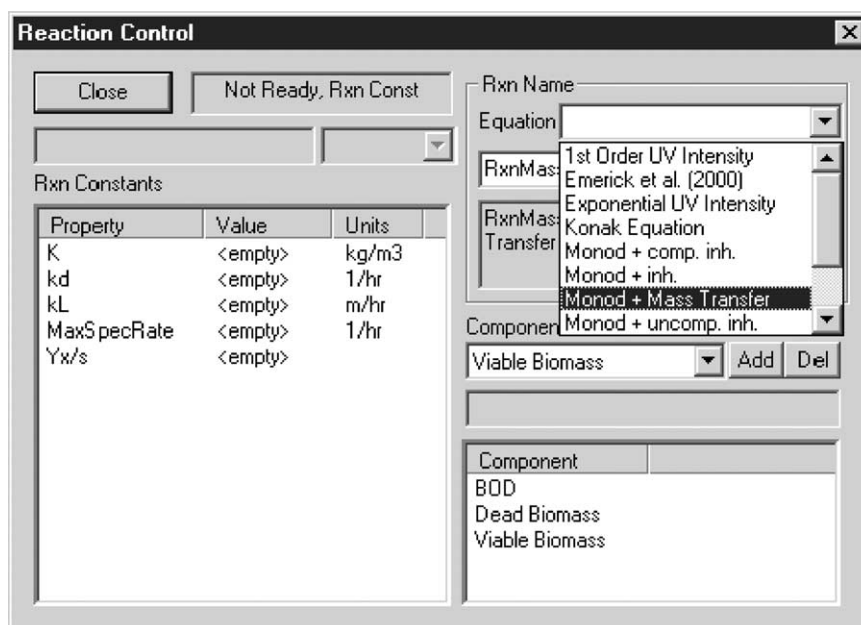

Fig. 6. Reaction control dialog box: the user can specify the reactions and their parameters.

that arise from the interaction of characteristic lines due to the non-linearity of the flux curve. The powerful classical Godunov numerical method was used in our simulation to address this challenge. At discontinuities of input and outputs, a mathematical condition developed by Diehl [5,6] picks up the stable points of the flux function, which gives uniqueness to Eq. (7) at these locations.

Zeidan et al. [7] developed a numerical procedure to apply Godunov and Diehl work to multi-particle suspensions using hydrodynamic and particle–particle interaction settling velocity equations. The work by Diehl and most other researchers was based on simulating the settler using flux-based settling velocity models, which require experimentally determined parameters. Our approach differed in that we used hydrodynamic-based settling velocity models, which predicted the settling velocity using particles and fluid properties such as the particle size, solid particles density, fluid viscosity, fluid density and hydrodynamic effects. These settling velocity models along with Zeidan et al. [7] procedure were found to be useful in determining the effluent concentration and particle size distribution. The flux-based settling velocity models provide a more accurate settling flux curve, but generally speaking, they cannot be used to predict effluent concentration with particle size distribution.

The steady state solution is obtained using criteria presented by Diehl [8]. Diehl used typical flux curve charts and the feed input conditions to predict the outputs and interior concentration profile of the settler. Our simulation required the use of flux curves that continuously change because of the change of particle size distribution inside the settler and at the feed. In order to adapt the steady state solutions to our changing flux curves, an iterative procedure was used. The flux curve of the feed is used to construct initial estimate of steady state solution. Then the flux of a stage that contains a concentration profile or blanket under the feed point is used to construct another better estimate of steady state solution. The re-construction of steady state solution using the interior concentration is repeated until the mass balance between outputs and inputs converges. The solution

is an approximation and requires further refinement and investigation as discussed by Zeidan et al. [7].

BioSys currently supports a wide range of settling velocity models and concepts by Richardson and Zaki (1954) [9], Garside and Al-Dibouni [10], Barnea and Mizrahi [11], Smith [12], Dallavale (1948), Lockett and Al-Habbooby [13], Mirza and Richardson [14], Masliyah [15], Selim et al. [16], Patwhardan and Tien [17], Zimmels [17] and Williams and Amarasinghe [18]. Critical review of these models as well as other hydrodynamic and flux-based models is available in the article by Zeidan et al. [19].

Another feature by BioSys is the Settling Predictor Utility through which the user can observe the change of settling velocity and flux with concentration of a single particle type in a suspension. The utility is useful for observing which particles will settle and which will not at a certain superficial velocity. The utility could be used for comparing settling models predictions with experimental data, which will allow the user to select the best model for the simulation. It could also be useful for design and gaining further insight about the suspension under investigation. Fig. 7 shows an example of flux curves simulated using the Settling Predictor Utility.

5.4. UV disinfection unit

The user can define multiple equations for UV disinfection reactions. The reaction vessel is simulated as a plug flow reactor

$$\frac{\partial X}{\partial t} = \frac{Q}{A} \frac{\partial X}{\partial z} + r \tag{8}$$

$$\frac{\partial l}{\partial t} = \frac{Q}{A} \frac{\partial l}{\partial z} + k_d \tag{9}$$

where X is the viable biomass concentration, l is the dead biomass concentration, Q is the flow rate, A is the cross sectional area of the tubular reactor, z is the length of the reactor and r is the reaction rate. The UV PFR is divided into completely mixed sections and simulated
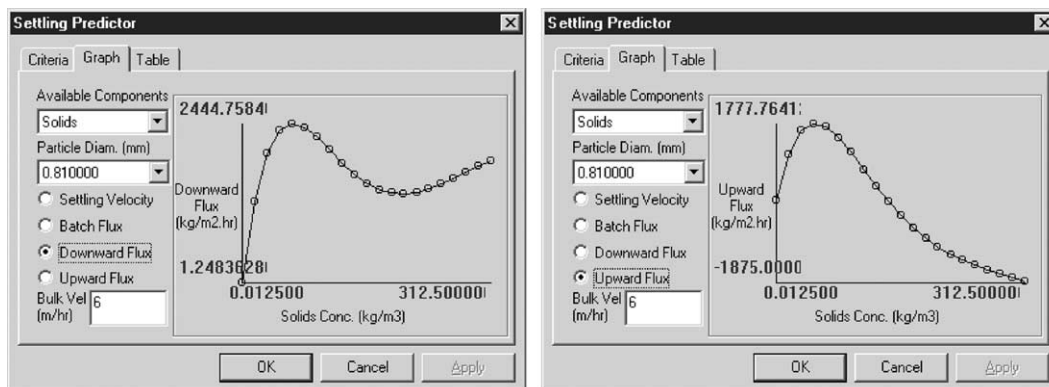

Fig. 7. Settling predictor utility: flux curves of a particle (diameter: 0.81 mm) within a suspension of solid particles in a liquid medium with a bulk velocity of 6 m/h. Left, downward flux. Right, upward flux.

using the Runge–Kutta method. The reaction rate equations and their parameters should be defined in the property package dialog box. The UV intensity is specified directly in the UV unit dialog box. Currently, the following reaction rate equation by Emerick et al. [20] is used, but other models will be added later

$$N(t) = N_{D}e^{-kIt} + N_p \frac{(1 - e^{-kIt})}{kIt} \tag{10}$$

where $N(t)$ is the number of viable microorganisms, N_D is the initial number of non-shielded microorganisms, N_p is the initial number of shielded microorganisms, I is the UV intensity, k is the inactivation rate coefficient and t is time. The reaction rate at continuous mode is evaluated by taking a small step change of time. Thus, the equation is modified as follows.

$$\frac{dN}{dt} = N_{D,t}e^{-kI\Delta t} + N_{p,t} \frac{(1 - e^{-kI\Delta t})}{kI\Delta t} \tag{11}$$

where Δt is a very small step change, $N_{D,t}$ is the current number of non-shielded microorganisms and $N_{p,t}$ is the current number of shielded microorganisms. The number of microorganisms was obtained from the user-specified viable biomass concentration in units of (mass/length^3) using the following basic relationship

$$N = \frac{XQ}{\frac{4}{3}\pi\left(\frac{d}{2}\right)^3 \rho_S}$$

where X is the biomass concentration, Q is the flow rate, d is the microorganism diameter, and N is the number of microorganisms. The UV transmittance in the liquid medium is taken into account by using exponential relationship to relate substrate and dissolved material concentrations to effective UV transmittance

$$I_{eff} = Ie^{KS} \tag{12}$$

where I_{eff} is the effective UV intensity, I is the normal UV intensity specified by the user, K is a constant and S is the substrate and dissolved material concentration. The effective UV intensity is then used in place of I in Eq. (11).

5.5. Mixer

The mixer works both as a mixer vessel (if a volume is specified) and a combiner of two or more material streams. The mixer unit operation can handle up to 10 streams and produces one output. The mixer vessel uses the basic material balance. If the user does not specify the volume of the vessel or if the volume is set to zero, then BioSys treats the unit as a combiner rather than a mixer. The fourth order Runge–Kutta numerical method is used to simulate the mixer dynamic behaviour

$$V\frac{dS_o}{dt} = QS_i - QS_o \tag{13}$$

5.6. Splitter

The splitter generally splits a stream into more than one output stream. Currently, the splitter handles up to 10 material streams. The outputs would have the same compositions of the input but each output would have a fraction of the total flow rate. The user is given the option of specifying all flow rates of exiting streams except one stream or specifying the split ratios between streams. Both options solve the splitter with different implication. Specifying the outputs flow rates means that only the non-specified stream will be calculated and affected by changes in the feed flow rate. On the other hand, specifying split ratios means that calculations are done to all output streams. Thus, a change of feed flow rate forces all streams to be recalculated based on the specified ratios.

5.7. Recycle logical operator

The recycle logical operator checks if its input and output match each other in composition and flow rate within a certain tolerance and a maximum iteration supplied by the user. It is always a good idea to start the simulation without any recycling. Then the recycle should be added along with the recycle logical operator. As mentioned earlier and as shown in Fig. 1, the recycle operator allows the simulation to run continuously until input and output streams to the operator match, which indicates that a steady state is reached. If not, the recycle operator copies data from the input stream to the output stream and allow the simulation to resume until the recycle operator is checked again. Sophisticated commercial software uses the recycle operator with mathematical techniques that accelerates convergence to a steady state mode. The recycle operator is only active in steady state simulation and is ignored at dynamic mode, where it copies the data wither input and output streams match in flow and composition or not.

5.8. Material stream

The material stream is a holder of information such as concentration and particle size distribution. It holds all necessary information and passes them to the destination unit. Unit operation will not start unless the process is connected to the required number of input and output streams except for mixers and splitters, which require at least one input and one output.

The material stream could be considered an ideal pipe with no pressure drop. In fact properties such as pressure

and temperature are not supported in BioSys. When new unit operations that require such information are added to BioSys, these properties would then be supported accordingly.

6. Case study

6.1. Case 1

One of the most commonly used and simulated processes is the activated sludge process. Fig. 1 shows a flow sheet of an activated sludge unit, which is presented here as a case study of steady state solutions for two different scenarios. All the components were predefined in the property packages dialog box as shown in Table 1. Table 2 shows the specification for the input flow. The reactor first searches for a guess value in the internal solution concentration by default. If that was not provided, it will take the output concentrations as the initial guess. Otherwise, it will go to the last resort and will take the input concentrations as the initial guess.

The biological reaction was defined using the Monod equation and three components: BOD (in kg mass/m^3), viable biomass and dead biomass. The maximum specific growth was set to $0.3\ h^{-1}$, the Monod constant to $0.06\ kg/m^3$, the death specific rate to $0.0025\ h^{-1}$ and the yield to 0.6.

Table 3 shows the specifications of the clarifier. It should be noted that double clicking the settling velocity model item or the interaction model item will launch a dialog box

Table 1
Components description

Component	Description
BOD	Aqueous substrate
Viable biomass	Biomass particle diameter = 0.08 mm and density = 1060 kg/m^3
Dead biomass	Solid particles of particle diameter = 0.08 mm and density = 1060 kg/m^3
Liquid	Liquid with density = 1000 kg/m^3 and viscosity = 0.001002 kg/m s
Solids	Solid particles of particle diameter = 0.01 mm and density = 1100 kg/m^3

Table 2
Feed material stream to the wastewater specifications

Property	Value
Flow (m^3/h)	500
BOD concentration (kg/m^3)	0.220
Viable biomass/microorganisms concentration (kg/m^3)	0
Dead biomass concentration (kg/m^3)	0
Liquid medium concentration (kg/m^3)	1000
Solids	0.250

Table 3
Clarifier specifications

Property	Value
Under-flow (m^3/h)	300
Number of stages	10 (default)
Height (m)	5
Depth (m)	5
Diameter (m)	30
Cut	1.0
Settling velocity model	5 (corresponds to Garside and Al-Dibouni correlation)
Interaction model	1 (corresponds to Selim, Kothari and Turian model)
Tolerance %	5
Maximum iterations	3

that will display all available models and options. The cut represents the maximum volume fraction after which the suspension will have a settling velocity of zero. Table 4 shows the bioreactor specifications required to run the simulation. The tolerance represents the allowable deviation of the accumulation (differential) term of the mass balances. The recycled material was set to a flow rate of 290 m^3/h and the tolerance of the recycle operator was set to 0.1%, which represents the percentage of deviation of any output value from the corresponding input value.

Simulating the activated sludge using steady state mode revealed that the settler successfully removed all dead and viable biomass. Table 5 shows simulation results of the clarifier overflow concentration, which is sent later for further treatment using UV disinfection or chlorination.

The activated sludge process also degraded the substrate material by 99.8% from 0.220 to 5.17×10^{-4} kg/m^3. The low presence of biomass materials means higher UV transmittance in water, resulting into higher rate of microorganisms kill in a downstream UV disinfection

Table 4
Reactor specifications

Property	Value
Tolerance (kg/h)	0.001
Maximum iterations	100
Solution volume (m^3)	10,000

Table 5
Settler results at steady state simulation

Property	Input	Overflow	Underflow
Flow rate (m^3/h)	790	490	300
BOD concentration (kg/m^3)	0.000517	0.000517	0.000517
Viable biomass concentration (kg/m^3)	2.567	0	7.009
Dead biomass concentration (kg/m^3)	2.282	0	6.010
Solids	0.256	0.248	0.265

Table 6
Clarifier results at steady state simulation at wet weather conditions

Property	Input	Overflow	Underflow
Flow rate (m^3/h)	1290	990	300
BOD concentration (kg/m^3)	0.0147	0.0147	0.0147
Viable biomass concentration (kg/m^3)	0.09685	0.0462	0.264
Dead biomass concentration (kg/m^3)	0.00387	0.00185	0.0105
Solid particles concentration (kg/m^3)	0.127	0.125	0.132

unit. The solid particles present also affect UV disinfection and shield the bacteria from the required UV killing dose. The settler is clearly unable to remove the small solid particles efficiently, even though the solids have a higher density than the BOD. On the other hand, the clarifier reasonably enabled the removal and recycling of viable biomass with a concentration higher than that in the bioreactor by a factor of 2.74. The same behaviour was observed for dead biomass. The settling velocity of a particle is not only a function of density, but also a function of particle diameter, fluid viscosity, fluid bulk flow and interaction with other particles. The solid particles are of a much smaller diameter than the biomass cells. From Table 1, multiplying the density of the particle by its volume gives a total mass per particle of 2.84×10^{-7} g for a biomass cell and 5.6×10^{-10} g for a solid particle. Thus, gravitational forces have a greater impact on the heavier biomass cells than the solid particles. Also, as the heavier cells settle down, fluid particles move in the opposite direction providing an upward drag force on the solid particles. Zeidan et al. [19] has provided a comprehensive insight of the models that predict the hydraulic and physical factors governing the settling velocity of solid particles. The ability of the software to predict overhead concentrations of light components is a direct result of implementing these settling velocity models along with the sedimentation model by Diehl and Jeppsson [4].

To study the effect of wet weather condition on such a process, we assumed that the input flow rate has doubled to 1000 m^3/h and the input solid particles and substrate concentrations were reduced by a factor of one half because of dilution. Simulation was performed at steady state mode keeping the same underflow and recycle flow rates. Looking at the results in Table 6, we notice that the BOD concentration entering the clarifier–thickener unit at wet weather condition has increased by 2700% from dry weather condition, indicating a decrease of efficiency of the bioreactor because of the higher dilution rate and lower recycled biomass concentration. Also, the percentage of materials removed by the settler decreased from 100 to 65.0% for viable biomass and 63.1% for dead biomass. This indicated that a significant amount of viable and dead microorganisms would go to the disinfection unit at a higher flow rate and lower UV transmittance, which would have a negative impact on a UV disinfection located downstream.

6.2. Case 2

To show the ability of the sedimentation model to handle a particle size distribution of viable biomass cells, a settler was modelled with one input and two outputs. The dimensions and specifications of the settler are shown in Table 3. The feed to the settler consist of a 500 m^3/h of feed with viable biomass of a density of 1060 kg/m^3. The underflow was set at 300 m^3/h. The viable biomass feed particle size distribution was taken to range between 0.01 and 2.00 mm of diameter. The particle size distribution represents an assumption of an instantaneous flocculation/coagulation of particles in the settler since the current model does not predict such phenomenon. The goal of the simulation is to show the ability of the sedimentation model to predict the presence of smaller biomass cells in the overflow. Fig. 8 shows the simulated particle size distribution of input, overflow and underflow.
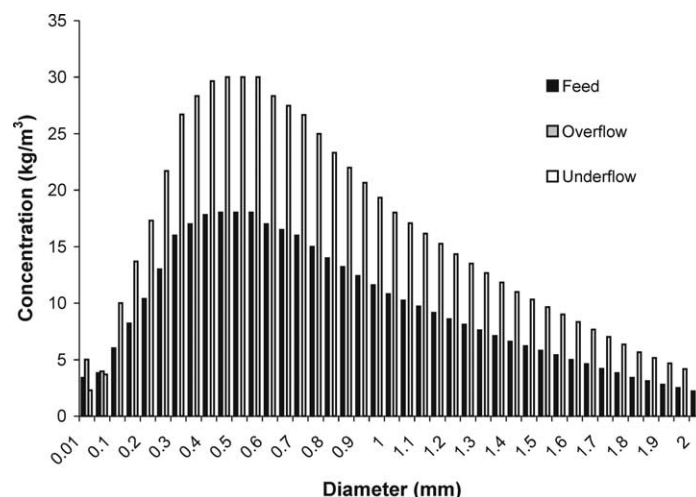

Fig. 8. Chart of particle size distribution of viable biomass cells at the settler's feed and outputs for case 2.

Thes simulation successfully predicted the separation of a feed viable biomass concentration of $227.6-8.980$ kg/m^3 in the overflow and 373.4 kg/m^3 in the underflow.

The reader is encouraged to refer Ref. [21] for further case studies and dynamic simulation of the activated sludge process.

An option to solve the overloading problem is to use a water storage facility, if present in the plant, as a temporary sedimentation unit to reduce the load the settler handles.

7. Conclusion

Simulating a wastewater treatment process is a powerful technique for optimization and improvement of current and under-construction wastewater facilities. Of particular interest is the prediction of how changes in the upstream feed conditions would impact the UV disinfection unit. BioSys was thus developed to be a flexible and multi-purpose software useful for the simulation of wastewater treatment processes.

The case study presented has shown impact of wet weather condition on the parameters affecting UV disinfection. A study of various process handling alternatives might have a direct effect on reducing the cost and improving efficiency. Designing and operating UV disinfection units should not be done in isolation from the surrounding processes.

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