# Development of an activated sludge software environment for application in operation, training, and education

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Activated sludge simulation modeling is now considered an accepted tool in engineering practice. However due to the complexity involved these models are only extensively used within a limited scientific community. There is a true need to leverage the use of these models among environmental engineering students and average plant operators to make them better understand the interactions of various factors on this process. A user friendly software environment that enables an ordinary user access and use these models to simulate a system without the need for either a complete understanding of the models behind or any special programming skills will certainly help promote models application. This paper defines the broad architecture of such an environment and identifies other applications that should be integrated to the simulator such as expert systems and database systems. Then it discusses the steps necessary to develop a reliable site-independent activated sludge simulator. Finally the paper points out that to introduce mathematical model simulations to traditional treatment plants, a how-to-do protocol is needed to adjust routine operating data for model use.

تعتبر برامج نمذجة ومحاكاة الحمأة المنشطة أداة هامة بالنسبة لتطبيقات الهندسة الصحية ولكن نظرا للصعوبات التي تشتمل عليها النماذج الرياضية الخاصة بهذه البرامج فان استخدامها يقتصر على فئة محدودة من المتخصصين في هذا المجال. وفي المقابل فان هناك حاجة ماسة ألي تشجيع مشغلي المحطات ومهندسي التصميم والطلاب على استخدام نظم المحاكة والنمذجة وذلك سواء لأغراض التحكم أو التدرب والتعلم. يهدف هذا البحث إلى تطوير برنامج متكامل سهل التشغيل يشتمل على عددة برامج تحتية هي برنامج نمذجة ومحاكاة و نظام خبير وقاعدة معلومات ليكون قادر على خدمة عدة أغراض مثل الستحكم في هذا التشغيل و التصميم و التدريب والتعليم. وتطوير مثل هذا البرنامج عملية معقدة يجب أن تتم على عدة ماراحل ويستم تقيم م مرحلة مرة على حدة ومرة من خلال البرنامج الرئيسي و هنا يجدر الإشارة إلى أن هذا البحث هو واحد من الأبحاث مرحلة مرة على حدة ومرة من خلال البرنامج الرئيسي و هنا يجدر الإشارة إلى أن هذا البحث هو واحد من سلملة من الأبحاث يقوم بها الباحث سواء منفردا أو مع آخرين بدأت عام ١٩٩٣ وماز الت مستمرة وقابلة للتطوير . يقدم مدر الأبحاث البرنامج الرابح المرة الرياضي مع التركير على خلال البرنامج المواز الت مستمرة وقابلة للتطوير . يقدر من سلملة من الأبحاث والذي يقوم بها الباحث سواء منفردا أو مع أخرين بدأت عام ١٩٩٣ وماز الت مستمرة وقابلة للتطوير . يقدم هما البحث مكون البرنامج الرئيسي مع التركيز على خطوات التطوير وتفاصيل برنامج المحاكاة و النمنجة الرياضية وهو الجزء الأكثر تعقيدا والذي يتم تطويره وتعديله على مراحل متعددة بدأت منذ أكثر من عشر سنوات وماز الت مستمرة.

**Keywords:** Activated sludge models, Control, Operation of traditional treatment plants, Training

#### 1. Introduction

Currently the activated sludge process is the most widely used biological unit process for secondary wastewater treatment worldwide for its high performance. Many models were proposed to provide a description of the complex biological reactions that take place within the process until in 1987 the International Water Association (IWA formerly IAWQ and IWPRC) task group for mathematical modeling for design and operation of biological wastewater treatment introduced the Activated Sludge Model no.1 (ASM1) to unite many of the previous scientific efforts in what was considered then as the state of the art model (Henze et al. [1]). ASM1 allows the simulation of the behaviour of nitrifying and denitrifying activated sludge systems, which treat primarily domestic wastewater. ASM1 immediately gained wide acceptance and became a major reference for further research work as well as the basis for many software programs applied for design and operation of treatment plants. Since then practice has taken ASM1 proposed primarily for nitrogen control- as many activated sludge plants are now modified to allow for phosphorous removal as well. This called the task group to present model 2 (ASM2) in 1995 and its minor extension (ASM2d) in 1999 to provide an understanding of the processes involved in

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biological phosphorous removal (Gujer et al. [2] and Henze et al. [3]). To accommodate for these mechanisms more components and processes were added leading to a more complex structure model compared to ASM1. The task group realized that the level of understanding of phosphorous removal processes is not very reliable and as such hoped that ASM2 would encourage scientific debate leading to further developments towards a more reliable model (Gujer et al. [2]). Finally in 1999, the task group proposed model ASM3 to correct some of the apparent defects of ASM2 returning to the structure of the less complex model as phosphorous removal was not considered (Gujer et al. [4]). All this enhanced the use of activated sludge models within the scientific community and among consulting engineers for a variety of purposes ranging from research to treatment plant design, operation, control and troubleshooting. Many software packages built on these models especially model ASM1- are available today. However most of these software tools were developed for research or for practical applications in consulting companies and are not well suited for application by average operators or for teaching purposes (Morgenroth et al. [5]). This paper aims to raise attention to this important aspect, to identify the means to achieve wide application of complex models among environmental engineering students and plant operators, and to present a proposed software environment.

### 2. Objectives

Operational practice shows that operators are among the important factors influencing the monitoring of activated sludge plants and coping with emergency situations. Skillful operators tend to develop an understanding of how to monitor their plants by taking advantage of mere observations related to colour, foam and odour [6]. Then as their experiences grow they get to know when the plant is in actual need of corrective measures and when it is best to leave what seems to be a problematic situation pass with no interference [7]. Evidently their performance will certainly be improved if they are equipped with computer systems such as process simulators and expert systems that provide rapid access to information about the plant state. A process simulator can predict how the actual system reacts under various conditions. Thus providing operators with a deep insight into the internal workings of the physical system and helping them avoid many unfavorable situations before actually turning into operational problems. Similarly if environmental engineering students were allowed to use simulation tools without having to understand every specific detail about the implemented models or about the numerical solution procedures involved this will certainly enhance their level of understanding of the physical wastewater system. Later on this would encourage them to experiment with the implemented models i.e. change model parameters, evaluate different process configurations and operating strategies or even select a completely different model. This would eventually promote model use within students and upgrade environmental engineering education as a whole.

On the other hand expert systems condense all the knowledge and experience about the treatment process in an easy to use means that provides immediate advice whenever human experience is a must. This may be considered as an invaluable tool for user's information training if the is continuously tested against the system's advice for a variety of practical cases. Whenever these systems are inter-linked with other information sources they get more powerful. For example if an expert system is linked to a database system in a way that lets the expert system directly access data records, a sort of an intelligent database will be developed. This enables the expert system to arrive at a decision based on the latest available data and makes the most out of the plant's routine data records. A similar approach was adopted during the development of an expert system called the Activated (ASExpert) dedicated Sludge Expert for inexperienced activated sludge plant operators [8]. A direct interface was established between the expert system and the database and as a future step it was recommended to integrate a simulation-modeling tool to ASExpert to test the validity of the expert system's advice before actual execution [8, 9]. Now this paper

aims to build on the previous work and presents the architecture of a complete software environment that incorporates both the system ASExpert and a process simulator as one information system's toolbox.

# 3. Architecture of the proposed software environment

Fig. 1 represents the complete architecture of the proposed environment where a well-designed Graphical User Interface (GUI) is the means of user interaction with essential components:

1. The readily available component or system ASExpert [8]:

- a. the expert system tool, and
- b. the database tool (record manipulation, report generation and graph representation sub-systems).

2. The simulation-modeling program made up mainly of a model library, numerical integration solver and a graphical output facility [10, 11].

ASExpert's internal architecture is made up of several elements. Typical to any other expert system the knowledge base and inference engine are the system's main building blocks. First the knowledge base is the system's repository of domain knowledge coded in the form of rules. Rules take the form of (If-Then) associations i.e. two-part conditional statements that represent heuristics or rules of thumb. The antecedent expresses a situation or a premise while the consequent states a particular action or conclusion that applies if the situation or premise is true. Second the Inference engine is the system's control mechanism that makes inferences and decides which rules are satisfied by facts, prioritizes the satisfied rules on a list called the Agenda and then executes the rule with the highest priority. The working memory works in harmony with the inference engine to model human short-term memory. It contains the facts of the current situation whether entered through user input or inferred as a result of rules firing. Finally the inference engine can also be programmed to provide the explanations behind the system's reasoning which is usually achieved through the explanation facility block [12]. Other external programs such

as the database tool and rule editor provide additional support to the main program. As stated earlier, there is an established interface between the expert system and database system [8, 9]

# 4. The main building blocks of an activated sludge simulator

To adequately simulate an activated sludge system, a simulation tool should mainly account for a model library, numerical solution procedures and a graphical representation output facility.

The model library: A straightforward simulator that can be easily implemented by inexperienced users should adopt a closed model structure. Accordingly the simulator model library provides the user with a set of predefined models that can be used to implement a specific activated sludge system. The user has no choice but to select a predefined model or coupled models (reactor/ settler model) from a set of available models. Model parameters may also be predefined or the user may be allowed to introduce his values (within the range of accepted values).

Simulated configuration setup facility: Usually a basic simulator will adopt a predefined process scheme regarding the type and number of reactors; connection between different units and the user has no freedom to define his own specifications other than manipulating a few variables. Thus this component may be regarded as a future enhancement and not as an essential part of the simulator's architecture.

Numerical solvers: Models describing activated sludge systems involve non-linear processes mass balance equations that and are represented mathematically as a set of Ordinary Differential Equations (ODEs). These ODEs are complex and can only be solved by numerical integration methods [11] Today there is an advanced software that facilitates the numerical solution of these complex systems and this software can also be easily incorporated within any new application to do the necessary computations efficiently. For example simulation languages such as Simnon, more details can be found elsewhere [11]. Graphical result output facility: To promote user acceptance in today's world of sophisticated applications, graphical representation of results is very much desired.

### 5. The simulator's development procedure

The development of an activated sludge system simulator is certainly no trivial task due to the complexity of the models used. If it is required to simulate a specific plant, the plant's site-specific control procedures must be included in the simulation. Finally computer simulations must be validated with experimental or full-scale data. This calls for a well-defined framework or methodology to identify the simulation model(s), plant layout, evaluation and test procedures and all other elements necessary to facilitate introducing the developed simulator for use in real plants as a future step. Recent technical literature strongly reveals a trend towards similar standardized procedures. Although the reported protocols were developed to serve different aims, all were triggered by one common motive: to provide a how-to-do practical protocol that benefits of the accumulated experiences, unifies inconsistent available knowledge and most importantly to set some form of quality control. Thus the COST simulation benchmark was implemented as a test vehicle for activated sludge control strategies [13-15]. This benchmark is a methodology not only comprised from a simulation model but also of a complete protocol on how to run tests and document results. Hulsbeek et al. [16] reported a protocol set to aid in the introduction and acceptance of dynamic models in fullscale plants in the Netherlands. Similarly in reporting experiences with computer simulation at two large wastewater treatment plants in Poland, Makinia et al. [17] stressed the need for a methodology to adjust routine operating data for modeling purposes. The simulator's main requirements were identified and the plan for development was set after a careful study of these research experiences.

### 5.1. The proposed model

In order to adequately describe an activated sludge process it is required to take into consideration a large number of phenomena such as: characterization of the influent wastewater, hydraulics of each tank, hydrolysis of different substrates present in the influent, carbonaceous, nitrogenous and phosphorous removal mechanisms, organism growth and decay and sludge clarification and thickening mechanisms [18]. Influent wastewater is characterized not only by its composition in organic carbon, nitrogen and phosphorous fractions but also in soluble, particulate, biodegradable and non-biodegradable fractions. Organisms are represented by at least one class of hetertrophs and one or two species of nitrogen consuming autotrophs. Then the main reactions are added for each class of organisms and each class of available substrate [18].

Many activated sludge models have been presented, but the Activated Sludge Model No. 1 (ASM1) -since it was proposed in 1986- has been widely accepted and is currently used all over the world -despite its limitations- to provide realistic predictions of a single sludge carrying carbon system out oxidation, nitrification and denitrification. This model focuses on a single unit process -the aeration basin in an activated sludge system- to describe the reactions that lead to carbon and nitrogen removal. It ignores the effects of sedimentation and treats the settling tanks as perfect splitters. It uses COD as the measure of concentrations of organic material in wastewater [1, 19]. Later on, more advanced models were presented that started to include phosphorus removal or sludge bulking [19].

Most growth models also share the basic assumptions of ASM1 where the reaction mechanisms are modeled by non-linear Monod-type equations or by simple extensions of these equations. The bi-substrate model and death regeneration hypotheses are used to describe biological growth of biomass, hydrolysis and decay [1]. Accordingly two fractions of biodegradable organic matter in influent wastewater are adopted: readily and slowly biodegradable COD. When microorganisms die, decayed cell material is recycled to the process as a slowly biodegradable COD that could then be used by the remaining microorganisms as substrate through hydrolysis, non-biodegradable whereas the fraction remains as an inert residue. In a similar



Fig. 1. The architecture of the proposed software environment.

way the transformations of nitrogen can be described by the death regeneration hypothesis [1, 20].

Based on mass balance equations these models relate changes of the state of the system (concentrations of model components) to transport and transformation processes. Transport processes are characteristic for the design of a system (reactor configuration, distribution of influent, excess sludge removal, etc.) and leave the chemical structure of all materials unchanged. On the other hand transformation processes involve the change of the chemical structure of the components [20]. Typically the number of states varies between ten and fifteen for each completely mixed reactor for models described in literature. A complete description of model ASM1 can be found in ref. [1]. ASM1 uses 13 model components or state variables both soluble to represent substrate, and particulate biomass, oxygen and alkalinity using the following symbols (S<sub>I</sub>, S<sub>S</sub>, X<sub>I</sub>, X<sub>S</sub>, X<sub>B,H</sub>, X<sub>B,A</sub>, X<sub>P</sub>, S<sub>O</sub>, SNO, SNH, SND, XND, SALK) and 8 transformation processes (i.e. growth, decay and hydrolysis) described in a matrix notation.

• For each of these model components (states) the rate of accumulation within a system boundary (a completely mixed reactor) can be calculated as follows:

Rate of accumulation = Rate of Input – Rate of Output + Rate of reaction  $r_i$ .

 $r_i$  is the result of the conversion of component *i* due to its involvement in several processes. Mass balances of all components form a set of simultaneous non-linear (because  $r_i$  is usually non-linear) Ordinary Differential Equations (ODEs) or the mathematical representation of the model. Traditionally the calculation of  $r_i$ has been simplified through model representation in matrix format that defines fundamental reactions and that shows the stoichiometric relationships relating the state variables to process rate equations [20]. Matrices not only represent a convenient way to store data and complex relationships but most importantly matrices can be easily manipulated by computers [21].

### 5.2. Reactor/ settler representation as one integrated unit

### 5.2.1. Using ASM1 to model a reactor and model solution via numerical integration

The following points show how the mathematical equations comprising the model are formulated:

• As stated earlier performing a separate mass balance over each reactor for each model component and adding the input/output terms, results in a set of non-linear ODEs of the form:

$$\frac{dZ}{dt} = \frac{Q}{V} (Z_{in} - Z) + r_z ,$$

where Z represents the concentration of a specific component inside the reactor,  $Z_{in}$  is the concentration of the same component in the influent to the reactor, Q, V and  $r_z$  represent the flow rate, the reactor's volume and the rate of reaction of component Z, respectively [22]. These ODEs define the system state and when solved characterize its behavior.

• In a similar way if the reactor is divided to separate anoxic and aerobic zones, each zone will be treated as a *separate* unit with its own characteristics such as volume, flows and process constants.

• The entire ASM1 model, except the reactions related to alkalinity (component no. 13) should be implemented. However it may be more practical to combine the two state variables  $X_I$  and  $X_P$  in one variable  $X_{IP}$  to decrease the number of ODES to 11 equations for each zone whether anoxic or aerobic.

• As it is currently a common practice in all plants to control the concentration of oxygen in aerobic reactors thus a mathematical expression that calculates the increase of oxygen concentration due to added air through the aeration system must be included in the differential equation that describes the change of oxygen concentration in any aerobic zone. This mathematical description is usually achieved by multiplying the oxygen transfer rate from gaseous to dissolved state  $(K_L a)$  with the subtract of  $(S_{o,sat} - S_o)$  where  $S_{o,sat}$  is oxygen saturation concentration and  $S_o$  is the actual oxygen concentration in the reactor.  $K_{L}a$  is usually a non-linear expression that calculates the transfer rate according to the air flow rate from the compressors.

• The set of non-linear ODEs comprising the model are usually very complex and can't be solved analytically. Therefore after determining appropriate initial conditions of model components, numerical integration techniques based on Euler and the classical 4<sup>th</sup> order Runge-Kutta methods [21] are adopted for model solution.

# 5.2. Modeling of the settlement process using one-dimensional multi-layer models

In addition to oxygen transfer mechanisms in the aeration basin; to obtain realistic results from model ASM1, it has to be used in combination with models capable of describing the settlement process efficiently [1]. The settlement process can be fairly represented using one-dimensional multi-layer model that model dynamics according to the solids flux theory in the vertical direction only leaving the cross-sectional area and depth as design parameters. Fig. 2 shows the basic idea behind one-dimensional multi-layer models.

• The settler is divided into a number of completely mixed layers (1:n) where the inflow and suspended solids are homogeneously spread over the horizontal cross section. The sludge transport between the layers is assumed to depend on two mechanisms; bulk movement and gravity settling. The bulk movement is caused by the hydraulic flow and hence is directed upwards and downwards. A feed layer (m) must be determined. At the feed layer the entering fluid is divided to an upward flow that depends on the rate of the effluent flow  $Q_e$ and a downward flow that depends on the rate of the underflow  $Q_u$  whereas the gravity settling flux is always directed downwards [23]. The solid flux due to the bulk movement of the liquid whether upward or downward is straightforward to assess as shown on the left side of fig. 2.

• The solid flux of particles due to gravity sedimentation  $J_s$  is calculated according to Kynch's solid flux theory such that  $J_s = V_s(X) * X$  where the gravitational settling velocity  $V_s(X)$  depends only on the local solids concentration X and was traditionally calculated as either a power or an exponential function.

• In the region above layer m, the solids are assumed to have a gravitational settling velocity greater than the upward movement of fluid in order to be separated from the overflow. According to Vitasovic's model an empirical threshold concentration  $X_t$  is defined and whenever the solids concentration is greater than  $X_t$ , it is assumed that the settling flux in that layer will affect the rate of settling within adjacent layers. For example above layer m,

the flux out of layer j is restricted if the concentration in layer j+1 is greater or equal to  $X_t$ , in which case the flux out of layer j is set to the minimum of [J(j), J(j+1)] as summarized in fig. 2. This threshold concentration  $X_t$  corresponds to the onset of hindered settling behaviour and the top of the sludge blanket height corresponds to the highest layer with concentration equal to or greater than  $X_t$  [23].

• Although the original model of Vitasovic set the work for practically all current multi-layers models, it remained to be ineffective for realistic predictions of effluent suspended solids because it uses the Vesilind's traditional exponential function  $v = ke^{-nX}$  to calculate the settling velocity. This settling velocity function is prone to give unrealistic high settling velocities for low concentrations of solids likely to be found in the clarification zone [23, 24]. It was found that the settling

**Bulk Movement Gravity Settling** Q<sub>e</sub>X<sub>e</sub>/A  $J_{s,1} = \min(v_{s,1}X_1, v_{s,2}X_2)$  $J_{up,2} = Q_e X_2 / A$ or  $J_{s,1} = v_{s,1} X_1$ , if  $X_2 \le X_t$  $J_{s,2} = \min(v_{s,2}X_2, v_{s,3}X_3)$  $J_{up,3} = Q_e X_3 A$ or  $J_{s,2} = v_{s,2}X_2$ , if  $X_3 \le X_t$  $J_{s,m-1} = \min(v_{s,m-1}X_{m-1}, v_{s,m}X_m)$  $J_{up,m} = Q_e X_m / A$ or  $J_{s,m-1} = v_{s,m-1}X_{m-1}$ , if  $X_m \le X_t$ Feed layer QfXf/A  $J_{s,m} = \min(v_{s,m}X_m, v_{s,m+1}X_{m+1})$  $J_{dn,m} = Q_u X_m / A$ **m**+]  $J_{dn,m+1} = Q_{u,X_{m+1}}/A$  $J_{s,m+1} = \min(v_{s,m+1}X_{m+1}, v_{s,m+2}X_{m+2})$  $J_{dn,n-1} = Q_u X_{n-1} / A$  $J_{s,n-1} = \min(v_{s,n-1}X_{n-1}, v_{s,n}X_n)$ Q<sub>u</sub>X<sub>u</sub>/A

Fig. 2. The general principal of the traditional one-dimensional layer settler model [11].

velocity function need to be modified and several functions were proposed until Takacs and co-authors proposed to use the double exponential velocity. The double exponential velocity model gained wide acceptability because unlike the standard model it is applicable to both the hindered and flocculent settling conditions. A complete description of Takacs modified model can be found in [24].

• Assuming complete mixing within each layer the complete set of equations comprising the settler model can be obtained by performing mass balance for each layer.

#### 5.3. Reactor/ settler models coupling

To represent both reactor and settler as an integrated part of the activated sludge process the reactor and settler models must be coupled. This coupling can be achieved mathematically if the following conditions are met.

• The complete set of reactor/ settler non-linear ODEs is solved simultaneously.

• All particulate state variables of the reactor's last compartment are converted into one composite term  $X_f$  (see fig. 2) that represents the total suspended solids in the feed to the settler. A well-known conversion relation proposed by [25] is  $X_f = 0.75^*(X_S + X_{IP}) + 0.9(X_{BH} + X_{BA})$  where  $X_{ND}$  is not included because it is considered to be initially a part of  $X_{BH}$  and  $X_{BA}$ . In the mean time the ratio of each particulate variable to this composite term is also recorded.

• During the ongoing numerical integration the total suspended solids in the settler's bottom layer  $X_u$  (see fig. 2) is divided again into particulate fractions to define the composition of the recycle flow entering the anoxic zone (knowing the ratios computed in the previous step of each particulate fraction to the total suspended solids in the feed to the settler). The flow sheets of table 1 and table 2 summarize the steps needed for the formulation of the set of derivative equations, which comprise the coupled reactor/settler model. More details on Reactor/Settler models coupling can be found elsewhere [10]. The proposed model was calibrated and verified using data from the Hamilton Wastewater Treatment Plant, Canada [11].

# 5.4. Main requirements of the proposed simulator

After this quick review of the nature of the system to be modeled, the simulator's main requirements can be summarized in the following points:

• To act as a site independent tool capable of simulating process mechanisms of an integrated activated sludge system (a coupled reactor/ settler system).

• To enable the users conduct "what-if" analysis by letting them view the response of the system when changes are introduced to the variables they are authorized to manipulate such as recycle and re-circulation rates, hydraulic and organic flows that may be adjusted to represent peak values, and to switch on/ off oxygen dynamics etc.

• To display the parameters used within the model, the plant's physical data (volumes, flows etc.) and the state variables initial conditions in each case.

• To produce realistic simulation data outputs by using real dynamic data as input.

• To represent simulations results graphically and provide the user with the facility to print these results or save them as computer files.

• As a future requirement, practical real world application of the simulator stresses the need for a customized Graphical User Interface (GUI) that allows the user to represent an activated sludge plant of his own specifications as a schematic diagram on the monitor's screen as well as to interactively manipulate this diagram. Such an interface should provide the user -through simple mouse clickswith the versatility to customize the plant's modes of operation and control -to some permissible range- according to his desire and to set the simulation start-up conditions. This enables the user to conduct extensive "what if" investigations to inspect the effect of different operating conditions or throughputs etc. Typical to fig. 3 the number of anoxic and aerobic zones may be set according to user input. In addition he may switch process modes of operation between (pre-denitrification/ post-denitrifaction). Accordingly the plant's schematic diagram should be immediately redrawn on the screen to reflect these modifications (highlight active pumps, dim inactive pumps, show air bubbles in aerobic zones and remove air bubbles from anoxic ones etc.). Eventually simulations start upon user request when the user is completely satisfied with his selections.

# 6. An outline of a four-stage plan for the development of the simulator

The development procedure is organized in four well-defined stages that follow the 3 development stages of ASExpert (fig. 4):

• Stage 1: setting up a development framework.

• Stage 2: implementation of system's models and verification of initial results.

• Stage 3: implementing a GUI for the simulator and linking it with the numerical solver.

• Stage 4: future simulator improvements and possibility of embedding it within a multi-system information toolbox.

Stage 1. The overall simulation model (process models to be implemented, influent model, parameter values and initial values) and verification procedure are set in accordance with the COST simulation benchmark [4].

• *Implemented models* are ASM1 and the double exponential settling velocity model of Takacs et al. [24].

• *Parameter values* of kinetic and stoichiometric are chosen as the default values of these models at a temperature of 20 °C.

• *Plant layout* is the COST simulation benchmark default plant layout, which is a commonly used pre-denitrification configuration, comprised of two anoxic reactors followed by three aerobic ones and then a sedimentation unit.

• Influent data files. 3 files were developed within the COST simulation protocol to represent normal dry weather inflow, storm and rain disturbances. These files contain data (model fractions ready for use in the simulations) taken at 15 minutes intervals for a 14day period in a way that represents a fair description of a true influent profile (regarding expected diurnal variations in influent flow and COD as weekly data patterns) of a plant of the chosen size [14]. These files used to verify the results of developed simulator and can be downloaded from the COST benchmark web site [14]. 

 Table 1

 Flow sheet for the formulation of reactor's derivative equations

• Calculate particulate state variables in the recycle flow, knowing the ratios of the particulate state variables to the total suspended solids in the feed ( $X_S/X_f$ ,  $X_{IP}/X_f$ ,  $X_{BH}/X_f$ ,  $X_{BA}/X_f$  and  $X_{ND}/X_f$ ) and the total suspended solids at the bottom of the clarifier  $X_u$ .

• Use ASM1 matrix to calculate the conversion rates of the model components where: the conversion rate of each component  $(r_i) = \sum_j v_{ij} * \rho_j$  i.e. summation of the products of the stoichiometric coefficients  $v_{ij}$  and the process rate equations  $\rho_j$  describing that component.

• Perform mass balance for the model components to formulate the differential equations of the state variables derivatives.

• Direct the set of ODEs to be solved by the numerical integration solver.

Reactor

Table 2

Flow sheet for the formulation of the settler's derivative equations

• For simplicity, one can use the composite variable  $X_f$  to represent all different particulate components within the model such that  $X_f = 0.75^*(X_S + X_{IP}) + 0.9(X_{BH} + X_{BA})$ .

- Assume that soluble components are not affected by sedimentation.
- Calculate the settling velocity for each layer with respect to the layer concentration.
- Calculate the solids fluxes from one layer to the next (settling zone) or the previous (clarification zone)
- For each layer of the settler (1 to n):
- Calculate the total suspended solids derivative depending on the continuity equation:
- Rate of mass increase per unit time = rate of flux in rate of flux out

• Direct the set of ODEs to be solved by the numerical integration solver.

Settler



Fig. 3. The basic capabilities of a GUI simulator for an activated sludge system.

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Fig. 4. Stepped procedure for the development of the proposed environment.

• Simulator verification procedure. To ensure a consistent starting point and to eliminate the influence of starting conditions on the generated dynamic output the COST simulation benchmark describes a two-step procedure that involves simulation to steady state followed by dynamic simulations using the three defined influent files. According to Copp [14] initial states for dynamic simulations can be obtained by simulating the set of ODEs under an input of constant flow and composition provided in the benchmark- for a period of 100 days. Following simulation to steady state, the generated output data must be compared to the standardized output that is included in the benchmark description. Only when similar steady state results are attained should dynamic simulations be initiated using the 3 dynamic input files. For a complete description of the verification procedure see Copp [14].

Stage 2. The tasks dedicated to this stage include the selection of the development languages or software tools to be used for implementation regarding the simulator's requirements and the capabilities of available tools. The following section discusses available possibilities.

The need for built-in stiff numerical integration solvers. As stated earlier the models of the present system take the form of non-linear ODEs and as such to cut down development time considerably there is a demand for readily available numerical integration solvers that could be directly used as built-in routines or functions. In this respect MATrix LABoratory (MATLAB) by Mathworks is a general, high-performance technical computing language that provides easy access to a whole suite of ODEs solvers capable of efficiently solving a variety of differential equation systems including initial value problems typical to the present activated sludge system. Some of these solvers are also based on algorithms specifically dedicated to deal with stiff systems (Hanselman and Littlefield [26]) similar to the present system where the time constants for the different processes of the simulated model vary significantly and require special integration algorithms to handle. MATLAB is also equipped with an integrated simulation toolbox called Simulink capable of providing real time graphical representation of simulation results. Finally it is worth to mention that MAT-LAB may be considered as the easiest and most straightforward method for implementing complex mathematical models even for the inexperienced programmer. All this makes MATLAB one highly suitable candidate for implementation.

The need for a GUI. Requirements indicate that the simulator should use a user-friendly interface capable of interactively taking in user input and providing a graphical result output and as a future requirement of providing some means of plant layout definition. Although MATLAB can be used for GUI implementation but the real-time update of a complex interface would be too time-consuming in such a case. Thus a general purpose programming language such as VC++ or Java will be more suitable to fulfill these requirements. This raises another issue, which is the necessity for establishing some means of connection between MATLAB that acts as the background engine, and the interface.

Reasons that favour choosing Java for the implementation of the interface. Java contains a rich set of GUI components that can handle most of the fundamental requirements of programs, which makes it easier and faster to use [27, 28]. Java is a multithreading language where multiple tasks can be run simultaneously in one program, thus satisfying the needs of a responsive user interface. Despite being an interpreted language Java has a relatively high speed sufficient to handle most real time interactive applications [22, 28]. In addition, there is currently an enormous worldwide interest in Java and there are a lot of powerful Java Integrated Development Environments (IDEs), which speed up coding, debugging and facilitate the development process to a great extent by freeing the developer from time-consuming tasks thus enabling him to focus on providing the real solutions.

Establishing an interface between Java and MATLAB. Software public domain currently provides a Dynamic Link Library (DLL) called JMatLink.dll that is capable of integrating Java with MATLAB without much programming effort. Although this DLL is still not supported by Mathworks, it may be tried as a quick step towards fulfilling objective.

Results of initial model implementation. The reactor/ settler (ASM1/ Takacs et al. double exponential velocity) coupled models were coded using MATLAB. The 2-step simulation-verification procedure was conducted. Obtained results were evaluated in the light of the provided standardized output. Initial testing shows that MATLAB numerical integration solvers are capable of satisfying requirements [29].

*Stage 3.* After verification of initial model implementations, effort was directed towards fulfilling the simulator's GUI requirements. A

Java GUI was hastily developed and used to build up the simulated system typical to user desire. Using the public domain DLL file (*JmatLink.dll*), user input was directed to MAT-LAB environment to do the necessary computations and save output as a text file. Initial testing of the developed application gives a promising indication that this technique is capable of satisfying requirements, which should encourage the development of a more functional GUI in the future.

Stage 4. Tasks of stage 4 aren't completely fulfilled yet. Attempts are dedicated to encourage more interactive manipulation of the simulator's GUI and to modify current database system to incorporate data necessary to start simulations (influent files) and save results for future use. Effort will focus on selecting adequate calculation procedures from literature to convert traditional plant parameters e.g. COD and TSS into model fractions. These procedures can then be introduced to the system to directly do the required conversion to model fractions ready for use in the simulations. Finally attempts will be directed towards integrating the developed simulator together with ASExpert in one environment. However it is not apparent, at present, whether a direct interface can be established between both systems and whether this capability would be of any specific advantage. Nevertheless the environment may be regarded as a multi-system information toolbox that provides access to several tools capable of satisfying different needs. The expert system is the tool to use when human experience is sought whereas the simulator is employed to visualize the effect of variable conditions on the process and to test whether the expert system's advice is sound before putting it to actual execution in the plant.

### 7. Conclusions

• Simulation models of activated sludge plants are still not very much used by plant operators nor by environmental engineering students. The barriers behind this situation could be related to the level of complexity of the simulation software mainly to the unavailability of ready to use data in traditional treatment plants. • In cases where it proves to be economically infeasible to upgrade old plants to automatic control facilities the one possible alternative to improve plant operation is to leverage the skills of operators. This can be achieved through effective computer systems that provide rapid access to information about the plant's state in a visual, easy to grasp graphical form. Appropriate information sources are primarily simulators and expert systems. Moreover if these powerful systems are integrated in one environment this would yield the ultimate software tool capable of making operators take decisions with confidence in the outcome.

• Technical literature strongly reveals a trend towards practical how-to-do protocols that provide maximum benefit of accumulated experiences, eliminate knowledge inconsistency and set measures of quality control. Although the motive behind each protocol is different still the need and benefit of standardization is apparent. This is especially emphasized if mathematical model simulations are to be introduced into traditional treatment plants because a great effort must be dedicated to adjust routine operating data for model use.

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