Coupled Systems Mechanics, *Vol. 5, No. 1 (2016) 21-39*
DOI: http://dx.doi.org/10.12989/csm.2016.5.1.021

Wastewater process modeling

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(Received December 28, 2015, Revised February 9, 2016, Accepted February 13, 2016)

Abstract. Wastewater process models are the essential tools for understanding relevant aspects of wastewater treatment system. Wastewater process modeling provides more options for upgrades and better understanding of new plant design, as well as improvements of operational controls. The software packages (BioWin, GPS-X, Aqua designer, etc) solve a series of simulated equations simultaneously in order to propose several solutions for a specific facility. Research and implementation of wastewater process modeling in combination with computational fluid dynamics enable testing for improvements of flow characteristics for WWTP and at the same time exam biological, physical, and chemical characteristics of the flow. Application of WWTP models requires broad knowledge of the process and expertise in modeling. Therefore, an efficient and good modeling practice requires both experience and set of proper guidelines as a background.

Keywords: wastewater treatment plant; modeling; activated sludge process; simulation

1. Introduction

The progressive deterioration of water resources and the large amount of polluted water generated in industrialized and urbanized countries put on the Wastewater Treatment Processes (WWTP) a fundamental importance in the water quality protection. Guidelines and regulations (Directive 91/271/CEE referring to the wastewater pollution control and treatment) enforce the adoption of specific quality parameters (maximum allowed concentration) for the treated wastewater. Processes are generally divided into the primary, secondary and tertiary stage/treatment technology, including appropriate facilities and equipment. The most common demand for municipality wastewater is a secondary treatment, including primary - mechanical treatment and secondary - biological treatment of wastewater. Inside a biological unit of the wastewater treatment plant, the Activated Sludge Process (ASP) is the most frequently used technology for the removal of the organic pollutant from wastewater. It is quite reliable, the most cost-effective and very flexible process. It is adaptable to any kind of wastewater and has the capacity of producing high quality effluent.

Taking into account current environmental problems and water scarcity, it is not unrealistic to believe that the trend of development of new WWTPs will be continued all over the world. At the

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http://www.techno-press.org/?journal=csm&subpage=7 ISSN: 2234-2184 (Print), 2234-2192 (Online)

same time, loads on existing plants are expected to increase due to the growth of urban areas. This situation demands more efficient treatment procedures for wastewater.

Therefore, experts have begun to explore how wastewater process modeling could be combined with computational fluid dynamics to further expand the capabilities of both tools. Also, modeling and simulation can significantly contribute to understanding and design of activated sludge wastewater treatment plants. Process models are the essential tools for understanding wastewater treatment system behavior. A wastewater treatment plant model describes the biochemical and physical processes involved in the technical purification of wastewater. Through the biochemical processes, the organic matter and nutrient content of the wastewater is eventually converted into carbon-dioxide, nitrogen and a particulate fraction (cell material). The step is a physical separation of exceeded sludge and removed cell material. Wastewater process simulators can provide insights for plant upgrades, new plant designs, and improvements of operational controls. The decisions made in the design and optimization of WWTPs have significant financial and environmental impacts.

The paper presents the mathematical models which are used the most for modeling of the biological processes for domestic wastewater treatment.

The overview of the Activated Sludge Models (ASM) and some of the commercial programs based on linear or non-linear dynamic models will be presented in this paper shortly.

2. Fundamentals of the wastewater biological treatment with activated sludge

The activated sludge treatment process is the process in which waste water is brought into contact with a suspended culture of microorganisms in an aerobic environment. The aerobic environment is achieved by the use of diffused air, or mechanical aeration, or even by pure oxygen. This operation takes place in a bioreactor known as an aeration basin. Microbiological reactions occur in the bioreactor, resulting in the growth of new bacteria and the oxidation of organic compounds in the waste water. The schematic flow diagrams shown in Fig. 1 include the nomenclature used in the following mass-balance equations. All designs of biological treatment reactor are based on using mass balances across a defined volume for each specific constituent of interest (i.e., biomass, substrate, etc.).

The mass balance includes the flow rates for the mass of the constituent entering and/or leaving the system and appropriate reaction rate terms for depletion or production of the constituent within the system.

Legend:
Q – influent (m^3/s),
S_0 – readily biodegradable substrate (mg COD/l),
X_0 - concentration of biomass in influent ($gVSS/m^3$),
V - reactor volume (aeration tank) (m^3),
X - concentration of biomass in the reactor (g/m^3),
S – concentration of biodegradable substrate in tank (mg BOD/l),
Q_w –waste sludge flowrate (m^3/d),
Q_r – return sludge (m^3/s),
X_R – concentration of MLSS (mg/l),(Biomass)
X_e – concentration of biomass in effluent ($gVSS/m^3$).

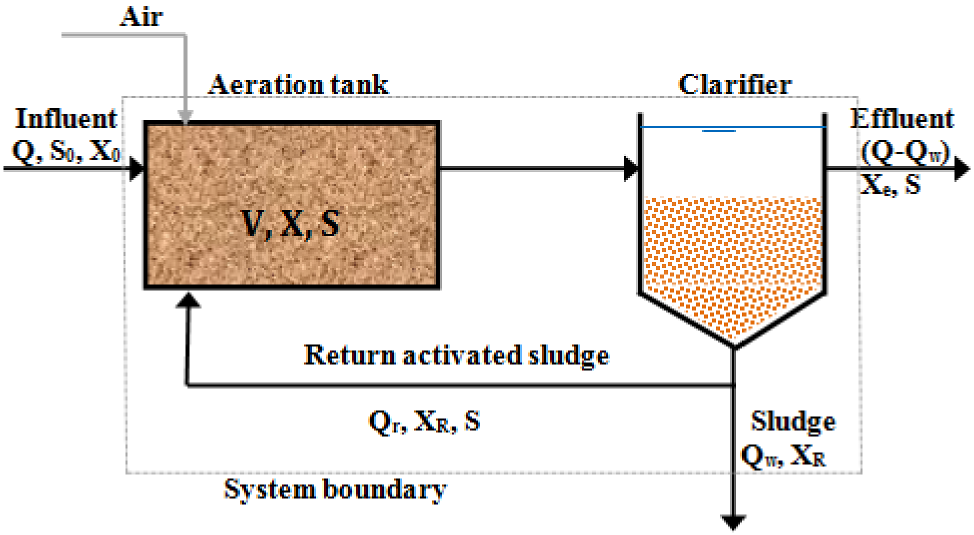

Fig. 1 Schematic diagram of activated sludge treatment process with model nomenclature with wasting from the sludge return line

Simplified word statement is:
Accumulation = inflow – outflow + net growth
Symbolic representation is

$$\frac{dX}{dt}V = QX_0 - [(Q - Q_w)X_e - Q_w X_R] + R_g V \tag{1}$$

Where is:
dX/dt - rate of change of biomass concentration in reactor measured as VSS/m^3*dR*$_g$ *- net rate of biomass production, gVSS/m*^{3}*d*

If it is assumed that the concentration of microorganisms in the influent can be neglected and that steady-state condition prevail (dX/dt =0), Eq. (1) can be simplified to yield

$$\frac{(Q - Q_w)X_e + Q_w X_R}{VX} = -Y\frac{r_{su}}{X} - k_d \tag{2}$$

Where is:
Y – synthesis yield coefficient, g VSS/g Bs COD
r_{su} *– rate of substrate concentration change due to utilization, g/m*^{3}*, d*
k_d *– endogenous decay coefficient, g VSS/g VSS, d*

The substrate utilization rate in a biological system can be modeled with the following expression for soluble substrates. Because the mass of substrate is decreasing with time due to substrate utilization and Eq. (3) is used in substrate mass balances, a negative value is shown.

$$r_{su} = -\frac{kXS}{K_s + S} \tag{3}$$

Where is:
*k – maximum specific substrate utilization rate, g substrate/g microorganisms*d*
Ks – half-velocity constant, substrate concentration at one-half maximum specific substrate utilization rate, g/m^3
S – growth-limiting substrate concentration in solution, g/m^3

The inverse of the term on the left-hand side of Eq. (2) is defined as the average solids retention time (SRT), as given below.

$$SRT = \frac{VX}{(Q - Q_w)X_e + Q_w X_R} \tag{4}$$

In the mass balance for the complete-mix reactor, presented above, the SRT was introduced as the fundamental process parameter that affects the treatment efficiency and general performance for the activated sludge treatment process.

Substrate mass balance:
The mass balance for substrate utilization in the aeration tank (see Fig. 1) is given by Eq. (5):
Accumulation = inflow – outflow + generation (Metcalf and Eddy 2003)

$$\frac{dS}{dt}V = QS_0 - QS + r_{su}V \tag{5}$$

Substituting the value for r_{su} (Eq. (3)) and assuming steady-state conditions (dS/dt=0), Eq. (5) can be written as:

$$S_0 - S = (\frac{V}{Q})(\frac{kXS}{K_s + S}) \tag{6}$$

The term 1/SRT is also related to μ, the specific biomass growth rate, as given by Eq. (7).

$$\frac{1}{SRT} = -Y\frac{r_{su}}{X} - k_d = \mu \tag{7}$$

Substituting Eq. (3) into Eq. (7) yields can be described with

$$\frac{1}{SRT} = \frac{YkS}{K_s + S} - k_d \tag{8}$$

The volume of the aeration tank divided by the influent flowrate is τ, the hydraulic retention time.

If Eq. (8) is solved for the term S/ (Ks+S) and substituted into Eq. (6), the following expression is obtained for the biomass concentration in the aeration tank

$$X = (\frac{SRT}{\tau})\left[\frac{Y(S_0 - S)}{1 + (k_d)SRT}\right] \tag{9}$$

As given by Eq. (9), the reactor biomass concentration is a function of the system SRT, the aerobic aeration tank τ, the synthesis yield coefficient, the amount of substrate removed (S0-S), and the endogenous decay coefficient.

As it shown in Fig. 1, part of the concentrated sludge is recycled in order to maintain enough mass of viable organisms in the bioreactor and reasonable food-to-mass (F/M) ratio (Metcalf and Eddy 2003).

$$F / M = \frac{S_0}{\tau X} \tag{10}$$

Where is:
*F/M=food to biomass ratio, gBOD or bsCOD/gVSS*d*
τ - hydraulic retention time of aeration tank, V/Q, d

Due to the fact that new cells are being continually formed, a portion of the total biomass must be continuously wasted from the system. Solids are usually wasted from the recycle line, but, alternatively, they could be wasted directly from the bioreactor. The sludge's age and solid retention time affect significantly the quality of the biological treatment. A system characterized by a large SRT would lead to deterioration of the quality of the process if subjected to mass loadings. Transient inputs are handled better with high solid levels and long hydraulic detention times. Shock loads of different types – hydraulic, quantitative, or in combination – do not produce equivalent disruptions of effluent quality for equal increases in the biomass loading rate. Other biochemical processes, such as nitrification and denitrification, may be developed in the bioreactor. Theory of the dynamic behavior of the activated sludge processes has been thoroughly investigated and presented in literature (Gujer *et al*. 1999).

The relationship between specific growth rate of microorganisms and substrate concentration is

$$\mu = \mu \max \frac{XS}{K_s + S} \tag{11}$$

Where is:
μ - the specific biomass grow rate,
μ_{max} *– maximum specific bacterial growth rate, g new cell/g cells, d.*

The modeling of the biochemical processes is based on several basic kinetic equations, describing bacterial growth, substrate utilization and the endogenous metabolism (decay) of bacteria, as well as the hydrolysis of entrapped organics. In the last 40 years, several activated sludge models have been developed, describing the biochemical processes in various manners (Eckenfelder *et al*. 2000).

Since the activated sludge treatment process is essentially composed of two main units, as it is shown in Fig. 1 (bioreactor and settling tank, linked together with a recycle line for returned sludge), a computation model for each unit is separately defined as a sub-model.

3. Modeling of wastewater treatment plant

3.1 Reasons and approach to modeling

Activated sludge wastewater treatment is a highly complex physical, chemical and biological process, and variations in wastewater flow rate and its composition, combined with time-varying reactions in a mixed culture of microorganisms, make this process non-linear and unsteady. The efficiency of the process is established by measuring the quantities that indicate quality of the treated wastewater, but that can only be determined at the end of the process. If the water quality is not acceptable, it is already too late for its improvement. Since there is no possibility of retracing the steps of the process back, all the mistakes in the control of the process could induce an ecological disaster on a small or big scale. Therefore, models that describe this process appropriately may be used as a basis for monitoring and optimal control of the process development.

Usually, engineers do not appreciate the dynamic character of the process, and steady-state procedures are still almost exclusively used to simplify the whole systems. The transient loading studies of activated sludge treatment process are the interest of technologists, microbiologists and engineers. The practical interest of engineers is focused on the design and control of the activated sludge process which is related to understanding of the mechanisms involved in biological growth and reproduction. It should be stressed that mathematical models are applicable both in the design and operation of treatment plants.

The main reasons for modeling wastewater treatment can be summarized as:

1. Research purposes (calibration and validation of the hydraulic model, biological model, aeration model, etc.)
2. Optimal selection of the best technology through more comparable options for WWTP
3. Cheaper than building/modifying the real system
4. Easier than carrying out testing on existing systems
5. Risk-free – see the consequences before implementation.

The approach to build a WWTP model includes the following steps:

1. Definition of the WWTP model purpose, or the objectives of the model application (design, reconstruction, control, learning).
2. Model selection, which means the selection of appropriate models needed to describe the different WWTP units that should be considered in the simulation, i.e. selection of the activated sludge model, the sedimentation model, etc.
3. Hydraulic determination of the models for the whole plant, or specific units of WWTP (i.e. hydraulics of the aeration tanks, secondary settling tanks, etc.).
4. Determination of the wastewater and biomass characterization, including biomass sedimentation (influent and effluent data, design parameters, etc.).
5. Calibration and verification of the activated sludge model parameters.
6. Evaluation of the different WWTP scenarios (i.e. optimization of the WWTP operation, process improvement, different technical (structure) solution, etc.).

In conducting process modeling to explore increasing a wastewater treatment system's capacity, process engineers first visit the existing plant to gather information and data. They determine the extent of model calibration and sensitivity analysis recommended for the specific objective, such as planning or detailed design. An existing flow and loading condition scenario is then analyzed using the simulator. Each model is calibrated to minimize observable discrepancies between field data and model predictions and can then be used to evaluate wet-weather treatment strategies. In addition, a sensitivity analysis can determine effects that different conditions have on plant capacity.

Wastewater process modeling can enhance projects involving an entire range of wastewater treatment processes, including physical-chemical; biological, such as activated sludge; and solids, such as thickening, digestion, and dewatering. It has become particularly useful to meet the effluent limits for nitrogen and phosphorus removal.

The mathematic modeling deals with static or dynamic behavior of activated sludge processes. Static models take some assumptions in the calculations, for example, constant hydraulic load, a constant concentration of biomass in the pool for a longer period, etc., which simplifies the whole system of calculation and interpretation of the results. As an example, there is a modelling according to ATV-A 131 standard, which is the most frequently used approach in design of WWTP larger than 500 PE (population equivalents) and describing the elimination of carbon, nitrogen and phosphorus compounds. It is based on the hydraulics and kinetics equation with determined values of the parameters, formed as a database of coefficients.

Dynamic simulation allows presentation depending on the biological treatment, as well as understanding and validation of certain processes in WWTP facilities. Approach to static modeling, based on some simplification and input assumptions, is not appropriate for understanding, researching and for prediction of the dynamic behavior of the system.

Dynamic models, such as the example of Activated Sludge Model 1 (ASM 1) describes the removal of carbon and nitrogen (nitrification and denitrification) in a system with activated sludge in the correlation with the variation of the whole system through the time. It is expected from the models to predict behavior of the chosen technology and system in different situations as well as designs, and to adjust WWTP facilities in the manner of optimization of each unit and provide the expected results of applied treatment processes.

Today, a lot of commercial computation softwares with wide and different possibilities are developed by different companies. Some of them are in the following list divided into the groups of static or dynamic programs:

- Simulation programs for steady (static) applications are: ANA / ANA win, Aqua Designer, ARA-BER, REVIVAL EXPERT, DENICOMP, Denika/Denika plus, Denni, SASS, etc.
- Simulation programs for unsteady (dynamic) applications are: AQUASIM, Arasim, ASIM, DENISIM, EFOR ApS, GPS-X, SASSPRO, SIMBA, STOAT, WEST, etc.

In the following chapter the focus will be on the overview of the Activated Sludge Model 1 (ASM1), which is the “state of the art” as theoretical mathematical model depicting the biological processes occurring in the activated sludge section of a wastewater treatment plant. As already mentioned above, it describes carbon oxidation, nitrification and denitrification process. Empirical models will also be mentioned, as well as commercial programs based on static models, which are very often used during the design process of the plants.

3.2 Review of the models development

Wastewater treatment plants are very complex hydro-technical facilities. Calculation and design of WWTP are based on a multidisciplinary approach, including knowledge of technology, hydraulics, biology, chemistry, physics, structure and math. Why do we need WWTP models? The WWTP models enhance the plant design and understanding of the process control.

Theoretical models are based on the physics and biochemistry principals involved in the descriptions of the behavior of the processes involved in activated sludge wastewater treatment.

Emphasis is usually put on the modeling of the processes in the biological reactor and on the hydrodynamic modeling of the secondary, settler tanks, and less on the hydraulic modeling of the whole wastewater treatment plant. WWTP models usually do not explicitly describe flow propagation through the reactors. Usually, hydraulics of the treatment plant is not sufficiently well known and can only be approximated or considered as a fix value for each unit. Frequently applied simplification is that the plant is considered as a few constant volume tanks with continuously complete mixing in series. The modeling of the biochemical processes is based on several basic kinetic equations, describing bacterial growth, substrate utilization and the endogenous metabolism (decay) of bacteria, as well as the hydrolysis of entrapped organics.

The first model which was developed in the early 20th century is the Activated Sludge Model (ASM). Developing the Activated Sludge Model No. 1 the IAWQ (International Association on Water Quality - now IWA), Task Group on Mathematical Modeling for Design and Operation of Biological Wastewater Treatment Processes introduced a new paradigm for the mathematical modeling of activated sludge systems. ASM1 as it was introduced in 1987 (Henze *et al*. 2000) has become a major reference for extensive scientific research and design of WWTP. The ASM1, ASM1, ASM2 and ASM3 are now widely used for wastewater treatment plant design, optimization, operation and training.

3.3 Dynamic simulation of wastewater treatment plants – ASM models

Activated sludge plants transform organic matter into biomass. The process is composed of two main units: a biological reactor and a settler. The effective operation of the process requires the biomass to be removed from the liquid stream (in the secondary settler) prior to being discharged in the receiving waters. The sedimentation of the particles in the liquor is achieved by gravity along with the density differences between the particles and the liquid. The complex behavior of the secondary settler and its importance for the successful operation of the ASP have made the settling process a great challenge for researchers working in the field of mathematical modeling. For that reason, different models are present in literature and usually combined with ASM models for research or design purpose. A significant problem in the evaluation of the activated sludge process is that it is difficult to separate the dynamics of the biological reactor from the settler, because of the recycle flow. From a modeling point of view, the components of the wastewater are described differently for the biological reactor and the secondary settler.

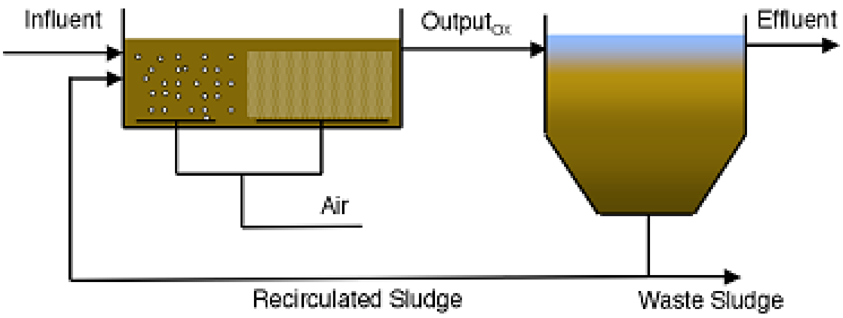

Fig. 2 Simple configuration for the activated sludge process

There are several models, proposed by the International Water Association (IWA), describing the biological process in the activated sludge plant (ASM1, ASM2, ASM3) (Mulas *et al*. 2006).

The ASM1, ASM2 and ASM3 models incorporate carbon oxidation, nitrification and denitrification, and ASM2 also describes the biological and chemical phosphorus removal. The ASM models have been "updated" several times since the first coming out of the ASM1 and most of the problems identified in the earlier versions have been corrected. The models are based on COD units (use chemical oxygen demand to define organic pollution) and ASM3 has a total organic carbon (TOC) based version as well.

• **ASM1**, the Activated Sludge Process Model No.1 can be considered as the reference model since it triggered the general acceptance of the biological process modeling. ASM1 was primarily developed to describe the removal of organic compounds and nitrogen with simultaneous consumption of oxygen and nitrate as electron acceptor. Furthermore, the model aims at yielding a good description of the sludge production. COD (Chemical Oxygen Demand) was adopted as the measure of the concentration of organic matter. Generally, the ASM1 model consists of 13 components or state variables (Table 1) involved in 8 reactions.

• **ASM2**, the Activated Sludge Process Model No.2 extends the capabilities of the ASM1 to the description of bio-phosphorus. ASM2 is the most complex model and it requires knowledge of the 19 concentration and 22 of biological processes.

• **ASM2d**, the Activated Sludge Process Model No.2d is built on the ASM2 model adding the denitrifying activity of Polyphosphate Accumulating Organisms (PAOs) to allow a better description of the dynamics of phosphate and nitrate removal.

• **ASM3**, the Activated Sludge Process Model No.3 was also developed for biological nitrogen removal, with basically the same goal as the ASM1. The major difference between the ASM1 and the ASM3 models is that the latter recognizes the importance of storage polymers in the heterotrophic activated sludge conversion. ASM3 model requires knowledge of the 13 components of wastewater and 12 processes.

The ASM models and the equations are publicly available. Mathematical models related to ASM1 are implemented in various computer codes for the simulation of the behavior of activated sludge systems treating municipal wastewater of mainly domestic origin.

Beside the very high complexity of these models, their main disadvantage is the fact that they are created especially for modeling of wastewater treatment process originated from households (municipal water). The principle application of ASM model is not exactly suitable for industrial wastewater and does not describe well enough all the dynamics of the processes.

Limitations of non-structural models could be overcome by using empirical models. These models are simple and do not require prior knowledge of the process. Development of the model is based on statistical analysis of experimental data, establishing a mutual dependence and relation of certain variables. Dependence is expressed by the function (equation model). There are two basic types of these models - linear and nonlinear.

Linear empirical models are most commonly used to describe linear, non-linear processes, or complex bioprocesses. Their application is based on the assumption that non-linear processes can be approximated by a linear function.

Development of linear models is based on the application of modeling methods such as Multiple Linear Regression (MLR) or the method of Partial Least Squares (PLS).

3.3.2 State Variables of ASM model

The ASM1 model allows us to describe phenomena of organic matter and nitrogen removal. In fact, the main classification of state variables in the model is based on organic matter, expressed in terms of COD and nitrogen compounds (Table 1). The organic matter is further divided into biodegradable COD (SS and XS), non-biodegradable COD (SI and XI) and active biomass (XBH and XBA).

The readily biodegradable substrate is assumed to be made up of simple soluble molecules that can be easily absorbed by the organisms and metabolized for energy and synthesis. In contrast, slowly biodegradable substrate consists of relatively complex molecules that require enzymatic breakdown prior to absorption and utilization. Non-biodegradable organic matter is biologically inert and passes through the system without change in form. It can be soluble (SI), which leaves the process at the same concentration as it enters and particulate (XI), becoming enmeshed in the activated sludge and leaving the system mainly as the wastage flowrate. Moreover, the biomass is divided into heterotrophic (XBH) and autotrophic biomass (XBA). As an extra component, XP is included to take into account the inert particulate arising from cell decay. As for the organic part, nitrogenous matter can be divided into two categories: non-biodegradable and biodegradable. With respect to the biodegradable part, the particulate portion is associated to the non-biodegradable particulate COD. The soluble portion is usually negligible and is not incorporated into the model. The biodegradable matter is divided into free and ionized ammonia (SNH), soluble organic nitrogen (SND), and particulate organic nitrogen (XND).

The last stage of the process is hydrolysis of soluble organic nitrogen in parallel with the hydrolysis of slowly biodegradable organic matter. The soluble organic nitrogen is converted into ammonia. For the sake of simplicity, the autotrophic conversion of ammonia to nitrate is considered to be a single step process which requires oxygen.

Table 1 ASM1 State Variables

State Variable	ASM1 Notation	
Soluble inert organic matter	S_I	$gCOD/m^3$
Readily biodegradable substrate	S_S	$gCOD/m^3$
Particulate inert organic matter	X_I	$gCOD/m^3$
Slowly biodegradable substrate	X_S	$gCOD/m^3$
Active heterotrophic biomass	X_{HB}	$gCOD/m^3$
Active autotrophic biomass	X_{BA}	$gCOD/m^3$
Part. Prod. From biomass decay	X_P	$gCOD/m^3$
Dissolved Oxygen	S_O	$gO2/m^3$
Nitrite and Nitrate Nitrogen	S_{NO}	gN/m^3
Free and Ionized Ammonia	S_{NH}	gN/m^3
Soluble biodegr. Organic N	S_{ND}	gN/m^3
Part. Biodegr. Organic N	X_{ND}	gN/m^3
Alkalinity	S_{ALK}	Molar units

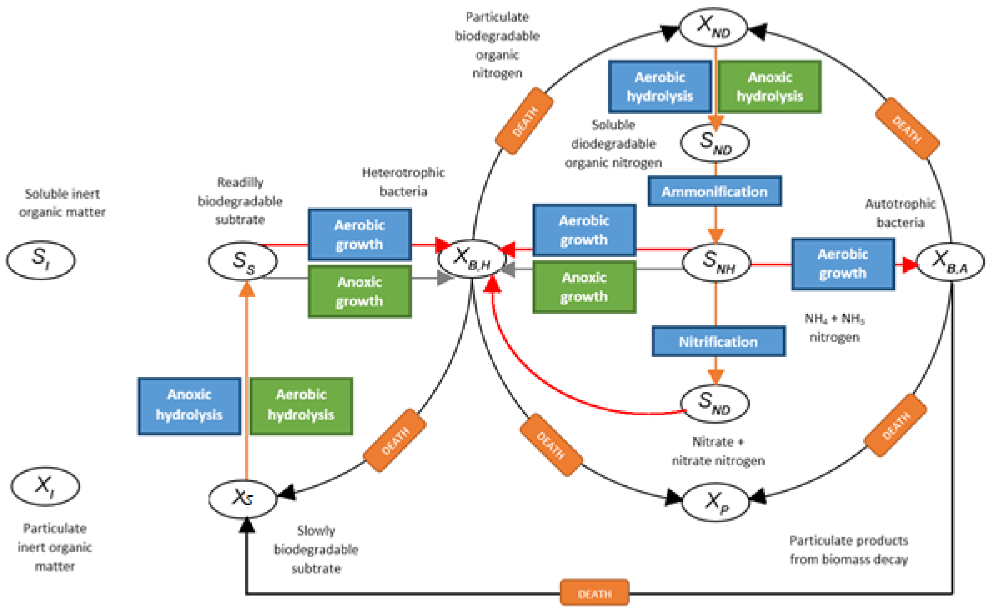

Fig. 3 Activated sludge model 1 – Model process

That means that a unique state variable (SNO) represents nitrate/nitrogen compounds in the activated sludge system. Furthermore, one variable is included to represent the dissolved oxygen consumption in the activated sludge system, SO.

Even if inclusion of alkalinity, SALK, in the conversion process is not essential, its inclusion in the model is also desirable because it provides information whereby undue changes in pH can be predicted.

Fig. 3 presents in a schematic way how different compounds participate in the conversion processes (Martinello *et al*. 2000). There is a list of model parameters, kinetics and stoichiometric, used in equations of the model (Henze *et al*. 2000).

Kinetic and stoichiometric parameters of the ASM1 models, shown on the Fig. 3 are listed below:

Activated Sludge Model 1 - Model parameters

The stoichiometric parameters are:		
Heterotrophic yield	(g X_{BH} COD_{formed} (g $COD_{utilised}$)$^{-1}$	Y_H
Autotrophic yield	(g X_{BA} COD_{formed} ($gN_{utilised}$)$^{-1}$)	Y_A
Fraction of biomass yielding particulate products	(dimensionless)	f_p
Mass N/mass COD in biomass	(g N (g COD)$^{-1}$ in biomass (X_{BA} and X_{BH}))	i_{XB}
Mass N/mass COD in products from biomass	(g N (g COD)$^{-1}$ in X_P)	i_{XP}
The kinetic parameters are:		
Heterotrophic maximum specific growth rate	(day^{-1})	μ_H
Heterotrophic decay rate	(day-1)	b_H
Half-saturation coefficient for heterotrophs	(g COD m^{-3})	K_s
Oxygen half-saturation coefficient for heterotrophs	(g O_2 m^{-3})	K_{OH}

Nitrate half-saturation coefficient for denitrifying heterotrophs	(gNO_3-Nm^3)	K_{NO}
Autotrophic maximum specific growth rate	(day^{-1})	μ_A
Autotrophic decay rate	(day^{-1})	b_A
Oxygen half-saturation coefficient for autotrophs	(g O_2 $m^{-3)}$	K_{OA}
Ammonia half-saturation coefficient for autotrophs	(gNH_3-Nm^3)	K_{NH}
Correction factor for anoxic growth of heterotrophs	(dimensionless)	H_g
Ammonification rate	(m^3(g COD day)$^{-1}$)	k_a
Maximum specific hydrolysis rate	$gX_S(gX_{BH}$ COD day)$^{-1}$)	k_h
Half-saturation coeff. for hydrolysis of slowly biodegradable substrate	$gX_S(gX_{BH}$ COD)$^{-1}$)	k_x
Correction factor for anoxic hydrolysis	(dimensionless)	η_h

The state variables included in the ASM1 are the fundamental components that act upon the process, but they are not always measurable or interpretable in many practical applications. Therefore, some composite variables can be calculated from the state variables in order to combine them into forms that are typically measured in reality, such as COD (Chemical Oxygen Demand), TSS (Total Suspended Solids) and TN (Total Nitrogen) with conversion coefficients 0.75 [gSS/gCOD] for the inert and particulate material and 0.9 [gSS/gCOD] for the heterotrophic and autotrophic biomass. Two types of microorganisms carry out the reactions in ASM1 processes: heterotrophs and autotrophs.

In literature, the kinetic and stoichiometric parameters are reported. The parameters selection of a mathematical model is known as model calibration and as a consequence of high interdependence of the state variables, troublesome nonlinearities, lacking identifiably and verifiability, the calibration of the model can be difficult and laborious. The calibration task becomes very hard especially because the data available from wastewater treatment plants are generally very variable and not always reliable.

Most of biological process models follow the standard matrix notation. The notation makes clear the processes incorporated in the model and the state variables involved. The matrix is usually referred to Petersen Matrix and is well known by the modelers of biological wastewater treatment system. Table –matrix for ASM 1 comprises the state variables (13) and important processes, (8) shown in separated rows.

The Activated Sludge Model 2 (ASM2) is an extension of the ASM1 model, but more complex and includes more components which are required to characterize the system. Additional biological processes are included, primarily in order to deal with biological phosphorus removal. The most significant difference between ASM1 and ASM2 is the fact that the biomass has a cell-internal structure, and therefore its concentration cannot simply be described with the XH (heterotrophic organisms) parameter. In addition, the model also contains two chemical processes which may be used to model chemical precipitation of phosphorus.

The ASM1 model was based entirely on COD for all particulate organic matter, as well as the total concentration of the activated sludge, whereas ASM2 includes poly-phosphates (XPP), a fraction of the activated sludge which is of primary importance for the performance of the activated sludge system, but which does not exert any COD. For this reason, the possibility of including total suspended solids (TSS) in the model was introduced. TSS allows for inclusion of mineral particulate solids in the influent to treatment plants, as well as generation of solids in the context of precipitation of phosphorus.

The matrix of ASM 1 is given in Fig. 4

Component i→ / Process j ↓		1 S_I	2 S_S	3 X_I	4 X_S	5 X_{HB}	6 X_{BA}	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	11 S_{ND}	12 X_{ND}	13 S_{ALK}	Process Rate, $[ML^{-3}T^{-1}]$
1	Aerobic growth of hetero-trophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_0}{K_{O,H}+S_O}\right)X_{B,H}$
2	Anoxic growth of hetero-trophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{286Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2,86Y_H}-\frac{i_{XB}}{14}$	$\eta_g\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_B X_{B,H}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57}{Y_A}+1$	$\frac{1}{Y_A}$	$i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\hat{\mu}_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
4	"Decay" of hetero-trophs				1-fp	-1		f_p					$i_{XB}-f_p$		$b_H \cdot X_{B,H}$
5	"Decay" of autotrophs				$1-f_p$		-1	f_p					$i_{XB}-f_p$		$b_A \cdot X_{B,A}$
6	Ammoni-fication of soluble organic nitrogen										1	-1		$\frac{1}{14}$	$k_a \cdot S_{ND} \cdot X_{B,H}$
7	"Hydro-lysis" of entrapped organics		1		-1										$k_h\frac{X_S/X_{B,H}}{K_X+\frac{X_S}{X_{B,H}}}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_H\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}$
8	"Hydro-lysis" of entrapped organics nitrogen												1	-1	$[process7]\cdot\frac{X_{ND}}{X_S}$

The actual process rate is shown in the far right column:

- 1 is the aerobic growth of heterotrophs;
- 2 is the anoxic growth of heterotrophs;
- 3 is the aerobic growth of autotrophs;
- 4 is the decay of heterotrophs;
- 5 is the decay of autotrophs;
- 6 is the ammonification of soluble organic nitrogen;
- 7 is the hydrolysis of entrapped organics;
- 8 is the hydrolysis of entrapped organic nitrogen.

Activated Sludge Model 3 (ASM3) was developed to correct some of the deficiencies of the earlier ASM1 and to include the advances in activated sludge modeling achieved in the decade following the publication of ASM1(Gujer *et al*. 1999). It includes 12 biochemical processes and 13 components. Neither biological nor chemical phosphorus removal processes are included in ASM3.

Today, the ultimate goal is to promote the correct use of ASM-type models by practitioners, and to overcome any major obstacles that prevent widespread use of Activated Sludge Modeling in practice.

The main objectives cited for building and using a model are: optimization (59%), design (42%) and prediction of future operations (21%).

The modeling tasks differ depending on the organization type as follows:

- Optimization (daily plant operation, control...) is the main objective regardless of the organization type (commercial simulation programs),
- Private companies use models for design (new plant design and expansion) more than any other organization types (usually commercials simulation programs),
- Universities are the only ones having a significant use of models for educational and research purposes.

3.3.3 Restrictions in implementation of activated sludge models

Regarding application of ASM in literature, some constraints are reported. The ASM1 (and ASM3) was developed for the simulation of the aerobic and anoxic treatment of domestic wastewater in activated sludge systems. ASM1 and ASM3 have been developed based on experience in the temperature range of 8–23℃. Outside of this range, model application may lead to very significant errors and even model structure may become unsatisfactory. ASM3 (and ASM1) does not include any processes that describe biomass behavior in an anaerobic environment. Development of ASM3 is based on experience in the range of pH values from 6.5 to 7.5. The concentration of bicarbonate alkalinity (SALK) is supplied to give early warnings when pH values below this range are to be expected. Alkalinity must be dominated by bicarbonate. ASM3 cannot deal with elevated concentrations of nitrite. ASM3 (and ASM1) is not designed to deal with activated sludge systems with very high load or small SRT (<1 day) where flocculation/ adsorption of XS and storage may become limiting.

4. Commercial software

Specific commercial software usually contains extended database and libraries of predefined process models referring to the whole wastewater treatment plant. The process configuration to be simulated can be easily designed and constructed by appropriate choosing of process unit blocks and connecting. Pop-up windows allow modifying the model parameters. Following is the list of some of the softwares, divided into static and dynamic applications (ATV-DVWK-A 131E, 2000; GPS-X, 2008):

- Simulation programs for steady (static) applications are: ANA / ANA win, Aqua Designer, ARA-BER, REVIVAL EXPERT, DENICOMP, Denika/Denika plus, Denni, SASS, etc.
- Simulation programs for unsteady (dynamic) applications are: AQUASIM, Arasim, ASIM, DENISIM, EFOR ApS, GPS-X, SASSPRO, SIMBA, STOAT, WEST, etc. An overall process model is developed by using some of commercial software (like GPS-XTM) which

solve a series of simulated equations simultaneously to propose a custom solution for a specific facility.

For instance, GPS-X is the most advanced tool available for the mathematical modeling, simulation, optimization and management of wastewater treatment plants. The user-friendly drag and drop interface and comprehensive database of unit processes allow users to quickly and easily assemble a treatment plant model, enter characterization data, and run simulations (Fig. 5). It can virtually cover all of the unit processes found in a wastewater treatment plant, including advanced nutrient removal models, fixed-film operations, anaerobic reactors, secondary settler and so on (GPS-X, 2008).

The GPS-X is a modular multi-purpose modeling environment for the simulation of municipal and industrial wastewater treatment plant. With regard to the bioreactor in the activated sludge process, the whole ASM family is included in the GPS-X library. For each process unit many different attributes and characteristics that uniquely describe the object must be specified. For this reason, physical parameters like the real dimension of the unit and kinetic and stoichiometric parameters for the biological reactor should be provided to the simulator. It should be also noted that the aeration basin model can be represented with different configurations. The GPS-X owns two important modules: the analyzer and the optimizing module (GPS-X, 2008).

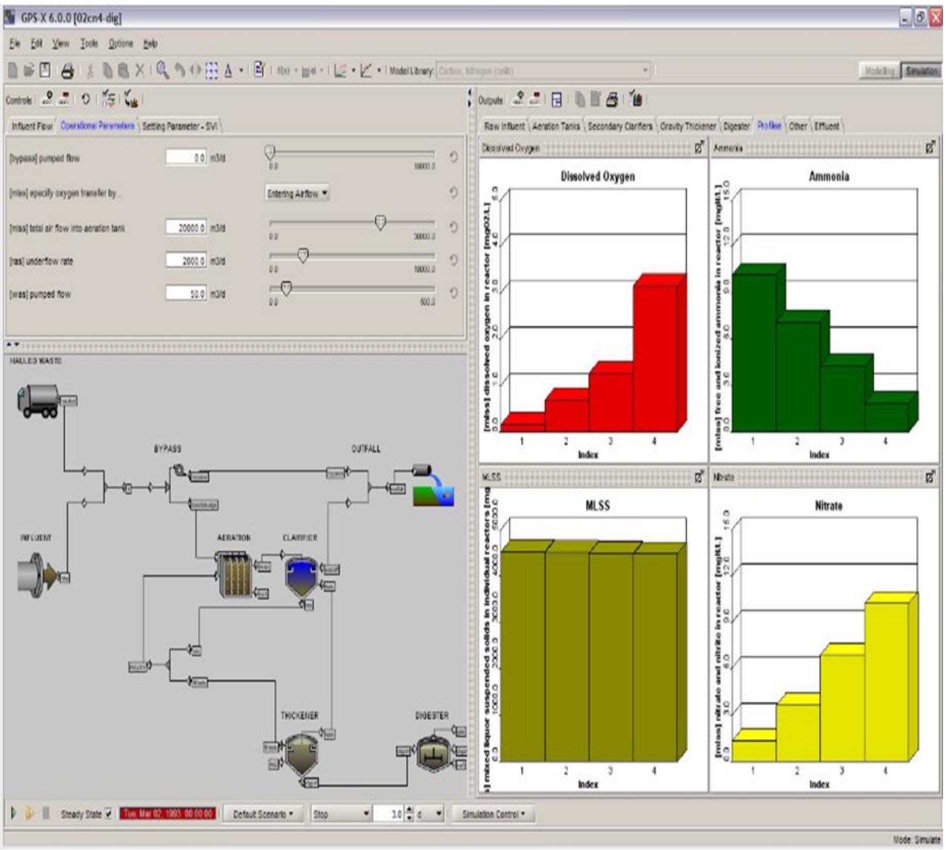

Fig. 5 GPS-X interface (GPS-X, 2008)

The improvement in WWTP design, analyses and optimization using GPS-X are following:

- Compare various design or operating strategies
- Verify existing plant capacity
- Isolate and quantify bottlenecks in liquid or solids lines
- Assess potential flow increases or regulatory changes
- Identify cost saving strategies (energy usage, reduction, ...)
- Evaluate impact of new technology
- Support regulatory decision.

4.1 Static simulations programs

Simulation programs are in general divided into two groups: static and dynamic. Previously, as example for dynamic software, GPS-X simulation program was briefly presented. In this section, simulation program developed by BITCom DE will be presented shortly. This software has been used for design and optimization of the process for several WWTP in FBiH in last few years.

AQUA DESIGNER is the powerful tool for the design of wastewater treatment plants, incl. preliminary treatment, biological and sludge treatment. AQUA DESIGNER provides numerous results for presentation and approval, including buildings, machines, operational costs and scaled drawings (Aqua Designer, Software, 2010).

With AQUA DESIGNER various processes for continuous flow plants with separate stage denitrification, intermittent denitrification or simultaneous denitrification, and also for carbon degradation, or only nitrification, can be calculated. Design includes the biological stage, but also preliminary treatment and sludge treatment. Sludge treatment includes thickener, digester with gas and heat production unit. Loads and balances for supernatant and dry solids are also displayed and reported. Operational costs, energy demand, consumables, sludge removal, energy production from the sludge treatment will also be taken into consideration.

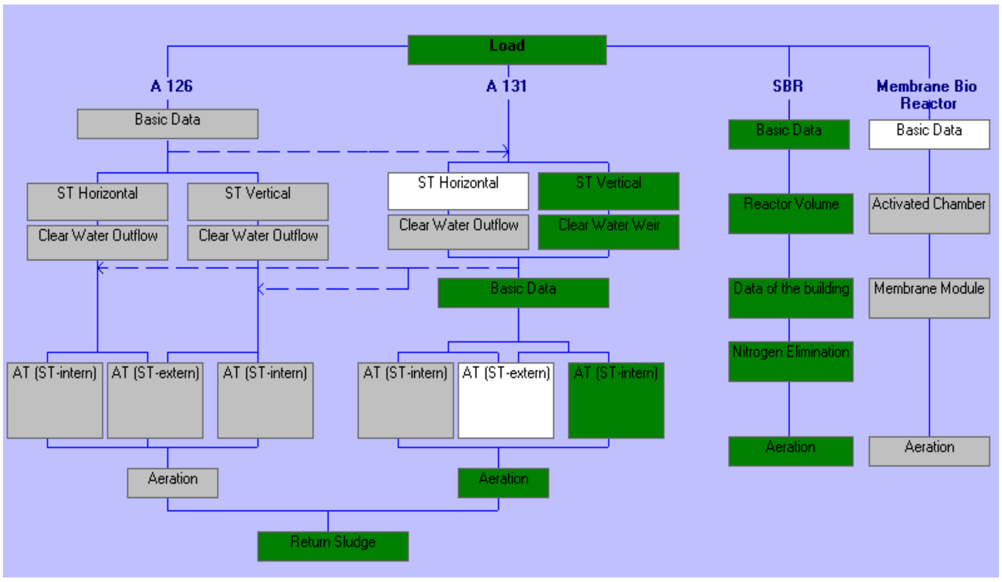

Fig. 6 AQUA DESIGNER flow diagram (Aqua Designer, Software, 2010)

Options for SBR or MBR technology for WWTP are included. Furthermore, other units of the plant, such as secondary sedimentation tank, sludge treatment and grit chamber, are the part of the design tools.

The aeration system is also included in modeling by Aqua Designer. The aeration system is the most important equipment of a wastewater plant. 75% of the energy used for the wastewater treatment is covered by the aeration system. The correct design of the aeration system is the basis for a good operation and the operational costs. As the energy costs are the main cost value of an aeration system, a real comparison of different systems must concern both the operation and the investment costs of the whole life cycle. Detailed reports, operational cost, key figures, drawings etc. are provided as results.

One of the special characteristics of AQUA DESIGNER is the consistent guidance of the user by a flow diagram. From the first sight, current processing status is visible, the selected way of design or process and the possible alternatives (Fig. 6). The flow diagram of the Aqua Designer software is shown in Fig. 6.

Opening the new windows, in order from top to bottom, is easy and selection is possible by click on the individual windows (Fig. 7), with defined parameters for the calculation of individual process and units. Also, it is possible to define and give the option of parameters (dimensions of specific facilities, equipment or characteristics of the process...).

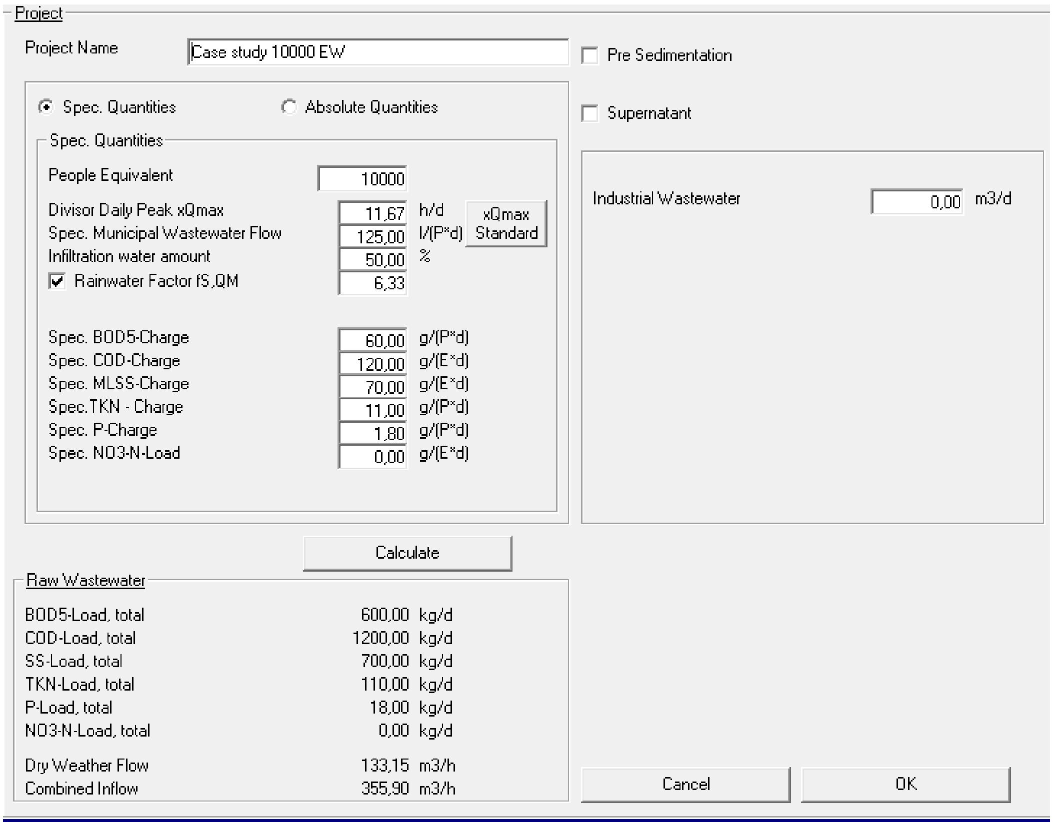

Fig. 7 AQUA DESIGNER – Calculation steps for WWTP (10.000 PE) (Aqua Designer, Software, 2010)

5. Conclusions

The wastewater treatment process is usually operated under highly variable loading conditions with the variability of influent and effluent quality because of the time-varying change in flow-rate and composition of wastewater. That is the reason why complexity of the activated sludge processes demands more and more accurate and well developed modeling techniques. Generally speaking, models are most often used by researchers for optimization purposes, while in public or private companies most models are used for design studies.

Activated Sludge Models and other commercial simulation programs are now widely used for wastewater treatment plant design, optimization, operation and training. Plenty of modeling software can be found on the markets which are based on the ASM modeling concepts and equations. There is a great interest for further testing of the process modeling concepts, as well as for required improvements of already existing models for WWTP modeling.

Engineers, mathematicians, technologists and other experts for wastewater have been developing wastewater process modeling aiming to further expand the capabilities of developed models. Working on various aspects of the same issues and technologies will enable engineers to examine and improve biological, physical and chemical characteristics of treatment, and also hydraulic and technical design of WWTP.

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