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Mathematical models for wastewater treatment plants: first applications in Friuli

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Abstract. The municipal or industrial wastewater biological treatment before discharge in rivers or other hydrological bodies, is the most common system to remove or minimize the pollution of wastewater. The activated sludge system is the most famous biological system for wastewater treatment. The activated sludge treatment removes the soluble organic and inorganic materials and coagulates unsettable and colloidal solids by the microorganisms that compose the sludge. The study of biochemical processes involved in wastewater biologic treatment has determined a new approach to planning: the modellistic approach. This article presents an introduction to the underlying mathematical theory and some real-case experiences with this model. The microorganisms that compose the activated sludge are called biomass, while pollutants are called substrate. The biomass is allowed to grow using pollutants as sources of carbon and/or energy, removing them pollutants from the wastewater by converting them in new biomass, H2O e CO_2. There are different kinds of microorganisms which are classified into heterotrophs and autotrophs as they utilize oxygen or carbon substance as electron acceptor. The main pollutant substances to be removed by biological treatments are carbon compounds, nitrogen and phosphate. This issues has been intriguing many universities and research centers abroad for a long time now. In particular, in 1987 the Task Group of I.A.W.Q. (International Association on Water Quality) formulated the Activated Sludge Model N. 1 that has been applied several times and whose validity and reliability has been demonstrated. The A.S.M. N. 1 considers removal of carbon and nitrogen. Increasingly complex models have been formulated in recent years which also consider removing phosphate (A.S.M. N. 2 and 3). The Chemical Department of the University of Udine has been studying the modellistic approach to planning/managing of wastewater treatment plants for some years now by the A.S.M. N. 1 which is described below.

Keywords. Activated sludge, Mathematical models, Dynamic simulations.

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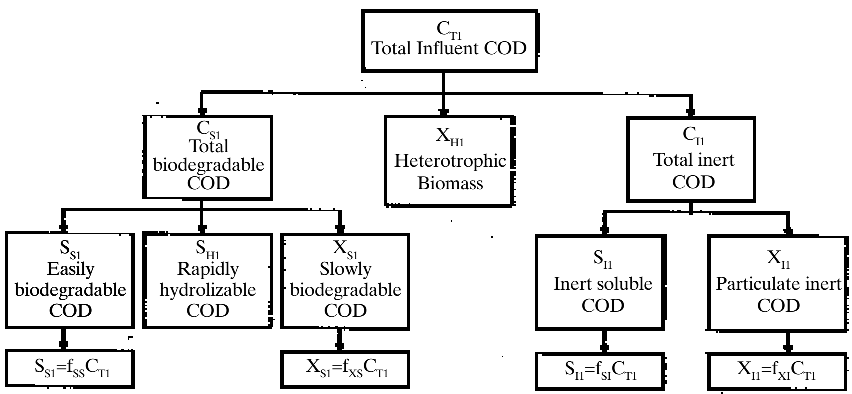
Introduction

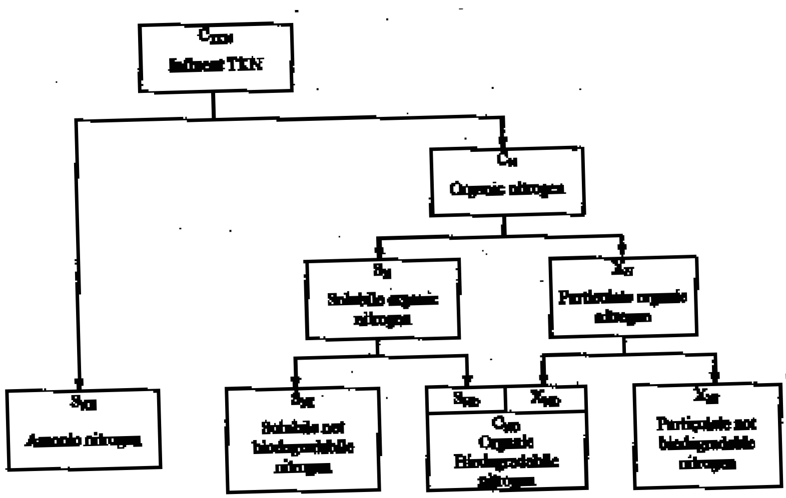
The pollutants. The parameter used for measuring the current pollution level is COD (Chemical Oxygen Demand). It refers to the quantity of oxygen required to oxidize the organic substance by a very strong oxidant reagent (e.g., potassic dichromate) in conditions of high acidity. It has demonstrated to be the best parameter because it is the only one correlating equivalent electrons in organic substrate, biomass and oxygen. Principally different forms of organic carbon are collected together and differentiated according to biodegradation features. The total influent COD has two components: total not biodegradable COD, or inert, and total biodegradable COD. Those fractions could be further divided into a soluble fraction and a particulate one. The easily biodegradable COD is perhaps composed by soluble elements such as volatile fatty acids, easy carbohydrates, alkali, amino acids, etc. and others that could be directly absorbed by synthesis.

The slowly biodegradable COD does not penetrate the cellular wall so it has to undergo the extracellular hydrolysis before being absorbed.



The nonoxydized nitrogen components are experimentally determined by the Total Kjeldahl Nitrogen (TKN) Test and by the ammoniac nitrogen test (reporting the free ammonia content as well as ammonia ion content). The TKN value refers to the sum of organic nitrogen and ammonic nitrogen. Organic nitrogen is the difference between TKN and ammonic nitrogen. Biodegradable organic nitrogen is composed by soluble biodegradable organic nitrogen and particulate biodegradable organic nitrogen. The ammonia nitrogen becomes available to incorporation into new cellular components or to nitrates and nitrites (NO_2^- and NO_3^-) by oxidation in the nitrification process. The particulate biodegradable organic nitrogen is hydrolyzed to organic nitrogen by the action of heterotrophic microorganisms. The further conversion of biodegradable soluble organic nitrogen to ammonia occurs by a process of ammonification regulated by a similar heterotrophic microbic activity.

In wastewater phosphate is pre-



sent in three forms: orthophosphate (PO_4^{-3}), polyphosphate (P_2O_7) and organically linked phosphate. Orthophosphates and simple polyphosphates or condensed phosphates make up the totally inorganic phosphate.

Materials and methods

The models. To explain the principles underlying the A.S.M. N.1 we consider, for example, the heterotrophic biomass, X_H, the most important particulate component in the activated sludge process responsible for the biodegradation of the organic carbon in aerobic conditions. The processes are:

Growth of the biomass. If growth is balanced, the utilization of one unit of substrate (carbon and/or energy source) by the biomass leads to the production of Y units of biomass (with Y smaller than one) as indicated in the following expression:

$\frac{dX}{dt} = -Y\frac{dS}{dt}$, where coefficient Y is known as "yield".

To correlate the growth with the concentration of substrate, the saturation curve with hyperbolic-rectangular expression proposed by Monod is applied.

The growth of the biomass including the influence of dissolved oxygen is expressed as follows:

$$\frac{dX_H}{dt} = \mu_H \left(\frac{S_S}{K_S + S_S}\right) X_H$$

$$= \hat{\mu}_H \left(\frac{S_S}{K_S + S_S}\right)\left(\frac{S_O}{K_{OH} + S_O}\right) X_H$$

where

μmax = greatest speed of heterotrophic growth [days-1];

K_S = substrate concentration of the substrate where μ = ½ μmax [mg COD/l];

K_{OH} = coefficient considering the switching effect of oxygen concentration [mg COD/l].

Death and decay. The life of particulate components in activated sludge systems is also influenced by the processes correlated to the loss of vital heterotrophic biomass.

It is supposed that the death or the loss of microorganisms occurs without electron acceptors:

$$\frac{dX_H}{dt} = -b'_H X_H$$

where: b'_H = speed of vital loss in heterotrophic biomass [d^{-1}].

The greatest part of the nonvital biomass becomes available as slowly biodegradable substrate, X_S, while the other part is present as endogen inert mass, X_P.

Denitrification. Denitrification is an anoxic process that requires the absence of oxygen and the presence of an adequate source of carbon as well as of electrons. The process is occurs by facultative heterotrophic bacteria.

The modelistic principle is based on a simplifying hypothesis: it utilizes the same expression used for heterotrophic growth plus an empiric correcting factor η_G<1

$$\frac{dX_{B,H}}{dt} = \hat{\mu}_H \left(\frac{S_S}{K_S + S_S}\right)\left(\frac{K_{OH}}{K_{OH} + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\eta_G X_H$$

For a dynamic model to be developed, it is necessary to set a control volume and to establish a mass balance for each component with regard to that volume:

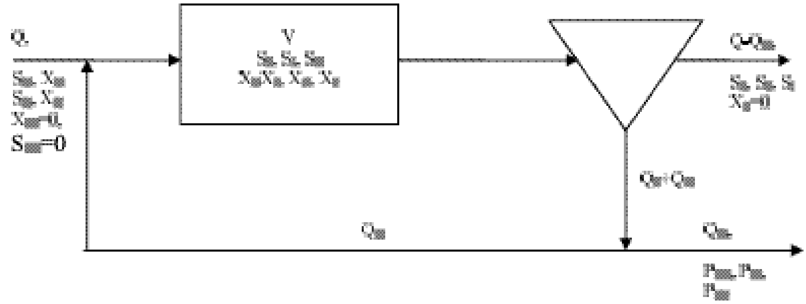
accumulation = input - output + generation

In carbon removal models it is necessary to consider at least eight components to reflect accurately wastewater characteristics:

- S_I, S_S, X_I, X_S, define the organic nature of water;
- X_H, S_P, X_P, represent the heterotrophic vital biomass as soluble and particulate microbic products;
- S_O indicates the oxygen concentration;
- S_I, e X_I are inert and are not indicated.

The relations between process components and the parameters of the model are derived on the basis of the continuity equations that define mass balance between input and output flows.

The diagram below shows a kinetic model for carbon removal.



1) Balance for S^S:

$$V\frac{dS_\blacksquare}{dt} = (Q+Q_\blacksquare)S_\blacksquare - V\left(\frac{\hat{\mu}_\blacksquare}{Y_\blacksquare}\frac{S_\blacksquare}{K_\blacksquare+S_\blacksquare}X_\blacksquare - (1-f_\blacksquare)K_\blacksquare X_\blacksquare\right)$$

$$-\frac{\hat{\mu}_\blacksquare}{Y_\blacksquare}\frac{S_\blacksquare}{K_\blacksquare+S_\blacksquare}X_\blacksquare + (1-f_\blacksquare)K_\blacksquare X_\blacksquare = \frac{1}{\vartheta_\blacksquare}S_\blacksquare = -\frac{1}{\vartheta_\blacksquare}S_\blacksquare$$

2) Balance for X^H:

$$V\frac{dX_\blacksquare}{dt} = (Q+Q_\blacksquare)X_\blacksquare + V\left(\hat{\mu}_\blacksquare\frac{S_\blacksquare}{K_\blacksquare+S_\blacksquare}X_\blacksquare - b'_\blacksquare X_\blacksquare\right)$$

$$\hat{\mu}_\blacksquare\frac{S_\blacksquare}{K_\blacksquare+S_\blacksquare}X_\blacksquare - b'_\blacksquare X_\blacksquare = \frac{1}{\vartheta_\blacksquare}X_\blacksquare = 0$$

3) Balance for X_S:

$$V\frac{dX_\blacksquare}{dt} = (Q+Q_\blacksquare)X_\blacksquare - V\left(K_\blacksquare X_\blacksquare - (1-f_\blacksquare)b'_\blacksquare X_\blacksquare\right)$$

$$(1-f_\blacksquare)b'_\blacksquare X_\blacksquare - K_\blacksquare X_\blacksquare = \frac{1}{\vartheta_\blacksquare}X_\blacksquare = \frac{1}{\vartheta_\blacksquare}X_\blacksquare$$

4) Balance for X_P:

$$V\frac{dX_\blacksquare}{dt} = (Q+Q_\blacksquare)X_\blacksquare + V\left(f_\blacksquare b'_\blacksquare X_\blacksquare\right)$$

$$f_\blacksquare b'_\blacksquare X_\blacksquare = \frac{1}{\vartheta_\blacksquare}X_\blacksquare = 0$$

5) Balance for S_P :

$$V\frac{dS_\blacksquare}{dt} = (Q+Q_\blacksquare)S_\blacksquare + V\left(\alpha_\blacksquare\hat{\mu}_\blacksquare\frac{S_\blacksquare}{K_\blacksquare+S_\blacksquare}X_\blacksquare + f_\blacksquare K_\blacksquare X_\blacksquare\right)$$

$$\alpha_\blacksquare\hat{\mu}_\blacksquare\frac{S_\blacksquare}{K_\blacksquare+S_\blacksquare}X_\blacksquare + f_\blacksquare K_\blacksquare X_\blacksquare = \frac{1}{\vartheta_\blacksquare}S_\blacksquare = 0$$

It is a five-equation system that require a simultaneous solution.

A matrix-based representation is used for a clear and univocal representation of the system.

Nitrification. There are two main ways to obtain nitrification in activated sludge systems.

Based on one of them, nitrification occurs in the same biological reactor used for carbon removal ("Combined carbon oxidation-nitrification system"), according to the other nitrification occurs by a separate-stage process, the first for organic carbon removal and the other for nitrification.

Below is a schematic representation of mass balance equations for nitrification.

Table 1. Kinetics and stoichiometrics of the carbon removal process and nitrification.

Component i → ↓process j	1 X_H	2 S	3 X_A	4 S_{NO}	5 S_{NO}	6 S_{NO}	Process velocity ρj
Heterotrophic growth	1	$-\frac{1}{Y_H}$		$-i_B$		$-\frac{1}{fY_H}-f_x$	$\hat{\mu}_H \frac{S_s}{K_S+S_S} X_H$
Heterotrophic decay	-1			i_B		$-f_x$	$k_d X_H$
Autotrophic growth			1	$-\frac{1}{Y_A}-i_B$	$-\frac{1}{Y_A}$	$-\frac{4.57}{Y_A}-f_x$	$\hat{\mu}_A \frac{S_{NH}}{K_{NH}+S_{NH}} X_A$
Autotrophic decay			-1	i_B		$-f_x$	$B_A X_A$
Parameters	VSS	BOD_5	VSS	NH_3-N	NO_3-N	O_2	

A.S.M. N. 1. The activated Sludge Model N. 1 consists of eight processes and thirteen components. For simplicity, the following matrix is used, where columns correspond to different components and rows correspond to different processes.

Some of the parameters indicated in the matrix can be obtained from the literature. Indeed, the parameters must generally be experimentally evaluated through sensitivity studies.

For the parameters below it is possible to use the indicated values as fixed ones because they have been demonstrated to be unaltered for all the analyzed systems. The others must be determined experimentally.

The law. The new law requirements, in particular Law Decrees 152/99 correcting and integrating provisions of Law Decree 258/00, concerning water saving from pollution, create new bounds on the water effluent quality of the treatment plant. Of particular interest is the reference to the yield of the treatment plants, as stated in Directive 91/271/EC, that requires maintainance of the above values.

In our region, as almost everywhere in Italy, there is a great number of wastewater treatment plants with medium or small potentiality that serve the different communities. Besides them, there are some industrial or handcraft entities with their own treatment plants. The greatest part of those plants are equipped with traditional technologies dating back to the 1970s-1980s. In the past years the Environmental Engineering Group of

Table 2. ASM No 1 Matricial structure.

Component i→ ↓Process j	1 S_I	2 S_S	3 X_I	4 X_S	5 X_{BH}	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 velocities ρj $[ML^{-3}T^{-1}]$
1 Aerobic growth of heterotrophs		[illegible]			1			[illegible]		[illegible]			[illegible]	[illegible]
2 Anoxic growth of heterotrophs		[illegible]			1				[illegible]	[illegible]			[illegible]	[illegible]
3 Aerobic growth of autotrophs						1		[illegible]	[illegible]	[illegible]		[illegible]	[illegible]	[illegible]
4 Decay of heterotrophs				[illegible]	–1		f_P					[illegible]		[illegible]
5 Decay of autotrophs				[illegible]		–1	f_P							[illegible]
6 Ammonificati of soluble organic nitrogen										1	–1		[illegible]	[illegible]
7 Hydrolysis of organic matter		1												[illegible]
8 Hydrolysis or organic nitrogen											1	–1		[illegible]
Observed conversion velocities $[ML^{-3}T^{-1}]$	[illegible]													

Symbol	*Units*	Value
	Stoichiometric coefficients	
Y_H	mg COD produced/ mg COD subtracted	0.60
f_P	mg COD produced by decay/ mg biomass COD	0.08
i_{XB}	mg N/ mg COD in activated biomass	0.086
i_{XP}	mg N/ mg COD in non-activated biomass	0.06
Y_A	mg produced biomass COD / mg oxidized N	0.24
	Kinetic coefficients	
$\hat{\mu}_H$	Maximum heterotrophic growth velocity d^{-1}	6.00
K_S	Mg/L as COD	20
K_{OH}	Mg/L as O_2	0.10
K_{NO}	Mg/L as N	0.20
b_H	Heterotrophic decay coefficient d^{-1}	0.408
η_G	Adimensional	0.8
η_H	Adimensional	0.4
k_a	L/(mg biomass COD ·h)	0.0067
k_h	mg COD/(mg biomass COD ·h)	0.092
K_X	mg COD/mg biomass COD	0.15
$\hat{\mu}_A$	Maximum autotrophic growth velocity d^{-1}	0.768
K_{OA}	Mg/L as O_2	1.0
K_{NH}	Mg/L as N	0.75
b_A	Autotrophic decay coefficient d^{-1}	0.096

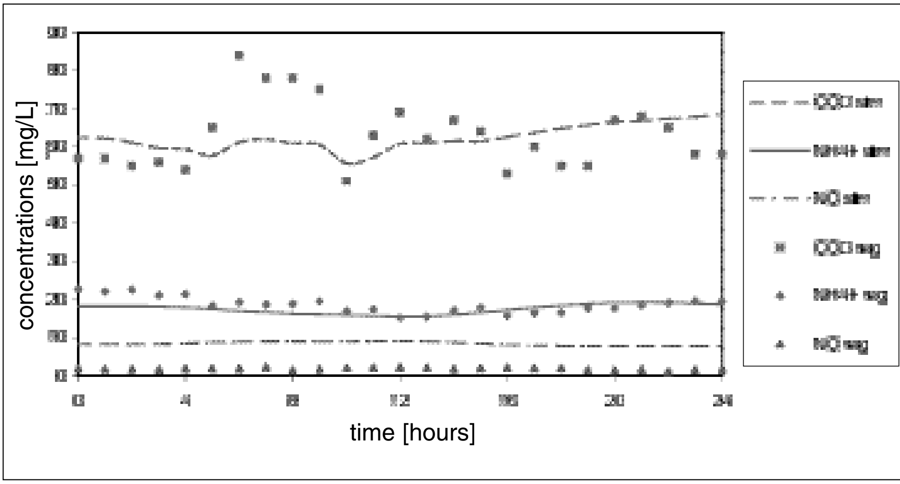
the University of Udine investigated the application of mathematical models to some local plants. This was possilble through the collaboration of some companies managing local plants.

Results

The first plant. In the first experience we have considered a medium-large size plant. This plant serves more or less 100 000 (one hundred) so-called equivalent inhabitants and presents different treatment lines. Equivalent Inhabitants is the conventional measure unit for the pollution load. Only the biological treatment line was considered.

We had two data series: a diurnal series of basal pollutant concentrations (COD, Suspended Solids and Nitrogen as TKN) and a diurnal series of flow values and the corresponding end-of-study data series.

We used a powerful software to implement the activated Sludge Model N.1 and dynamic simulations. The plant lay-out was developed following the indications of the original project. The data used for model calibration were taken as input and output data. As we showed above, the parameters included in the model are numerous. At first, parameters taken from the literature were considered and thereafter a series of sensitivity analyses were made to find out which factors influenced the system response to a greater extent.



The sensitivity analysis for ammonia are reported.

The solid points in the figure indicate the measured values and the curves indicate the simulated trends.

As you can see from the comparison between real data and the trends of the simulated parameters, an optimum level of approximation was reached.

The second plant. As a second step, we studied another plant present in our region with a potentiality of 62500 Equivalent Inhabitants. As in the previous case we used the same software for the implementation of the ASM N.1. We built up the plant lay-out following the indications of the original project. The managing society of the plant gave us the concentration data for the input and the output for a series of pollutants and the corresponding flow rate data. We reconstructed the unity of biologic treatment. This plant was not compliant with the law requirements about the yield of pollutant removal.

We wanted to demonstrate that this level of removal was a consequence of the low level of inlet load, caused by the fact that the existing infiltrations in the sewage net cause an excessive dilution in the wastewater. In this case, we determined the principal parameters by applying respirometric techniques.

Respirometry is a methodology that determines the kinetic parameters through the dissolved oxygen curves registered in a laboratory-scale plant.

In particular, the following values were determined:

- endogen respirometry coefficient, k_d, [dîs^{-1}];
- the specific heterotrophic growth coefficient, Y_H, [mg MLVSS/mg COD];
- the maximum heterotrophic growth velocity, μ_{max}, [dîs^{-1}];
- the substrate concentration where $\mu = \_\ \mu_{max} : K_S$, [, [mg COD/l]

Then, a sensitivity analysis was made on the secondary clarifiers.

As reference parameters for the

approximation evaluation, we considered the yield of total solids, carbon and TKN removal.

At the end, we reached an optimum reality approximation, with an error substantially lower than 10% for the first two parameters and a little higher for the third. Based on the principle that real yields are sensibly lower than those required by law we set out to understand, through sensitivity analysis, what type of actions were required to increase the plant efficiency. Some possible actions were suggested at a plant operating level such as variations of recycle flow rate from secondary clarifiers and increases in volumes for oxidation also by a third basin and the addition of a possible anoxic reactor.

The first action produced net increments of 5-10% in the removal of SSt and COD, the second did not produce any evident benefit. Already from the start we had observed that the plant was characterized by definitely low influent organic loads. Modelistic reconstruction demonstrated that this someway reduces the efficacy of the metabolic activity of the biomass with reduced feeding. Preliminary respirometric experiments and sensitivity analysis showed that autotrophic bacteria were not the optimal solution. As a consequence, a possible anoxic reactor for denitrification would also imply an additional supply of carbonic substrates, with few benefits.

We can conclude that low quality biomass negatively influences the process reducing the yield of the plant. We could conclude that the observed plant could not reach the yield limits required by the law even if it complied with pollutant concentrations in the effluent.

Discussion. The new bounds established by the law provide for maintaining the yield above the specified values. Therefore, the planning of a plant achieving predetermined yields through traditional systems may exhibit some major gaps stressing the need for these new tools.

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