### PAPER 11

# Using dynamic modelling to rethink wastewater treatment plant designs and augmentations

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### ABSTRACT

Population growth is on the rise. As a result, there is an increase in the development of urban housing and related infrastructure to meet the population demands, and subsequently, an increase in the wastewater (industrial effluent and sewage) generated, that would require treatment. As a result, municipalities are seeking to augment their treatment capacity, and often this is done through erecting a carbon copy of the existing plant, in an effort to double the treatment capabilities of the plant. This is not always the optimal solution.

The Integrated Regulatory Information System (IRIS), for 2019, issued by The Department of Water and Sanitation (DWS), revealed that nationally, only 69% of the wastewater treatment plants in South Africa adhere to the effluent discharge limits pertaining to microbiological composition; 69% adhere to the effluent discharge limits pertaining to the chemical composition and only 78% comply in terms of the physical composition of the discharge effluent.

The Green Drop Assessment reports suggests that a significant number of the treatment plants have "inefficient treatment processes". If in such circumstances, the plant is merely doubled in capacity, the municipality would have increased the plant inefficiencies twofold.

To increase a plant's treatment capacity, the current plant would require a comprehensive assessment in terms of hydraulic and process design, operation and maintenance regimes, the legislated effluent limits, conditional assessment of existing ageing infrastructure and plant footprint layout for future expansion. As part of the optimization process it may be concluded that the best way to cater for the need for augmented treatment is not to create a carbon copy of the existing infrastructure, but to rather be innovative with respect to technology and biological treatment processes.

A dynamic treatment model considers the current influent to the plant both in terms of composition and volume; the kinetic parameters and behaviour of the various microorganisms that degrade the influent biological matter, and from this information, key process components are able to be designed. The dynamic model provides a microscopic view into the activated sludge process and this tool is also used to troubleshoot any inefficiencies within the plant and provide an optimised design of the plant. The merit in using such a tool, is that a solution that requires a reduced capital cost may be found.

### **INTRODUCTION**

The state of wastewater and sanitation infrastructure in South Africa has been in a critical state in recent times. This is evidenced by reports from the Department of Water and Sanitation, and the latest Integrated Regulatory Information System results pertaining to the Green Drop status of treatment works in all nine provinces. The Green Drop report of 2013, which was the last report to be published and made public knowledge, showed that 30.1% of the treatment works assessed nationally were in a critical state and in need of an intervention and an additional 19.5% of sites assessed nationally were generally in a poor condition. It was found that only 7% of the treatment works assessed were granted a Green drop certification (Toxopeus, 2019). The 2019 preliminary results show an improved national functionality of the treatment works but, upon further investigation, some treatment works are still in a critical state and achieving only 25% compliance with the Green Drop requirements in terms of effluent quality.

Coupled with poor Green Drop results, an increase in the number of pollution incidents as a result of wastewater effluent discharges were noted. This prompted a case study by Mema (2010), to investigate four of the incidents and the factors that contributed to water body contamination, groundwater contamination and the resultant health issues that were reported in the areas of study.

The areas and plants investigated were Kieskammahoek treatment plant in the Eastern Cape, treatment plants in Buffalo City and Nkokobe municipalities also located in the Eastern Cape, Zandvliet and Cape Flats wastewater treatment plants in the Western Cape, and a study of the effluent quality that is received by the Mhlathuze River in Kwa-Zulu Natal.

The results from the case study indicated that three out of the four incidents of the poor-quality effluent discharge were due to inefficient treatment works, two out of the four were due to poor planning in terms of catering for projected developments, and three out of the four had limited skilled personnel, (Mema, 2010).

Aging infrastructure, the increase in demand for plants that have a higher treatment capacity due to industrial and population growth, and the need to meet effluent discharge regulations and improve the operation of treatment plants, presents itself as an opportunity to not only troubleshoot and mend current inefficiencies, but also to introduce innovative thinking into the design, augmentation and operation of treatment works.

Dynamic modelling allows for the identification of bottlenecks within a treatment plant and improve operation, it allows for what-if scenarios where a plants response to variations in biological and hydraulic loads may be modelled, and it is able to play a huge role part in optimizing plant designs.

### 1. Dynamic modelling

The mathematical modelling and simulation of the activated sludge process, which is the main unit operation in wastewater treatment, has been a complex study area for decades, with the mathematical representation of the treatment reactions being studied as early as about 1967 (Henze et al., 2015).

In 1985, the International Water Association (IWA) formed a Task Group which was tasked with creating a common model for treatment processes, that was less complex than the available models at the time. From this, the Activated Sludge Model No.1 (ASM1) was created.





The basic mass balance equation for any component in a defined system is defined as:

Accumulation= Input- Output + Reaction

If the changes in the concentration of particulate biodegradable organic nitrogen were computed using the ASM1 matrix shown in Table 1 below, the derived mass balance would be:

(1)

$$\frac{dX_{ND}}{dt} = X_{ND,in} - X_{ND,out} - \rho_7 \left(\frac{X_{ND}}{X_S}\right) + \left(i_{XB} - f_p i_{xp}\right) \left(b_A X_{B,A}\right) + (i_{XB} - f_p i_{xp}) \left(b_H X_{B,H}\right)$$
(2)

And the computation of the particulate products arising from biomass decay being:

$$\frac{dX_{P}}{dt} = X_{p,in} - X_{p,out} + f_{p}(b_{H}X_{B,H}) + f_{p}(b_{A}X_{B,A})$$
(3)

Where,

 $X_{ND}$ - particulate biodegradable organic nitrogen

 $\rho_7$ - process rate 7 in the matrix

 $X_S$ - slowly biodegradable substrate

 $i_{XB}$ - mass of nitrogen/ mass of COD in biomass

 $f_p$ - fraction of biomass leading to particulate products

 $i_{xp}$ - mass of nitrogen/ mass of COD in products from biomass

 $b_A$ - decay coefficient for autotrophic biomass

 $X_{B,A}$ - active autotrophic biomass

 $b_{H}$ - decay coefficient of heterotrophic biomass

 $X_{B,H}$ - active heterotrophic biomass

 $X_p$ - particulate products arising from biomass decay

The rest of the processes are modelled similarly. These processes occurring in the activated sludge process, as shown in the various matrices, form the basis for the dynamic simulation tools.

					TABL	.E 1:	The k	kineti	cs and s	toichiom	etry of the A	ASM1	model (H	lenze et al., 2	2015)
	Component + 1 Process 1	1 St	2 53	3 ,32	4 .33	5 Лан	6 .18.4	7 .X3	\$ .50	9 5300	10 Sын	11 SND	12 <i>X</i> ND	13 Salk	Process Rate, py [ML-3T-1]
	Aerobic growth of heterotrophs		$-\frac{1}{T_{\rm H}}$			1			$\frac{1-Y_{\rm H}}{Y_{\rm H}}$		-/308			-1/208	$\hat{\mu}_{H}\left(\frac{S_{S}}{K_{S}+S_{S}}\right)\left(\frac{S_{O}}{K_{O,H}+S_{O}}\right)Y_{B,H}$
	Anoxic growth of heterotrophs		- <u>1</u> Y <sub>H</sub>			1				<u>1-Г</u> <sub>Н</sub> 2.86Г <sub>Н</sub>	-1238			$\frac{\frac{1-Y_{\mathrm{H}}}{14\cdot 2.86Y_{\mathrm{H}}}}{\frac{-\frac{f_{\mathrm{M}}}{14}}{14}}$	$\frac{\hat{\mu}_{\mathrm{H}}\left(\frac{S_{\mathrm{S}}}{K_{\mathrm{S}}+S_{\mathrm{S}}}\right)\left(\frac{K_{\mathrm{O},\mathrm{H}}}{K_{\mathrm{O},\mathrm{H}}+S_{\mathrm{O}}}\right)}{\left(\frac{S_{\mathrm{S},\mathrm{O}}}{K_{\mathrm{N}\mathrm{O}}+S_{\mathrm{N}\mathrm{O}}}\right)\eta_{\mathrm{g}}X_{\mathrm{B},\mathrm{H}}}$
	Aerobic growth of autotrophs						1		$-\frac{4.57}{Y_A}+1$	$\frac{1}{Y_A}$	$-i_{\rm NB} - \frac{1}{Y_{\rm A}}$		l l	$-\frac{i_{\rm XB}}{14} - \frac{1}{7Y_{\rm A}}$	$\hat{\mu}_{A} \left( \frac{S_{NR}}{K_{NR} + S_{NR}} \right) \left( \frac{S_{O}}{K_{O,A} + S_{O}} \right) X_{B,A}$
1	'Decay' of beterotrophs				1-fp	-1		ſ₽					103-19100		b <sub>B</sub> X <sub>B.H</sub>
1	"Decay" of autotrophs				1-17		-1	ß					008-/900		balba
	Ammonification of soluble organic nitrogen										1	-1		1 14	Hallanda,
	'Hydrolysis' of entrapped organics		1		-1										$\begin{aligned} & k_{\mathbf{b}} \frac{X_{5} \langle X_{\mathbf{B},\mathbf{H}}}{K_{\mathbf{X}} + (X_{5} / X_{\mathbf{B},\mathbf{R}})} \bigg[ \left( \frac{S_{0}}{K_{0,\mathbf{H}} + S_{0}} \right) \\ & + \eta_{\mathbf{b}} \bigg( \frac{K_{0,\mathbf{H}}}{K_{0,\mathbf{H}} + S_{0}} \bigg) \bigg  \frac{S_{\mathbf{N}0}}{K_{110} + S_{1\mathbf{N}}} \bigg) \bigg  X_{\mathbf{B},\mathbf{R}} \end{aligned}$
the second se	'Hydrolysis' of entrapped organic nitrogen											1	-1		P7(35(2)(35)
Observed Conversion Rates [ML-9T-7]		$r_i = \sum_j v_i \rho_j$									$v_i = \sum_j v_{ij} \rho_j$				
H A Fi	toichiometric Parameters: idercotrophic yield: Ja utotrophic yield Ja nettion of biomass yielding particulate products: fo fass N/Mass COD in biomass: foa fass N/Mass COD in products from biocansi: fop	Soluble inert organic matter [M(COD)L-3]	Readily biodegradable urbarate IMiCODIL-31	Particulate stert organic matter IMCODIU-31	Slowly biodegradable substrate [M(COO)L <sup>3</sup> ]	Active heterotrophic biomass [MICOD]L-3]	Active automphic biomass [M(COD)L-3]	Particulate products arising from biomass decay [M(COD)L-3]	Oxygen (negative COD) [M(-COD)L-3]	Nitrate and njujie njinogen [M(N)L-3]	NH eNH nirogan [M(N)J]	Soluble bisdegradable organic nitrogen [M(N)L-3]	Particulate biodegradable organic nitrogen [M(N)L-7]	Alkalitäty – Molar units	Kinetic Parameters: Heterotrophic growth and decay: $\dot{\mu}_{B}$ Ks, Kos, Kso.bs Autotrophic growth and decay: $\dot{\mu}_{A}$ Kos, Kos, ba Correction factor for anoxic growth of beterotrophs: $\eta_{g}$ Ammonification: $k_{a}$ Hydrolysis: $k_{a}$ Kx Correction factor for anoxic hydrolysis: $\eta_{b}$

The ASM1 model presents, in matrix form, the kinetic and stoichiometric data for the various processes that occur in the carbon oxidation, nitrification and denitrification processes in an activated sludge unit (Henze et al., 2015).

As an extension to the ASM1 model, further models were developed to create more comprehensive modelling tools. These are:

- The ASM2 model is able to simulate nitrogen, chemical oxygen demand (COD) and phosphorus removal;
- The ASM2d model which is a development of the ASM2 model but accounts for denitrification by phosphorus accumulating organisms (PAOs)
- The ASM3 model being the main model that is used as it was developed to overcome the limitations that were present in the ASM1 model, (Henze et al., 2015).

The intention of dynamic modelling of the activated sludge process is to obtain a real-time understanding and behavior of the processes and constituents of wastewater, so as to optimize and better operate the plant. The ASM suite is used in mass balances.

### **1.1 Dynamic simulation tools in the market**

A variety of software has become available commercially for the dynamic simulation of wastewater treatment plants. Such modelling software is inclusive of BioWin, SIMBA, STOAT, WEST etc. The similarity in all the simulation tools is that they are developed with the ASM suite being the core tool, with additional features that have been added for competitive advantage. The differences and similarities between the available simulation packs are illustrated in Table 2 below:

Noting the subtle differences that are present in the simulation tools, and that one may not be able to make changes to the background intelligence and operation of the simulators; and noting further that the simulation programmes are based on the ASM suite. The research team set out to create an in-house simulation programme that would be unique.

### 1.2 The simulation model

Whilst taking cognizance of the commercially available simulation programmes, the research team created an in-house simulation tool with the intention of using dynamic modelling to offer prospective clients optimal designs for the treatment of wastewater.

Similar to the available simulation programmes as shown in Table 1, the in-house tool is modelled after the ASM suite of reaction kinetics, stoichiometry and processes occurring in the activated sludge unit. The tool is designed to account for the various process variations that are present in biological treatment and has both a steady-state and dynamic environment. The dynamic model was created using Scilab, an open-source, numerically-based software that is used for programming.

The ordinary differential equations arising from the ASM suite were coded into Scilab from first-principles to generate a representation of the processes. Due to the complexity of the equations and the simulation environment, several user-friendly tools were employed to allow for the easy navigation and use of the programme. To simulate a treatment plant, the initial step is to determine or obtain the influent stream constituents and data. The characterization and fractionation of the influent

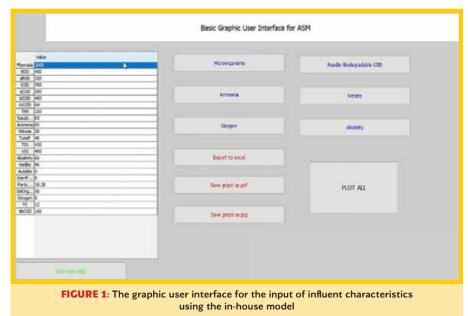


TABLE 2: The features of the different simulation packs that are commercially available.	Table extracted from Makinia, 2010
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Feature	BioWin	SIMBA	STOAT	WEST					
Activated Sludge Models	ASM suite	ASM suite, ASM3P	ASM suite and own model using a BOD balance	ASM suite, ASM3P, TUDP (Technical University Delft Phosphorus) model					
Reactor hydrodynamic model	Continuously-stirred tank reactor (CSTRs) or a series of CSTRs								
Petersen matrix editor	Yes	Yes	No	Yes					
Input data	Directly on the program or excel	Directly in the program, excel, text files or data bases	Directly on the program or excel	Directly on the program, excel or data bases					
Chemical Phosphorus precipitation	Model based on chemical equilibrium	ASM2	ASM2	ASM2					
Anaerobic digestion	General biokinetic model and ADM1	Two simplified models and ADM1	Simple and more complex models for mesophilic digestion	Three kinds including ADM1					



1 Charlentit	
2	
3 (AS&I: Model	
4 names- Hettin, Autobic, d	COD, 45COD, Instititionals, Fatte autoOpper, SoCophil, America, Initiale, Oxygen, Alkanity J ocamponation
5	
6 1/1. Influent properties	
7 Flowrate= 2000 //mil/day	
8 BOD= 250 Pimp/L	Bological Oxygen Demand
9 sBOD= 300 img/L	Solutin Bological Oxygan Demand
10 COD+ 300 //mg/L	Chemical Oxygen Demand
11 sCOD+ 250 //mpil.	Soldie Chemical Dxygen Demand
12/6COD= 600 //mg/l.	Exclegitutivite Citumical Citygen Demand
13 (BCOD= 150 // mgl.	Readly Biolegradeble Chemical Oxygen Demand
14 TKN= 60 // mg/L	Total Kyeldale Nilrogen
15 SolubleTKN= 40/mg/L	Eduble Total Kjetovni Nitrogen
16 Ammonia= 15 Umg/L	Anthonia
17 Nitrate= 5 Pmg/L	Nitrate
18 TotalP= 10 Jing/L	Total Phosphorus
19 TSS= 400 /mpl.	Total Suspended Solida
20 V85= 0.8 T58/mg1	Volutile Suspended Bolids
21 Akalinity= 10 Imolim*3	AlkalinBy
22 HetBio= 5 //mg/L	Heterotopic Microorganisma
23 AutoBio* 0 //mig/L	Autotropic Microorganiama
MinertPProducts= 0 //mg/L	Inert Particulain Products
25 ParticulateOrgNt= 5/imp/L 26 SolOrgNt= 0 //mp/L	Particulate Organic Nitrogen
	Baltible Organiz Mirogen
27 Oxygen= 0 //mgil. 28 T0= 12 //depC	Ovgen Feid Temperatum
	- Field Factorian
19 10/sbC00= 1/60 //mg/L1	
st nbCOD+ COD-bCOD impl.	
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FIGU	<b>RE 2</b> : Typical plant data input that may be used in the simulation

is important as the user is able to determine information such as the biodegradability of wastewater, determine the relevant fractions of components that assist in selecting the optimal process route, i.e. is the ratio of COD to total phosphorus sufficient for phosphorus removal?. Having obtained the relevant information, this is entered in the model using the graphic user interface or it may be entered through importing the data from Microsoft Excel, similar to the simulators in Table 2. The graphic user interface is shown in Figure 1.

The data loaded is received in the background where the relevant processes in the ASM suite have been coded.

The simulation environment is broken up to different sections. It begins with the fractionation and input of the wastewater received by the plant. The default ASM kinetic data and stochiometry follow as they will be used in the ordinary differential equations. The kinetic and stoichiometric data is set at default values but as each plant behaves different and has different inflow constituents, the kinetic information would have to be calibrated to suit the wastewater plant being simulated. After the kinetic and stoichiometric data input, the actual reactor environment where the interaction and relationship between one component and another is represented using the differential equations.

Having simulated the environment, the programme is then coded to provide the concentrations of the components in the effluent streams. The programme is coded to provide the parametisation of the components against important design variables so as to determine the parameters that are optimal to the operation of the plant. These design variables may be inclusive of the activated sludge recycle ratios (return activated sludge or internal recycles), the sludge retention times etc.

The output from the parametisation and

optimisation of the plant is provided through the user-interface and the output may also be exported to Microsoft Excel. The various sections of the modelling tool are shown in Figures 2-5.

The most crucial step in the dynamic modelling of treatment works, is that each plant behaves differently and it warrants a unique study of the influent and kinetic parameters. To better model a plant, a clear understanding of the actual behaviour in the treatment is required. This allows the model to better predict various scenarios that may be tested, i.e. would the plant be able to accommodate a variation in biological load and still produce a regulatory compliant effluent? Would the plant be able to accommodate a figure for Company X? If the plant influent were increased by 1.5 M&/day due to developments, would the existing infrastructure be able to cope?

The process of obtaining the plants' unique characteristics and using these in the model for better predictions, is called calibration. The

> process of calibration may be done through a series of experiments where the various process parameters that are specific to the plant may be measured, used in the model and the model output is then compared to the actual plant outputs to test how closely the data sets correlate. In a well-defined and controlled calibration procedure, the differences between the data sets and the model outputs should be minimal (Makinia, 2010).

> Having calibrated the model, the data would have to be validated and the model structure is then usable for the intended study. The model may be used to optimise process performance, it may be used during the expansion of existing treatment works, or the design of new treatment works.

## **1.3 Use of dynamic modelling in municipal treatment works**

Using dynamic modelling in municipal wastewater treatments has proven meritorious as was shown in the simulation of the Marianridge

36 44-0.67 // eCOD/ eCOD ordered 38 yA= 0.24// gCOD/ gN oxidised 39 40 XB=0.086; //gN/ gCOD XP+ 6.06; // gN/ gCOO uH= 6; // day-1 45 42 43 |bH= 0 62; //day -1 44 Kg= 45 KoH= 0 2 // gOZ/ m3 46 47 KNo= 0.5;//gNC uA=0.8//day~1 NO3-N/m 48 49 bA= 0 g02/ m3 g NHO-N/m3 50 KNh= 1 51 52 Ka= 0.08 //m3/ (gCOD, day)\*-1 54 Kx= 0.03 //gsbCOD/ (g COD, day)\*-1 56 CoAST=10 4,3,3,10,3,50,67 57 CI=[HetBio AutoBio rbCOD sbCOD InertPProducts ParticulateOrgNit SolOrgNit Ammonia Nitrate Oxygen Alkalinity ] 58 tau= 10 11 12 13 14 59 3 R. 60 1 function IdCdtl=cstn(t.C) r1= uH'(C(3)(Ks+C(3)))'(C(13)/(KoH+C(10)))'C(1) r2= uH'(C(3)(Ks+C(3)))'(KoH/(KoH+C(10)))'(C(3)/(KNo+C(3)))'ng'C(1) 3 r3= uA\*(C(5)/(KNh+C(5)))\*(C(10)/koa+C(10))\*(C(1)) r4=bH'C(1) FIGURE 3: Typical kinetic and stoichiometric data of the plant, default ASM values used

32

33

34

sCODe=sCOD-1

'sBOD

nbVSS= (1-(bpCODpCOD))"VSS

bpCODpCOD= ((bCOD/BOD)\*(BOD-sBOD)/(COD-sCOD)) //mg1

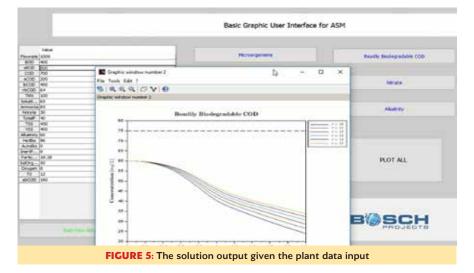
module of the Umhlathuze wastewater treatment plant by Mhlanga, 2008. The need for a dynamic simulation of the Marianridge plant arose due to the plant receiving industrial effluent whose effect on the treatment works had to be determined to ascertain that the effluent discharged to the receiving water bodies would still be compliant with regulations.

The modelling of the treatment works was done using the WEST simulator and ASM3 of the ASM suite was used, (Mhlanga, 2008). The wastewater influent was characterized and fractionated into components as required by ASM3, i.e. the COD is classified into readily biodegradable COD, slowly biodegradable COD, the inert fraction etc. Thereafter, experiments were conducted in an effort to calibrate the model for increased accuracy. During the calibration, difference between the experimentally-obtained kinetic data and the default ASM3 values were noted, however the difference was minimal. After the calibration of the model, the data obtained from the model output was validated against the plants' historic data. The results from the calibration, and validation step showed that the simulation was accurate enough to be used further in dynamic studies of the plant.

The steps taken towards the simulation of the plant show that it is a massive undertaking to correctly simulate a treatment plant and that the deployment of the correct people, tools, knowledge of the plant and simulators to perform this task is imperative.



FIGURE 4: Illustrating the coding of the ASM1 processes and simulation of the reactor environment



Municipalities need to be aware of the presence of dynamic simulators and the fact that municipal treatment plants can be augmented optimally and not through a method of doubling up on existing infrastructure without initially interrogating the system. If the plants investigated by Vusimzi Mema in 2010 had to be augmented and doubled-up to meet rising capacity, the current inefficiencies, groundwater pollution, water body pollution and the resultant health issues reported by residents, all reported incidents would be increased and intensified two-fold.

Erecting bigger but non-functional treatment plants is not the only answer to South Africa's sanitation issues. Consulting firms and municipalities jointly have to rethink the approach to wastewater treatment.

#### **CONCLUSION**

A concerted effort towards improving the state of sanitation in South Africa needs to be made Dynamic modelling offers a platform that takes the conceptual design and representation of wastewater treatment processes, and makes it a possible reality that could potentially result in an optimized plant with an effluent discharge that is able to comfortably meet the General and Special discharge limits, that is easily operable and where, if plant disturbances occur, there is comfort in the knowledge that the plant would be able to accommodate these.

> The benefits to using dynamic simulation tools is the improvement in everyday operation which may result in a reduction in operational costs. If the tool is used for the augmentation of existing works, it may result in a reduction in capital expenditure as a simulation study may conclude that a reduced volume than initially anticipated may be required. In addition, simulation models are ultimately decision-making tools that may assist in determining the plants' response to uncertainties such as variations in the feed that may result from emerging industries, and the surrounding community.

> The key to conquering municipal challenges, is to have an in-depth understanding of the challenges in order to determine the most appropriate solution to the problem.

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