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Contribution of Modelling to Enhancing the Operation of Wastewater Treatment Plants: Case Study of Maghnia and Tlemcen WWTPs

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Dedication

"I dedicate this thesis to my beloved mother for all the support she accorded to me since I was a little child."

"To my dear father for raising me to be the man I am now, his guidance continue to inspire me every day."

"Also, I dedicate this work to my beloved sister Wafaà for her continuous encouragement, my close friend and brother Bachir for being always there when I am feeling low, my adorable younger brother Abdelhak "Big Hurt", and last but not least my lovely little nephews Abderrahman and Zakaria."

"To my siblings, relatives, and friends who have stood by me through thick and thin, thank you for your unwavering belief in me. Your love and support have been invaluable."

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ABSTRACT

Mathematical modelling of activated sludge systems has become a widely accepted tool and is used in particular for optimization and upgrading of existing plants and for new facilities design, either by engineering and consulting companies, or university and research centres.

The adopted methodology in this study is based on numerical simulations conducted by the ASM1 model (Activated Sludge Model No. 1), which incorporates the kinetics of organic and nitrogen removal processes in association of the GPS-X simulator in order to obtain an optimal solution for treatment performances. Two treatment facilities were examined: the Maghnia wastewater treatment plant (MWWTP) and Tlemcen City's plant (Ain Elhoutz TWWTP), Data collection from these plants, coupled with statistical analysis of input and output quality, facilitated the completion of this study, allowing for a comprehensive evaluation of their performance.

After a successful steady state calibration of three effluent state variables (observed concentration values of chemical oxygen demand (COD), total suspended solids (TSS), and ammonium (NH4-N) parameters), the Maghnia WWTP ASM1 modelling yielded promising outcomes in predicting COD removal performance under dynamic conditions with some reservations regarding TSS, and NH4-N.

The second case study focused on assessing the dynamism of Chemical Oxygen Demand (COD) effluent quality, viewing it as a pivotal measure of plant performance. The application of ASM1 model in Ain Elhoutz TWWTP was guided by a sensitivity analysis approach and an optimization for dynamic calibration of the model. The results of model validation indicate that the calibration was performed properly with a good correlation coefficient (R^2).

The ASM1 model effectively reflects the dynamic fluctuations in COD effluent concentrations for both plants, the modelling of wastewater treatment plants (WWTPs) presented in this thesis represents a significant step forward in a relatively new field.

Keywords: Activated Sludge Process (ASP), Activated Sludge Model 1 (ASM1), Wastewater treatment plant (WWTP), GPS-X Software, Model Calibration, Dynamic Simulation, Model Validation, Sensitivity Analysis.

Résumé: La modélisation mathématique des systèmes de boues activées est devenue un outil largement accepté et est utilisée notamment pour l'optimisation et la modernisation des installations existantes et pour la conception de nouvelles installations, que ce soit par des entreprises d'ingénierie et de conseil ou par des centres universitaires et de recherche. La méthodologie adoptée dans cette étude repose sur des simulations numériques réalisées par le modèle ASM1 (Modèle de boues activées n° 1), qui intègre les cinétiques des processus de dégradation organique et de dénitrification, en association avec le simulateur GPS-X afin d'obtenir une solution optimale pour les performances de traitement. Deux installations de traitement ont été examinées : la station d'épuration des eaux usées de Maghnia (MWWTP) et celle de la ville de Tlemcen (Ain Elhoutz TWWTP). La collecte de données provenant de ces installations, associée à l'analyse statistique de la qualité des entrées et des sorties, a facilité la réalisation de cette étude, permettant une évaluation complète de leurs performances. Après un calage réussie en régime permanant de 3 variables d'effluent (concentrations observées de demande chimique en oxygène (DCO), de matières en suspension totales (MES) et de paramètres d'ammonium (NH4-N)), la modélisation ASM1 de la STEP de Maghnia a donné des résultats prometteurs pour prédire les performances de dégradation de la DCO dans des conditions dynamiques, avec quelques réserves concernant les MES et le NH4-N. La deuxième étude de cas s'est concentrée sur l'évaluation de la dynamique de la qualité de l'effluent en demande chimique en oxygène (DCO), le considérant comme une mesure pivot de la performance de l'installation. L'application du modèle ASM1 dans la station d'Ain Elhoutz a été guidée par une approche d'analyse de sensibilité et une optimisation pour le calage dynamique du modèle. Les résultats de validation du modèle indiquent que le calage a été réalisé correctement avec un bon coefficient de corrélation (R^2). Le modèle ASM1 reflète efficacement les fluctuations dynamiques des concentrations d'effluents en DCO pour les deux installations. La modélisation des stations d'épuration des eaux usées présentée dans cette thèse représente une avancée significative dans un domaine relativement nouveau.

Mots-clés: Procédé de boues activées (ASP), Modèle de boues activées 1 (ASM1), Station de traitement des eaux usées (STEP), Logiciel GPS-X, Calage du modèle, Simulation dynamique, Validation du modèle, Analyse de sensibilité.

الملخص: النمذجة الرياضية لأنظمة الحمأة المنشطة قد أصبحت أداة مقبولة على نطاق واسع وتستخدم بشكل خاص لتحسين وتطوير محطات معالجة مياه الصرف الصحي الحالية وتصميم اخرى جديدة، سواءً من قبل شركات الهندسة والاستشارات، أو مراكز الجامعات والبحوث. المنهجية المعتمدة في هذه الدراسة تعتمد على المحاكاة العددية التي يقوم بها نموذج ASM1 (النموذج الرياضي رقم 1 للحمأة المنشطة)، الذي يدمج حركية التفاعلات العضوية وإزالة النيتروجين بالتعاون مع محاكي GPS-X من أجل الحصول على الحل الأمثل لأداء المعالجة. تم فحص منشآت المعالجة الآتية: محطة معالجة مياه الصرف الصحي في مدينة مغنية ومحطة مدينة تلمسان "عين الحوت". جمع البيانات من هذه المنشآت، مع التحليل الإحصائي لجودة المدخلات والمخرجات، ساعد على إكمال هذه الدراسة، مما يتيح التقييم الشامل لأدائها. بعد الانتهاء الناجح من عملية المعايرة في الحالة المستقرة لثلاثة متغيرات (قيم التركيز المراقبة لطلب الأكسجين الكيميائي (COD) والمواد الصلبة العالقة الكلية (TSS) ومعلمات الأمونيوم (NH4-N))، أظهرت نمذجة ASM1 لمحطة مغنية نتائج واعدة في توقع أداء إزالة COD تحت ظروف ديناميكية مع بعض التحفظات بشأن TSS وNH4-N. الدراسة الثانية ركزت على تقييم ديناميكية جودة التراكيز لطلب الأكسجين الكيميائي (COD)، مع النظر إليها كمقياس محوري لأداء المحطة. تم توجيه تطبيق نموذج ASM1 في محطة "عين الحوت" عن طريق نهج تحليل الحساسية وتحسين المعايرة الديناميكية للنموذج. تشير نتائج التحقق من النموذج إلى أن المعايرة تمت بشكل صحيح مع معامل ترابط جيد (R^2). يعكس نموذج ASM1 بشكل فعال التقلبات الديناميكية في تراكيز مخلفات COD لكل من المنشآت، وتمثل نمذجة محطات معالجة مياه الصرف الصحي (WWTPs) التي قدمت في هذه الرسالة خطوة هامة في مجال جديد نسبياً.

الكلمات المفتاحية: عملية الحمأة المنشطة (ASP)، نموذج الحمأة المنشطة رقم 1 (ASM1)، محطة معالجة مياه الصرف الصحي (WWTP)، برنامج GPS-X، معايرة النموذج، محاكاة ديناميكية، التحقق من النموذج، تحليل الحساسية.

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NOMENCLATURE

ASM: Activated Sludge Model

ASP: activated Sludge Process

AST: Activated Sludge Tank

AOB: Ammonia Oxidizing Biomass

b_A: Decay coefficient for autotrophic biomass

b_H :Decay coefficient for heterotrophic biomass

BOD: Biochemical Oxygen Demand (in a 5-day incubation period)

COD: Chemical Oxygen Demand in mgO2/L

DO: Dissolved Oxygen

f_p: fraction of biomass leading to particulate products

HRT: Hydraulic Retention Time

HSVM: Hard Suspended Volatile Matter

IWA: International Water Association

K_S: Half-saturation coefficient for readily biodegradable substrate

MAE: Mean Absolute Error

MCRT: Mean Cell Resident Time

MLSS: Mixed Liquor Suspended Solids

MLVSS: Mixed Liquor Volatile Suspended Solids

NH4-N: Ammonia Nitrogen

NO2-N: Nitrite

NO3-N: Nitrate

pH: Potential of Hydrogen

Q: Inflow Rate

RAS: Recycle Activated Sludge (under flow)

r_i: Substrate utilization rate

r(ξ): Conversion vector of the variable ξ

S_I: Soluble inert organic matter

S_{ND}: Soluble biodegradable organic nitrogen

S_{NH}: Ammonia nitrogen

S_{NO}: Nitrate and Nitrite nitrogen

S_S: Readily biodegradable substrate

SD: Standard Deviation

SRT: Sludge Retention Time

t: Time (d)

T: Temperature (◦C)

TSS: Total Suspended Solids

TKN: Total Kjeldahl Nitrogen

TN: Total Nitrogen

V: Reactor Volume

VSS: Volatile Suspended Solids

WAS: Wasted Activated Sludge (pumped flow)

WWTP: Wastewater Treatment Plant

X_{BA}: Active autotrophic biomass

X_{BH}: Active heterotrophic biomass

X_I: Particulate inert organic matter

X_{ND}: Particulate biodegradable organic nitrogen

X_P: Particulate products arising from biomass decay

X_S: Slowly biodegradable substrate

Y_A: Growth yield of autotrophic biomass

Y_H: Growth yield of heterotrophic biomass

ξ: Vector of reactor and effluent concentration

ξin: Vector of influent concentration

$\mu_{-max\ H}$: Maximum specific growth rate for heterotrophic biomass

$\rho(\xi)$: Vector of reaction kinetics

ρj: Process rate

Θ: Hydraulic residence time, HRT

ν_{ij}: Stoichiometric coefficient

η_g: Correction factor of μ_H under anoxic conditions

η_h: Correction factor for hydrolysis under anoxic conditions

INTRODUCTION

Everywhere humans live and utilize water, we release wastewater. It results from basic water needs including those of sanitation, hygiene, cooking, agriculture, and industry. Huge amounts of wastewater build up when we stop having to manually gather water and now have tap water in or close proximity to our houses. Wastewater refers to any spent water that has become so polluted that it cannot be used for most purposes without treatment. Accumulating volumes of wastewater soon constitute a concern since the toxins typically cause both health hazards (the spread of infectious diseases) and environmental problems for both natural waterways (eutrophication and toxicity) and the air (greenhouse gas emissions) [1].

Historically, the major goal of wastewater collection was sanitation, which sought to prevent the spread of waterborne illnesses. For good cause, readers of the prestigious British Medical Journal named the hygienic revolution the greatest medical advancement since 1840 [2]. Many countries continue to struggle with providing adequate drinking water and sanitation. With the introduction of wastewater treatment plants (WWTPs), treatment objectives have expanded, and regulations continue to become more stringent. Currently, wastewater treatment facilities in developed nations not only eliminate disease-causing microorganisms, but also have a vital function in safeguarding the environment from a range of harmful discharges. Simultaneously, there is considerable pressure on wastewater utilities to recover resources, where reuse has been strongly encouraged in recent years.

Algeria currently operates 211 wastewater treatment plants, including 71 natural refinement stations, with a combined treatment capacity of up to 1 billion cubic meters according to a report of the Algerian National Sanitation Office [3]. However, the actual treated volume stands at approximately 480 million cubic meters, resulting in a treatment rate of 47% [3]. These treatment facilities, established primarily in the early 2000s, signify Algeria's recognition of the significant backlog it had accrued in wastewater management. Presently, 7 steps are operating beyond their designed capacity, while 16 others are underutilized, processing less than 30% of their potential capacity revealed the same source.

To address this gap, Algeria has initiated a comprehensive wastewater treatment program. This program involves the construction of 15 new treatment plants, the recent commissioning of 3 facilities, and the launch of 7 additional projects. Upon completion, these efforts are expected to increase the treated volume by 110 million cubic meters. Aligned with a national action plan, these initiatives aim to enhance the current treatment capacity of 1.16 billion cubic meters by an additional 140 million cubic meters annually. The overarching goal is to alleviate water stress and ensure sustainable water management practices.

Looking ahead to 2030, Algeria anticipates expanding its wastewater treatment network to accommodate a treatment capacity of 2 billion cubic meters. This increased capacity will primarily support agricultural irrigation across 160,000 hectares of arable land, promoting water reuse and resource conservation [3].

In addition to agricultural use, efforts are underway to explore other avenues for wastewater reuse, including industrial applications, public garden irrigation, and forest fire prevention. These initiatives are integral to Algeria's broader strategy for water resource management and environmental sustainability.

1. Problem Statement

Studying the operations of a treatment plant is a difficult undertaking. For first of all, the influent load varies in flow and concentration, is intrinsically uncontrollable, and comes at various hours of the day and year. It is imperative that a wastewater treatment plant be operational at all times, including during inspection and maintenance procedures. Furthermore, the utilization of sequential unit processes with different return feeds leads to many feedback effects, causing the processes to become intricately interconnected.

Given these complexities, the problem lies in the lack of comprehensive and accurate models that can capture the intricacies of WWTPs, accounting for the dynamic interactions between different treatment units, fluctuations in influent characteristics, and the impact of operational parameters on treatment performance and environmental impacts. The process of activated sludge is an intricate system where many bacterial conversion and transport activities take place. The conversion of pollutants is significantly influenced by kinetics, stoichiometry, and transport mechanisms.

In such circumstances, mathematical modelling proves to be a significant tool for assessing the efficiency of wastewater treatment plants. These models provide a comprehensive description of the processes and their interactions, taking into account ambient conditions in the goal of understanding the mechanisms of organic substance biodegradation, nitrogen, and phosphorus removal. The models developed are utilized to create simulation software, which serves as a tool for designing or managing treatment systems. Simulation allows for better planning of expansions, optimization, management, rehabilitation, or strengthening of various components of the station, biological models ASM (for "Activated Sludge Modelling"), the first of which was published in 1987 [4], have already proven their effectiveness for conventional activated sludge processes.

2. Hypothesis

The development and application of accurate and reliable models for WWTPs require a combination of theoretical knowledge, empirical data, and calibration techniques. Validating these models against real-world plant data is crucial to ensure their predictive capabilities and suitability for supporting decision-making processes. Biokenetic process models, in particular, can effectively assess the treatment performance of wastewater treatment plants by capturing the highly dynamic nature of the treatment processes.

The application of dynamic process models to the case studies of Maghnia and Tlemcen wastewater treatment plants can validate the utility of such models in accurately representing real-world scenarios and identifying opportunities for operational improvements. Through these case studies, it is possible to gain a comprehensive understanding of the complex interactions affecting treatment performance, ultimately contributing to the enhancement of plant operations at Maghnia and Tlemcen cities.

3. Objectives

To explore the potential of using the ASM1 (Activated Sludge Model No. 1) for modelling and simulation of wastewater treatment plants integrated within the GPS-X module, with a focus on the facilities in the Tlemcen region and Maghnia. The project aims to conduct a comprehensive study of the Maghnia wastewater treatment plant and the Ain Elhoutz WWTP in the Wilaya of Tlemcen, involving data collection and analysis of influent and effluent characteristics to evaluate the performance of the treatment processes.

To calibrate and apply the ASM1 model for simulating the biological processes occurring during treatment at the Maghnia and Tlemcen facilities. This involves identifying and understanding the crucial parameters and mechanisms influencing the alignment of key quality performance targets for these plants. The objective is to develop a better comprehension of the overall wastewater treatment process, particularly the ensemble of mechanisms involved in the activated sludge system.

The project aims to explore the opportunities and potential offered by such dynamic modelling approaches in enhancing the understanding and operation of wastewater treatment plants.

4. Outline of Thesis

This thesis is structured into five main sections:

- ***Literature Review:*** This section provides an overview of the activated sludge process, encompassing its fundamental aspects. It also introduces biological modelling using ASM-type models and examines previous studies on modelling activated sludge treatment plants. Additionally, it explores various simulation platforms used for modelling.
- ***Materials and Methods:*** Here, we detail the materials and methods utilized in this study. This includes information about the two treatment plants monitored, the statistical methods employed for data analysis, and a brief discussion on the performance of these plants.
- ***Application of ASM1 Model for Maghnia WWTP:*** This section focuses on the calibration of the ASM1 model specifically for the Maghnia Wastewater Treatment Plant (WWTP). It covers the estimation of kinetic and stoichiometric parameters, encountered issues during parameter fitting, and the subsequent resolution of these issues. Model validation will be the final step in this process.
- ***Sensitivity Analysis in Calibration of ASM1 Model for Ain Elhoutz WWTP:*** Similar to the previous section, this part of the thesis discusses the calibration of the ASM1 model, but for the Ain Elhoutz WWTP. It includes the incorporation of a sensitivity analysis module to identify parameters requiring adjustment during model calibration. These analyses will assess whether modifications to these parameters affect the model outputs concerning COD effluent quality.
- ***Conclusions and Future Research:*** Finally, this section presents essential conclusions drawn from the preceding chapters and offers some overarching insights. It also identifies areas for future research, summarizing the key needs and directions for further investigation.

CHAPTER I

LITERATURE REVIEW

I.1 Introduction

This chapter provides a comprehensive overview of the activated sludge system, examining its operation from microscopic to macroscopic scales. We will discuss the role of microorganisms within the system and explore its functioning in detail.

Furthermore, the chapter focuses on the state of the art in biological modelling, with a focus on the ASM1 model and its significance in wastewater treatment. We will highlight also the simulation environment used in this study.

I.2 Activated Sludge Process

I.2.1 History of Wastewater Treatment

In the very beginning of modern wastewater management, the collected wastewater was either released without any treatment into settlements downstream or spread over agricultural land. This approach helped improve urban health and living conditions by moving the problem away from populated areas. However, as cities expanded and water consumption increased, new challenges emerged. Individuals began experiencing illnesses like as typhus and paratyphoid fever. Regions having a lower number of wastewater treatment facilities exhibited a higher incidence of these illnesses [5].

Due to population growth, urbanization, and increased water consumption in the late 19th century, larger cities faced environmental issues in their aquatic ecosystems, regardless of how far the wastewater was relocated, as a result of industrialization and the implementation of improved building regulations, such as the introduction of water closets. Subsequently, wastewater treatment was implemented. Early treatment facilities utilized mechanical methods to separate sludge and visible impurities using coarse screens and primary sedimentation, occasionally supplemented with chemical treatment. Nevertheless, it became apparent that the presence of soluble pollutants required treatment due to the subsequent oxygen depletion and fish mortality in the receiving waters [6].

Historically, the initial modern treatment plants employed mechanical methods such as coarse screens and primary sedimentation to separate sludge and visible contaminants. In some cases, chemical treatment was also used as an additional measure. Nevertheless, the rapid occurrence of oxygen depletion and fish mortality in the receiving waters clearly indicated the necessity of addressing soluble pollutants. The activated sludge technique, developed in England in 1914

[7], was particularly effective at eliminating organic waste - measured as biological oxygen demand (BOD) - and was also found to oxidize ammonium (nitrification). The procedure immediately gained popularity, and by including additional biological therapy, oxygen deprivation could be prevented. In the mid-twentieth century, it was determined that not only organics but also soluble nutrients in wastewater contributed to the newly found problem of cultural eutrophication [8]. The process of nitrification was predominantly accomplished in the activated sludge system, and with improved supervision capabilities in the latter half of the twentieth century, it was successfully perfected to a significant extent. Denitrification was a well-known concept at that time, but it was not until Ludzack and Ettinger [9] proposed the placement of anoxic tanks before the aeration basins, with the return of nitrate to the anoxic tanks, that denitrification was accomplished in a controlled manner. Figure I.1 depicts a diagram illustrating a standard representation of a plant.

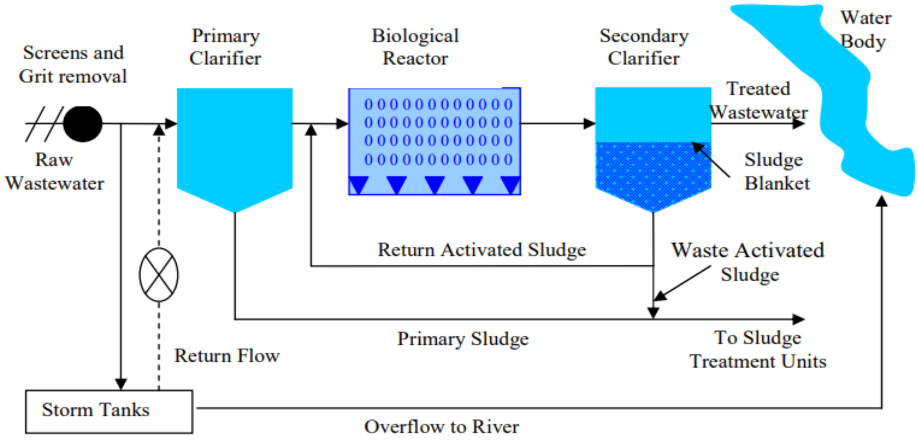


Figure I. 1 Schematic of a wastewater treatment plant based on the conventional activated sludge biological treatment [10].

I.2.2 Principles of the Activated Sludge Process

Activated sludge is the predominant technology used for biological wastewater treatment. Its primary components are solid-liquid separators (also known as secondary clarifiers or settlers) and multiple biological reactors, sometimes known as aerated tanks. It can carry out the following four vital tasks for wastewater treatment: it can break down or oxidize carbonaceous wastes, break down or oxidize nitrogenous wastes, remove fine particulates, and remove heavy metals. The major means by which these duties are accomplished is via the development and upkeep of a sizable, varied, and vibrant population of bacteria. As a result, it uses the dissolved oxygen provided by the aerators to change the biodegradable components (substrate) into fresh biomass, carbon dioxide, water, and leftover organic waste. The primary purpose of the clarifier is to segregate the suspended solids and biomass from the aerated sewage and increase the density of the sludge prior to its return to the reactor [1,11].

As was previously mentioned, the activated sludge process is a biological process where organic waste is mineralized and oxidized by microorganisms. Hence, the key requirement of the activated sludge process is to sustain a substantial concentration of a diverse community of microorganisms in a mechanically aerated reactor known as the mixed liquid suspended solids (MLSS) is the primary need of the activated sludge process. The functioning of the wastewater treatment plant as well as the influent wastewater have an impact on the species makeup of microorganisms. In the aerated tank, the microorganisms develop slowly and are maintained suspended by agitators or air flowing into the tank. The microbes oxidize organic materials by using oxygen. The MLSS is thickened and clarified in the secondary settling tank after exiting the aeration tank, where it is retained for an average of six hours. A portion of the thickened sludge from the secondary clarifier is cycled back to the aeration tank to sustain the microbial population there; the excess thickened sludge is disposed of. Typically, between 40 and 100 percent of the wastewater flow is returned as sludge to the aeration basin [11].

Numerous factors, including the amount of biomass, the substrate, temperature, pH, and the presence of toxins, affect the pace at which biomass grows. As the sludge ages or the mean cell resident time (MCRT) increases, bacteria multiply and become more diverse. During this stage, the biochemical oxygen demand (BOD) undergoes a transformation into extra bacterial cells or sludge, as well as new, less harmful waste products. The bacteria selectively remove minuscule particles and toxic heavy metals from the large volume of liquid, aiding the metazoan and ciliated protozoa. The ciliated protozoan and metazoan play a crucial role in consuming the dispersed cells. The term "cropping activity" refers to the feeding behaviour of these organisms, where they consume dispersed germs. Bacteria are separated from the waste stream by the process of cropping [1,11,12]. Non-biodegradable substances are generated as a result of bio-reduction, which is the breakdown of microorganisms. The incoming wastewater may also contain inert materials, which remains unaffected during the process and is subsequently collected and removed in the settler.

I.2.3 Operation of Activated Sludge System

Achieving optimal performance in an activated sludge system requires maintaining a delicate balance among three key factors: the amount of organic matter (food), the population of microorganisms (activated sludge), and the level of dissolved oxygen (DO). Imbalances in these parameters are the primary cause of most issues encountered in activated sludge processes [1]. Activated sludge systems are primarily controlled by three factors: aeration and the maintenance of appropriate levels of dissolved oxygen, the rate of recirculation of activated sludge (RAS) from the secondary clarifier to the aeration tank, and the management of excess sludge extracted from the system (WAS), which is usually pumped from the secondary clarifier to sludge treatment facilities. Figure I.2 depicts a fundamental diagram of the operational mechanism of the biological process in an activated sludge system.

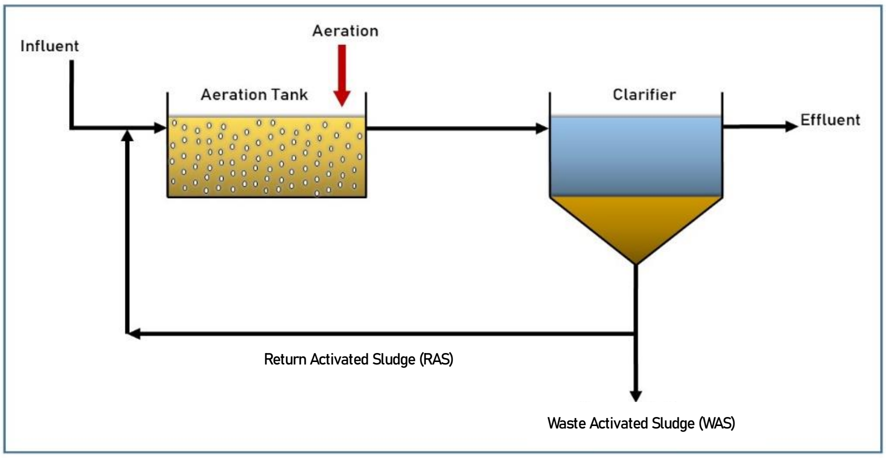


Figure I. 2 Basic schematic of the biological process in an activated sludge process [13].

Aeration and maintaining proper dissolved oxygen levels serve two primary purposes: firstly, to sustain the activity of microorganisms by keeping the oxygen concentration within the appropriate range, typically around (2 mg/l), and secondly, to ensure effective mixing of tank contents to keep solids suspended [14]. Inadequate dissolved oxygen levels can hinder microbial growth and promote the dominance of filamentous bacteria, leading to a decline in effluent quality, as discussed earlier. Conversely, excessive dissolved oxygen levels result in wasteful energy expenditure, particularly with mechanical aerators, which may disrupt the biological floc, leading to poor settling characteristics and elevated solids concentration in the effluent.

The return activated sludge (RAS) rate plays a crucial role in the activated sludge process by transferring sludge between the secondary clarifier and the aeration tank, ensuring a healthy population of microorganisms in the aeration basin [12]. It's essential for operators to maintain a consistent flow of activated sludge back to the aeration tank to prevent a significant drop in system performance. Insufficient RAS rate results in the accumulation of solids in the settling tank, causing a reduction in treatment efficiency and loss of solids. Alternatively, if the rate is very high, the aeration tank may get overwhelmed, leading to a decrease in aeration time and subpar performance. Hence, it is essential to maintain a harmonious equilibrium between the return activated sludge and wastage in order to attain the desired treatment performance.

However, due to the presence of live organisms in activated sludge that undergo growth and produce waste, its volume steadily expands. Prolonged retention of activated sludge in the system can result in diminished process efficiency. Conversely, removing too much activated sludge can result in lightweight solids that settle too slowly in the secondary clarifier [15]. Therefore, the rate of waste activated sludge (WAS) removal is an important operational parameter. It enables operators to maintain the desired concentration of mixed liquor suspended solids (MLSS), the food-to-microorganisms ratio, and the sludge age [15]. Additionally, in the secondary clarifier, solids and liquid are separated, forming a solid blanket. If the rate at which solids are removed from the clarifier is not equal to the rate at which they enter, the depth of the blanket increases, this can result in the transportation of solid particles into the effluent of the operation. Various factors, such as temperature fluctuations or sludge bulking, can affect the depth of the sludge blanket.

I.2.4 The Secondary Clarifier

The secondary clarifier is a crucial component of the activated sludge system. The primary purpose of this process is to separate the biomass from the water, resulting in a high-quality effluent that is free from settleable solids. Additionally, it also serves to thicken the biomass (Figure I.3). A portion of the densified biomass is discarded as sludge, while another portion returns into the biological reactor to ensure a suitable biomass concentration.

The key aspect of secondary treatment for domestic sewage is the inclusion of a biological phase, while preliminary and primary treatments mostly rely on physical processes, the elimination of organic substances in the secondary stage takes place through biochemical reactions mediated by microorganisms. Secondary treatment processes are designed to expedite decomposition mechanisms that naturally occur in receiving bodies of water. Consequently, the degradation of degradable organic pollutants is achieved under controlled conditions and within shorter time frames compared to natural systems [16].

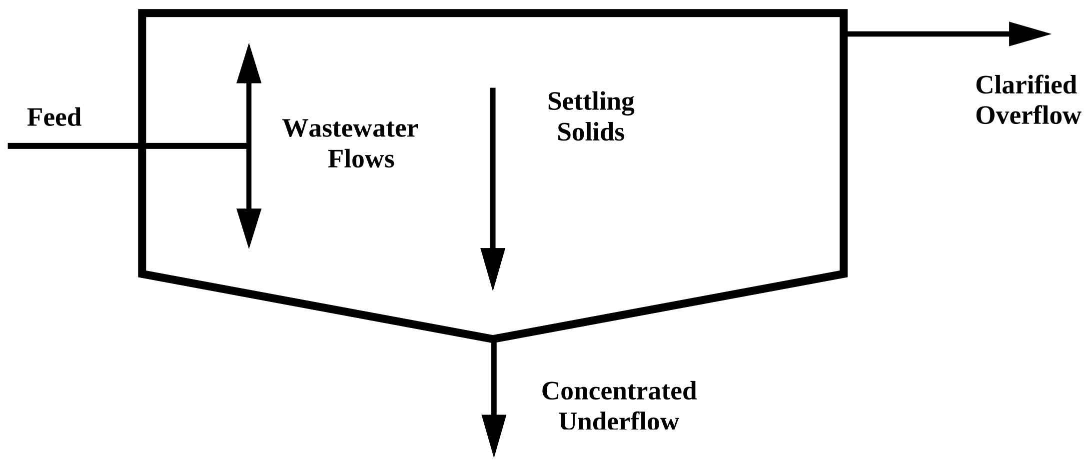


Figure I. 3 Clarifier flows.

I.3 Modelling of Biological Processes

Modelling and simulation are valuable tools for comprehending and designing activated sludge wastewater treatment facilities (WWTPs) [17]. A mathematical model of a WWTP that can anticipate how the WWTP would behave under different operating situations is a useful tool for WWTP design, analysis, control, forecasting, and optimization, hence ensuring high effluent quality.

A wastewater treatment plant model represents the biochemical and physical processes that are part of the technical process of treating wastewater. The biochemical processes convert the organic substances and nutrients present in wastewater into carbon dioxide, nitrogen, and a solid component consisting of cell material [18]. The latter can be eliminated from water by physical separation techniques. Therefore, the activated sludge WWTP models typically comprise two interconnected sub-models: the activated sludge model and the settler model [19–21].

Mathematical modelling involves creating a virtual representation of a system by solving equations that describe its functioning using computer algorithms. This virtual representation allows for the study and experimentation, known as simulations, of the system, mirroring real-world scenarios. The advantage lies in the ability to conduct numerous experiments efficiently, saving time and resources compared to traditional on-site experimentation. Mathematical modelling is widely applied across scientific and technical domains, utilized by both researchers and operational staff such as managers and technicians.

Beyond enhancing the understanding of phenomena through interpretation and extension of experiences, modelling serves as a predictive tool, enabling scenario testing and process optimization. In the treatment of liquid effluents, dynamic operation modelling of wastewater treatment plants integrates variations over time, encompassing biological (microbial population growth), physical (aeration, hydraulics, decantation), and chemical (precipitation, oxidation-reduction, etc.) phenomena that occur within the system. Among these processes, activated sludge treatment stands out as an area where knowledge and applications are particularly advanced [22].

I.3.1 Input Data

In addition to the physical layout and operational parameters, the characterization of influent wastewater is vital for modelling wastewater treatment plants effectively. Comprehensive data on the quantity and quality of influent water, including variations in flow rates, pollutant concentrations, and seasonal fluctuations, provide critical insights into the dynamic behaviour of the treatment process.

Furthermore, detailed information on the characteristics of pollutants, such as biochemical oxygen demand (BOD), chemical oxygen demand (COD), total suspended solids (TSS), nutrients (nitrogen and phosphorus compounds), heavy metals, and emerging contaminants, is essential for understanding the treatment requirements and predicting the performance of treatment units.

Moreover, factors such as hydraulic loading rates, hydraulic retention times, temperature variations, and influent pH levels significantly influence the efficiency and effectiveness of wastewater treatment processes. Therefore, incorporating these parameters into the modelling framework enables engineers and researchers to simulate various operating scenarios, optimize treatment strategies, and assess the resilience of treatment systems to changing conditions.

Furthermore, advancements in sensor technology, data acquisition systems, and online monitoring tools facilitate real-time data collection and continuous monitoring of treatment plant performance. Integrating these technologies into modelling platforms enables dynamic modelling and adaptive control strategies, enhancing the operational efficiency and sustainability of wastewater treatment facilities.

In summary, accurate modelling of wastewater treatment plants requires a comprehensive understanding of the physical, chemical, and biological processes involved, as well as access to high-quality data on plant operations and influent characteristics. By integrating these elements into the modelling framework, engineers and researchers can develop robust and reliable models that support informed decision-making, optimize resource allocation, and enhance environmental stewardship in wastewater treatment.

I.3.2 Mass Balance

The models, composed of a series of nonlinear differential equations, are derived from the dynamic balance equations on the bioreactor. A mass balance describes the fluctuation in the quantity of a compound as the total of what is introduced or created, subtracted by what is removed, as stated by [23]:

Accumulation = (Input + Production) - (Output + Consumption)

Drafting a balance for each chemical results in the suggestion of a global process model, with the part representing biological responses represented by the words production and consumption.

I.3.2.1 Reaction Scheme

In summarizing synthetically and from a macroscopic perspective all the biological and chemical reactions, the reaction scheme defines the terms production and consumption of the mass balance. It is these reactions that determine the biological dynamics of the process, with their speed generally corresponding to the growth rate of the involved bacteria.

The reaction scheme is thus constructed based on available phenomenological knowledge. Furthermore, its level of complexity depends on the precision desired. It involves selecting the predominant reactions for the studied process and the compounds present. Its formulation is not unique; the main reactions involved in a biological treatment process are schematized below:

$$\text{Substrate} + \text{biomass} \xrightarrow{\rho} \text{biomass} + \text{product}$$

With:

ρ: The kinetics of the reaction.

We can write this reaction more synthetically, according to [24], as:

$$\text{Substrate} \xrightarrow{\rho} \text{biomass} + \text{product}$$

The arrow indicates that biomass utilizes the substrate to generate new biomass (both as a product and catalyst biomass). In essence, biomass growth does not occur without an initial biomass presence.

For every biological reaction, the consumption and production rates of the compounds involved are determined by the product $\boldsymbol{Y} \times \boldsymbol{\rho}$ with the '-' sign preceding consumption and the '+' sign preceding production. The aggregate rates affecting compound ($\boldsymbol{j}$) which align with the term Production '-' Consumption in the material balance, constitute the overall biological speed denoted (r_j). Its expression takes the form (Equation I.1)):

$$r_j = \sum_i \nu_{i,j} \rho_j \tag{I.1}$$

Therefore, the reaction scheme enables the definition of:

- State variables, representing the compounds involved in the reactions.
- The kinetics associated with each state variable based on the biological reactions in which it participates.

It can also be represented in the form of a functional diagram which contains the same information but which, visually, makes it possible to better highlight the reaction sequences [25].

I.3.2.2 Kinetics of Reactions

The kinetics, or reaction rates, play a crucial role in understanding system dynamics. However, determining how each compound affects the reaction kinetics can be challenging. The equations representing these kinetics often stem from empirical considerations, resulting in approximate relationships.

The expression of kinetics is:

$$\rho = \mu \times [biomass] \tag{I.2}$$

(μ) is a parameter that might be represented by a constant, a time-varying parameter, or a combination of the other state variables of the system. For biomass mortality, a constant coefficient is adequate:

$$\rho = -b \times X_B \tag{I.3}$$

With:

b: Mortality coefficient of biomass (d^{-1});

X_B: Biomass concentration (mgO2/l)

The parameter (b) offers the advantage of direct measurability through the respirometric method [26], unlike kinetic coefficients, which are generally not directly measurable. However, the representation of complex kinetics, such as the oxidation of biodegradable organic matter, nitrification, denitrification, and hydrolysis, remains challenging. Complex kinetics require determining whether a compound, based on its concentration in the reaction medium, inhibits, activates, or limits the reaction, and to what extent. Empirical models proposed by Monod [27], inspired by previous work by Michaelis and Menten [28], provide solutions to this challenge, primarily focusing on the biomass growth reaction, which is one of the most intricate reactions in the treatment process.

$$\rho = \mu \times X_B \tag{I.4}$$

$$\mu = \mu_{max} \cdot \frac{[Substrate]}{K_S + [Substrate]} \tag{I.5}$$

With:

μ**:** Specific growth rate (d^{-1});

μ_{max}: Maximum growth rate (d^{-1});

K_S: Substrate half-saturation constant (mg O2/L).

The half-saturation constant (K_S) represents the substrate concentration at which the growth rate (μ) equals half of its maximum value (see Figure I.4). The value assigned to the (K_S) coefficient determines the point at which substrate concentration begins to saturate, directly influencing the shape of the Monod's law curve. Understanding the value of this parameter is crucial as it indicates the substrate concentration relative to the saturation level. However, estimating this parameter requires specific experimental tests and is highly sensitive to operating conditions [4].

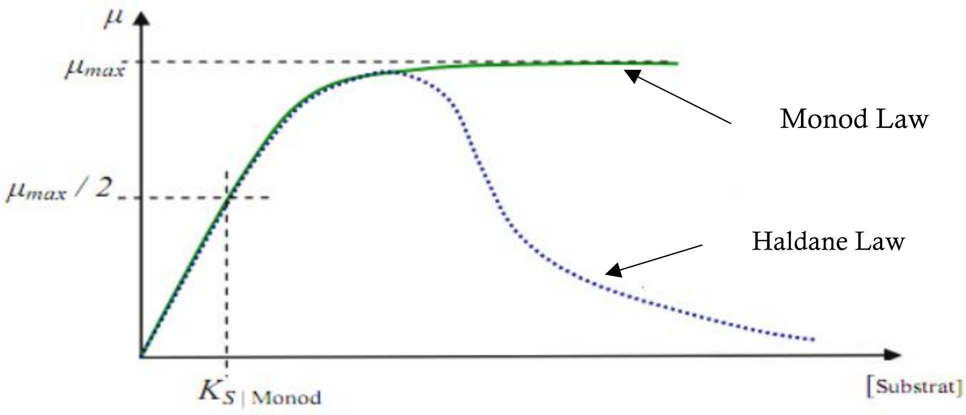


Figure I. 4 Graphical representation of Monod's and Haldane's laws.

When the concentration of certain compounds becomes too high, they can inhibit a reaction. Monod's law does not account for this phenomenon, so it is preferable to use Haldane's law Equation (1.6):

$$\mu = \mu_{max} \cdot \frac{[Substrate]}{K_S + [Substrate] + \frac{[Substrate]^2}{K_{inhib}}} \tag{I.6}$$

Where

K_{inhib}: Inhibition constant (mg/l).

To facilitate bacterial growth, besides biodegradable organic matter, nutrients like oxygen (in aerobic reactions), ammoniacal nitrogen, nitrates, nitrites, etc., are required. The specific growth rate expression must incorporate these elements as limiting factors, taking the following form:

$$\mu = \mu_{max} \cdot \prod i \left[\frac{(Composite_i)}{K_i + (Composite_i)}\right] \tag{I.7}$$

The formulation of reaction kinetics is inherently approximate due to the complexity of reactions and the challenge of precisely identifying the influence of each compound on reaction dynamics. As a result, while the formulation of biological conversion rates within a model is relatively reliable, the formulation of kinetics remains imprecise.

I.4 Activated Sludge Model N °01 by IWA (International Water Association)

Biokinetic models describe the changes in wastewater substrates of interest as a result of chemical reactions and the action of bacterial biomass in activated sludge. Since the mid-1960s, approximately ten biokinetic models of activated sludge have been developed [29]. These models incorporate biological processes such as bacterial growth through the consumption of organic or mineral substrates, hydrolysis, and bacterial death, all of which occur within the bioreactors of the treatment plant.

To build models tailored to the objectives and treatment conditions, (Vanrolleghem and Dochain [30]) propose a methodology (Figure I.5) based on the model's objectives, prior knowledge of the system to be modelled, and available data.

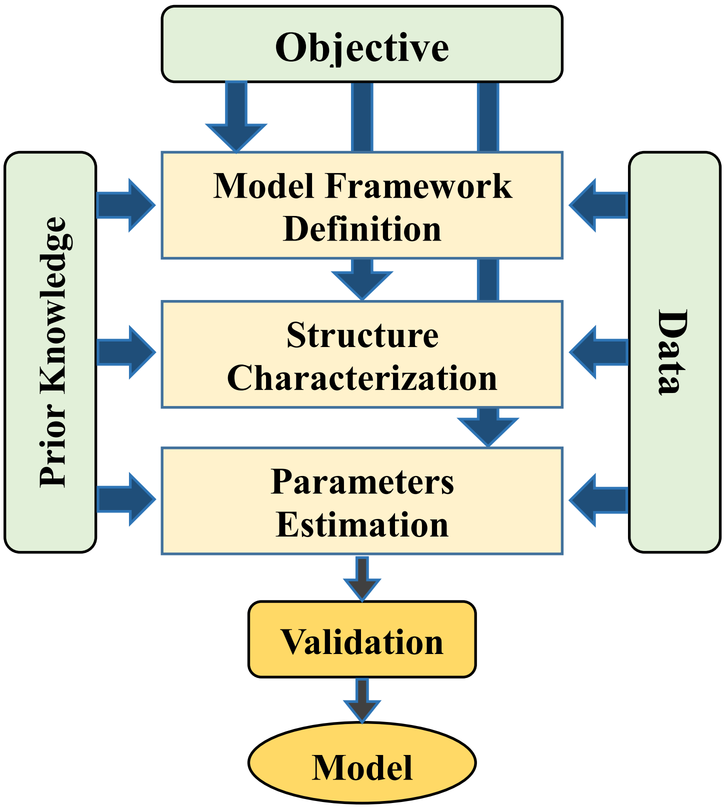


Figure I. 5 Steps to build a model (according to Vanrolleghem and Dochain [30])

These endeavours aimed to acquire knowledge on managing, predicting, and controlling functional strategies under various conditions [31]. The activated sludge process may be described using various mathematical expressions and models, activated sludge models (ASM) proposed by the International Water Association (IWA) have emerged as the most commonly used for designing, operating, and optimizing biological wastewater treatment plants [32]. In particular, the ASM1 model (Henze et al. [4]) holds a special status as the primary reference model, leading to the universal recognition of activated sludge system (ASS) modelling. By adopting chemical oxygen demand (COD) as a parameter to represent the concentration of organic matter in wastewater, the ASM1 model provides a valuable framework for understanding and simulating the complex dynamics of the activated sludge process, thereby contributing to the efficient and effective management of wastewater treatment operations worldwide.

I.4.1 The ASM1 Model Matrix

The ASM1 model incorporates 13 state variables to describe eight pollution degradation processes. Each component, such as biomass (X_{BH}) and substrate (S_S), is denoted by indices **(i)**, while processes like bacterial growth, bacterial mortality, and hydrolysis of particulate organic matter are represented by **(j)**. The kinetic expressions for each process are outlined in the right column of their respective lines within the matrix (Table I.1).

The ASM1 model matrix is structured as a three-entry table:

The first entry comprises the first column, listing the processes utilized in the model.

The second entry is represented by the first row, which denotes the characteristic variables of the effluent. It is noticeable that the fractions (S_I) and (X_I) are not involved in any equations, yet they are included in the matrix because of their significance. Fraction (S_I) contributes to the quantity of COD leaving the station, while fraction (X_I) constitutes the Hard Suspended Volatile Matter (HSVM). The other columns of the matrix involve other variables that participate in various equations. The last column represents the alkalinity of the environment, which is not essential for the model but provides information during its evolution regarding nitrification capacity. A low pH (pH < 7) reduces the nitrification rate and can cause other issues such as deflocculating or bulking of sludge.

The third entry is materialized in the last column by a set of kinetic equations that relate the processes and variables. The "interior cells" of the matrix are completed with various stoichiometric parameters.

This matrix enables the involvement of all relationships occurring in biological processes, with the simplest model considering three components: biomass, substrate, and dissolved oxygen [33]. The Monod and Herbert equations are used. The Monod equation states that biomass growth is proportional to biomass concentration in a first-order connection and substrate concentration in a mixed-order relationship. The Herbert equation states that biomass decomposition is first-order with regard to biomass concentration. The interpretation of the matrix can be illustrated with reaction rates concerning the rapidly biodegradable fraction (S_S).

Table I. 1 Peterson States variables and processes matrix. Components are recorded in columns and processes are identified in rows.

i Component	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**
j Process	S_I	S_S	X_I	X_S	X_{BH}	X_{BA}	X_P	S_O	S_{NO}	S_{NH}	S_D	X_{ND}	S_{ALK}
1-Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$\frac{-i_{XB}}{14}$
2-Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14*2.86Y_H}-\frac{-i_{XB}}{14}$
3-Aerobic growth of autotrophs						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$\frac{-i_{XB}}{14}-\frac{1}{7Y_A}$
4-Decay of heterotrophs				$1-f_P$	-1		f_P					$-i_{XB}-f_P i_{XB}$	
5-Decay of autotrophs				$1-f_P$		-1	f_P					$-i_{XB}-f_P i_{XB}$	
6-Ammonification of soluble organic nitrogen										1	-1		$\frac{1}{14}$
7-Hydrolysis of entrapped organics		1		-1									
8-Hydrolysis of entrapped organics nitrogen											1	-1	

I.4.1.1 COD Components in ASM1

COD is selected as the most appropriate measure for identifying carbon substrates because it connects electron equivalents in the organic substrate, biomass, and oxygen consumption. In ASM1, COD is separated into four categories: solubility, biodegradability, biodegradation rate, and viability (biomass):

• The overall chemical oxygen demand (COD) is separated into two distinct components: soluble (S) and particulate (X).

• The COD is further classified as non-biodegradable organic waste and biodegradable materials. The non-biodegradable matter is biologically inert and remains unaltered through an activated sludge system. The inert soluble organic matter (S_I) exits the system with the same concentration as it entered. Inert suspended organic matter in the wastewater influent (X_I) is formed by decay, whereas (X_P) becomes entangled in the activated sludge and is eliminated from the system by sludge wastage.

• The biodegradable matter is classified as soluble quickly biodegradable (S_S) and slowly biodegradable (X_S) substrate. Already, it should be noted that certain slowly biodegradable substances may be soluble. The quickly biodegradable substrate is thought to be made up of relatively simple molecules that heterotrophic organisms may consume directly and use to create new biomass. In contrast, the slowly biodegradable substrate is made up of very complex molecules that must be broken down by enzymes before they can be used.

Finally, heterotrophic biomass (X_{BH}) and autotrophic biomass (X_{BA}) are formed by growth on the readily biodegradable substrate (S_S) or by growth on ammonium nitrogen (S_{NH}). The biomass is lost during the decay process, where it is changed to (X_P) and (X_S) (death regeneration, see below) [4,34].

Summarising, the total COD balance of ASM1 is defined by (Equation I.8) and further illustrated in Figure I.6:

$$COD_{tot} = S_I + S_S + X_I + X_S + X_{BH} + X_{BA} + X_P \qquad (I.8)$$

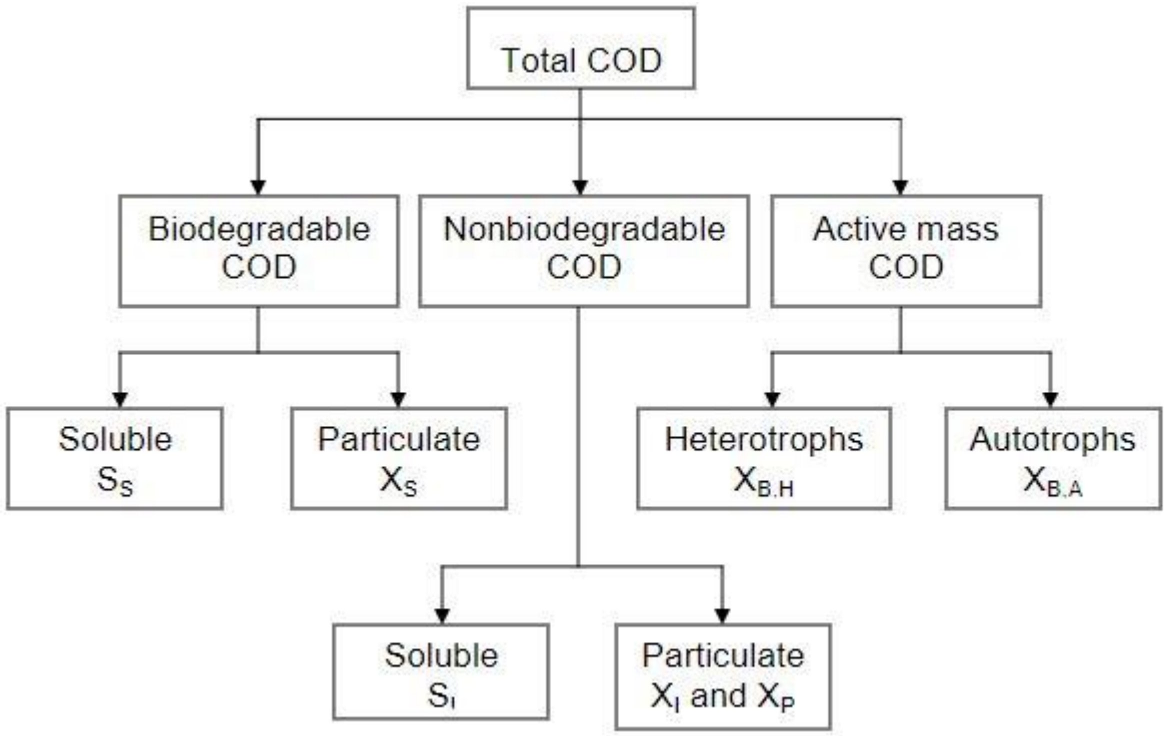


Figure I. 6 COD components in ASM1 [32].

I.4.1.2 Nitrogen Components in ASM1

Like organic matter, total nitrogen can be categorised according to its (1) solubility, (2) biodegradability and (3) biodegradation rate:

• Total nitrogen can be subdivided into soluble (S) and particulate (X) components.

• Nitrogen is classified as non-biodegradable and biodegradable materials. The non-biodegradable particulate organic nitrogen (X_{NI}) is related with the non-biodegradable particulate COD (X_I or X_P), whereas the soluble non-biodegradable organic nitrogen (S_{NI}) is believed to be minimal and so not included in the model.

• The biodegradable nitrogen is classified as ammonia nitrogen (S_{NH}), nitrate + nitrite nitrogen (S_{NO}), soluble organic nitrogen (S_{ND}), and particulate organic nitrogen (X_{ND}). Particulate organic nitrogen is hydrolysed to soluble organic nitrogen in tandem with the hydrolysis of slowly biodegradable organic matter (X_S) (either existing in wastewater or created during the decay process). Ammonification converts soluble organic nitrogen into ammonia nitrogen. Ammonia nitrogen is used as a nitrogen source for biomass growth (i_{XB} represents the quantity of nitrogen incorporated per COD unit). Finally, the autotrophic conversion of ammonia produces nitrate nitrogen (S_{NO}), which is considered a one step process in ASM1 [4,34].

In summary, the overall nitrogen balance for the components in ASM1 is determined by Equation 1.9 and visually represented in Figure I.7.

$$N_{tot} = S_{NH} + S_{ND} + S_{NO} + X_{ND} + X_{NI} + i_{XB}.(X_{BA} + X_{BA}) + i_{XP}.X_P \qquad (I.9)$$

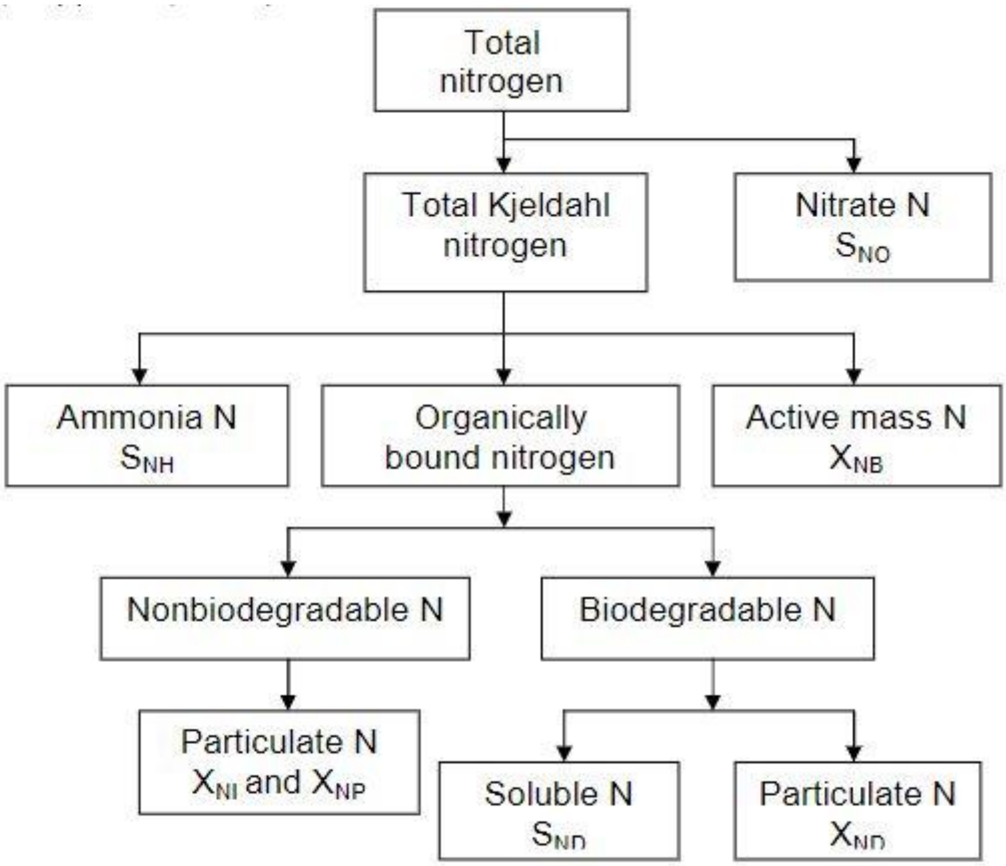


Figure I. 7 Nitrogen components in ASM1 (modified from Jeppsson [32]).

Based on the information provided in the two previous sections **(1.4.1.1 and 1.4.1.2)** regarding the fractionation of organic and nitrogen matters, Table I.2 summarizes the ASM1 model, which consists of 13 state variables.

Table I. 2 State variables of the biological model (ASM1)

Component Nbr	Component symbol	Definition
1	S_I	Soluble inert organic matter $M(COD).L^{-3}$
2	S_S	Readily biodegradable matter $M(COD).L^{-3}$
3	X_I	Particulate inert organic matter $M(COD).L^{-3}$

4	X_S	Slowly biodegradable substrate $M(COD).L^{-3}$
5	$X_{B.H}$	Active heterotrophic biomass $M(COD).L^{-3}$
6	$X_{B,A}$	Active autotrophic biomass $M(COD).L^{-3}$
7	X_P	Products from biomass decay $M(COD).L^{-3}$
8	S_0	Dissolved oxygen $M(COD).L^{-3}$
9	S_{NO}	Nitrate and nitrite nitrogen $M(N).L^{-3}$
10	S_{NH}	Ammonia nitrogen $M(N).L^{-3}$
11	S_{ND}	Soluble biodegradable organic nitrogen $M(N).L^{-3}$
12	X_{ND}	Particulate biodegradable organic nitrogen $M(N).L^{-3}$
13	S_{ALK}	Alkanity - Molar units

I.4.2 Processes in ASM1

ASM1 defines four distinct primary processes [4]:

• Growth of biomass

• Decay of biomass

• Ammonification of organic nitrogen

• Hydrolysis of particulate organic matter

The substrate flows in ASM1 are illustrated in Figure I.8.

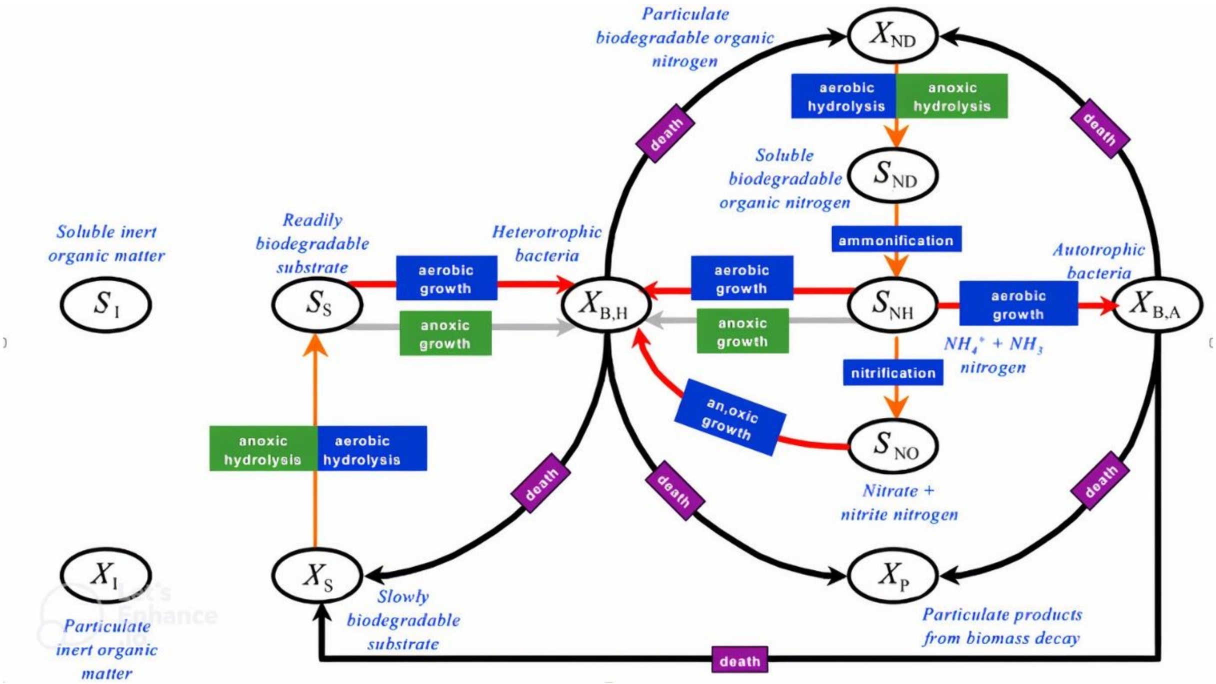


Figure I. 8 Substrate flows in ASM1 (General overview) [32].

I.4.2.1 Growth of Biomass

- Aerobic growth of heterotrophic biomass

The breakdown of readily degradable substances that can be broken down by living organisms in the presence of oxygen results in the growth of heterotrophic biomass. Ammonia is employed as a nitrogen supply and absorbed into the cell mass. In general, the procedure contributes significantly to biomass generation and COD elimination.

- Anoxic growth of heterotrophic biomass

Heterotrophic organisms utilise (S_S) as a substrate and nitrate as an electron acceptor when there is no oxygen present. Denitrification causes biomass growth and the generation of nitrogen gas.

- Aerobic growth of autotrophic biomass

Nitrification is the process by which ammonia nitrogen is transformed to nitrate. As a consequence, there is a rise in autotrophic biomass and an elevated need for oxygen. Ammonia serves as a nitrogenous compound for cellular synthesis and is taken up by the cellular biomass.

I.4.2.2 Decay of Biomass

- Decay of heterotrophic biomass

The organisms are anticipated to die at a specific rate, and when they decompose, some of the degradation will lead to the release of slowly degradable compounds. The remaining portion is considered non-biodegradable and adds to the (X_P) component. The process is anticipated to exhibit equivalent rates under aerobic, anoxic, and anaerobic conditions.

- Decay of autotrophic biomass

This process can be similarly described as the decay of heterotrophs.

I.4.2.3 Ammonification of Soluble Organic Nitrogen

During a first-order process, biodegradable soluble organic nitrogen is transformed into free and saline ammonia.

I.4.2.4 Hydrolyses

- Hydrolysis of entrapped organic matter

Slowly biodegradable substrate entrapped in the sludge degrades extracellularly. This process generates easily biodegradable substrate that is accessible to organisms for growth. It happens in both aerobic and anoxic environments and is based on surface reaction kinetics.

- Hydrolysis of entrapped organic nitrogen

The process by which biodegradable particulate organic nitrogen decomposes into soluble organic nitrogen is referred to as the rate of entrapped organics.

I.4.3 Kinetics of the Reactions Involved

The reactions involved are expressed by speeds ρ_1*(j = 1 … 8)*:

j = 1: Aerobic growth of heterotrophs

$$\rho_1 = \mu_H \left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{OH}+S_O}\right) X_{BH} \qquad \text{(I.10)}$$

j = 2: Anoxic growth of heterotrophs

$$\rho_2 = \mu_H \left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{OH}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{BH} \qquad \text{(I.11)}$$

j = 3: Aerobic growth of autotrophs

$$\rho_3 = \mu_A \left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{OA}+S_O}\right) X_{BA} \qquad \text{(I.12)}$$

j = 4: Mortality of heterotrophs

$$\rho_4 = b_H X_{BH} \qquad \text{(I.13)}$$

j = 5: Mortality of autotrophs

$$\rho_5 = b_A X_{BA} \tag{I.14}$$

j = 6: Ammonification of soluble organic nitrogen

$$\rho_6 = K_A S_{ND} X_{BH} \tag{I.15}$$

j = 7: Hydrolysis of absorbed organic matter

$$\rho_7 = k_h \frac{X_S/X_{BH}}{K_X+(X_S/X_{BH})}\left[\left(\frac{S_O}{K_{OH}+S_O}\right)+\eta_h\left(\frac{K_{OH}}{K_{OH}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{BH} \tag{I.16}$$

j = 8: Hydrolysis of absorbed organic nitrogen

$$\rho_8 = k_h \frac{X_S/X_{BH}}{K_X+(X_S/X_{BH})}\left[\left(\frac{S_O}{K_{OH}+S_O}\right)+\eta_h\left(\frac{K_{OH}}{K_{OH}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{BH}\frac{X_{ND}}{X_S} \tag{I.17}$$

I.4.4 Conversion Rate and Parameter Values

The observed conversion rates (r_i) result from combinations of fundamental processes and are expressed by:

- i = 1 (S_I) :

$$r_1 = 0 \tag{I.18}$$

- i = 2 (S_S) :

$$r_2 = -\frac{1}{Y_H}.\rho_1 - \frac{1}{Y_H}.\rho_2 + \rho_7 \tag{I.19}$$

- i = 3 (X_I) :

$$r_3 = f_\mathrm{p}\,.(\rho_2 + \rho_7) \tag{I.20}$$

- i = 4 (X_S) :

$$r_4 = \left(1 - f_\mathrm{p}\right).\rho_4 + \left(1 - f_\mathrm{p}\right).\rho_5 - \rho_7 \tag{I.21}$$

- i = 5 ($X_{B,H}$) :

$$r_5 = \rho_1 + \rho_2 - \rho_4 \tag{I.22}$$

- i = 6 ($X_{B,A}$) :

$$r_6 = \rho_3 - \rho_5 \tag{I.23}$$

• i = 7 (S_{NO}) :

$$r_7 = -\frac{1-Y_H}{2.86.Y_H}.\rho_2 + \frac{1}{Y_A}.\rho_3 \tag{I.24}$$

• i = 8 (S_{NH}) :

$$r_8 = -i_{\mathrm{XB}}.\rho_1 - i_{\mathrm{XB}}.\rho_2 - \left(i_{\mathrm{XB}} + \frac{1}{Y_A}\right).\rho_3 + \rho_6 \tag{I.25}$$

• i = 9 (S_{ND}) :

$$r_9 = -\rho_6 + \rho_8 \tag{I.26}$$

• i = 10 (X_{ND}) :

$$r_{10} = \left(i_{\mathrm{XB}} - f_{\mathrm{p}}.i_{\mathrm{XP}}\right).\rho_4 - \left(i_{\mathrm{XB}} - f_{\mathrm{p}}.i_{\mathrm{XP}}\right).\rho_5 - \rho_6 \tag{I.27}$$

• i = 11 (S_O) :

$$r_{11} = -\frac{1-Y_H}{Y_H}.\rho_1 - \frac{4.57-Y_H}{Y_H}.\rho_3 \tag{I.28}$$

I.4.5 Values of Biological Parameters

In Table I.3 the kinetic and stoichiometric parameters are reported, the process of selecting these parameters is referred to as model calibration [35].

Table I. 3 Kinetic and Stoichiometric coefficients in ASM1.

Parameter	Symbol	Unit	Range	Default Values
		Stoichiometric Parameters		
Yield for heterotrophic biomass	Y_H	g(cell COD formed)/g(COD oxidized)	[0.57 - 0.67]	0.67
Yield for Autotrophic biomass	Y_A	g(cell COD formed)/ g(N oxidized)	[0.15 - 0.24]	0.24
Fraction of biomass yielding part. prod.	f_p	dimensionless	-	0.08

(Mass N)/(Mass COD) in biomass	i_{XB}	g N/g COD	-	0.086
(Mass N)/(Mass COD) prod. from biomass	i_{XP}	g N/g COD	-	0.06
volatile suspended solids/ total suspended solids	VSS /TSS	g VSS/ g TSS	-	0.70
particulate COD to total COD	XCOD/VSS	g COD/ g VSS	-	1.48
Kinetic Parameters				
Maximum specific growth rate for heterotrophic biomass	$\mu_{max\ H}$	d^{-1}	[0.6 - 13.2]	6
Heterotrophic decay coefficient	b_H	d^{-1}	[0.30 - 1.20]	0.62
Half saturation constant	K_S	g COD/ m^3	[10 - 40]	20
Oxygen hsc for heterotrophs	K_{OH}	g O_2/ m^3	[0.01 - 0.20]	0.20
Nitrate hsc for denitrifying heterotrophs	K_{NO}	g NO_3^-N/ m^3	[0.10 - 0.50]	0.50
Autotrophic maximum specific growth rate	$\mu_{max\ A}$	d^{-1}	[0.6 - 13.2]	6.0
Autotrophic decay rate	b_A	d^{-1}	[0.05 - 0.20]	0.20
Oxygen hsc for Autotrophs	K_{OA}	g O_2/ m^3	[0.40 - 2.0]	0.40
Ammonia hsc for Autotrophs	K_{NH}	g NH_3^-N/ m^3	-	1.0
Correction factor for anoxic growth of heterotrophs	η_H	Dimensionless	[0.60 - 1.0]	0.80
Ammonification rate	K_a	g O_2/ m^3	-	0.08

Maximum specific hydrolysis rate	k_h	g(slowly biodegr.COD)/g(cell COD)/d	-	3.0
Hsc for hydrolysis of slowly biodegradable (biodeg.) substrate	K_X	g(slowly biodegr.COD)/g(cell COD)/d	-	0.03
Correction factor for anoxic hydrolysis	η_h	Dimensionless	-	0.40

I.4.6 Mass Balance in the Clarifier

The total flow (Φ) of particulate compounds in a given section of the clarifier, which results from the superposition of the liquid flow (Φ_l) and the sedimentation flow (Φ_s), is defined by:

$$\Phi = \Phi_l + \Phi_s \tag{I.29}$$

$$\Phi_t = \begin{cases} X_t^{dec} v_{up} \text{ if } z < z_a \\ X_t^{dec} v_{dn} \text{ if } z > z_a \end{cases} \tag{I.30}$$

$$\Phi_s = X_t^{dec} v_s\left(X_t^{dec}\right) \tag{I.31}$$

Where (X_t^{dec}) denotes the sludge concentration in the section considered. (v_{up}),(v_{dn}) the ascending and descending velocities of the liquid in the decanter. (v_s) the sedimentation velocity and (z_a) the depth of the clarifier feed (axis facing downwards).

The upward velocity (v_{up}) and downward velocity (v_{dn}) of liquid in the clarifier are written:

$$v_{up} = \frac{Q_0 - Q_w}{A} \tag{I.32}$$

$$v_{dn} = \frac{Q_0 + Q_w}{A} \tag{I.33}$$

Where:

A: the surface area of the clarifier.

Q_0: the inlet flow rate.

Q_w: the sludge extraction flow rate.

In order to get accurate outcomes in the modelling of wastewater treatment plants, it is recommended to integrate the ASM1 model with a model of a decantation system. Takaçs [36] has developed a standardized layered settler model, which effectively describes the processes of clarification and thickening. This model depicts the settler as a tank with 10 horizontal levels and assumes total mixing inside each layer, the sedimentation velocity is calculated using the double exponential velocity approach provided by [36] (Equation I.34):

$$u_{\mathrm{s}}(X_t^{\mathrm{set}}) = max\left[0, min\left[u'_{\mathrm{s},0}, u_{\mathrm{s},0}\left(e^{-r_{\mathrm{h}}X_t^{\mathrm{set}}(1-f_{\mathrm{ns}})} - e^{-r_{\mathrm{p}}X_t^{\mathrm{set}}(1-f_{\mathrm{ns}})}\right)\right]\right] \tag{I.34}$$

The settling parameters ($u_{\mathrm{s},0}$), ($u'_{\mathrm{s},0}$), (r_{h}), (f_{ns}), (r_{p}) and (X_t^{set}) are defined in Table I.4.

Table I. 4 Settling model parameters.

Parameter	**Symbol**	**Unit**	**Default Value**
Theoretical maximum sedimentation rate.	°F	$m.j^{-1}$	712
Maximum effective sedimentation rate.	$u'_{\mathrm{s},0}$	$m.j^{-1}$	340
Sedimentation parameter for highly concentrated suspensions.	r_{h}	$m^3.g^{-1}$	$4.26\ 10^{-4}$
Sedimentation parameter for weakly concentrated suspensions.	r_{p}	$m^3.g^{-1}$	$5.0\ 10^{-3}$
Unsettled fraction of incidental solids.	f_{ns}	-	$5.0\ 10^{-4}$
Limit concentration of suspended solids.	X_t^{max}	$g.m^{-3}$	3000

I.4.7 Restrictions of ASM1

A number of restrictions concerning ASM1 are summarized below [4]:

- The system must maintain a consistent temperature.
- The pH remains stable and close to neutral. It is known that the pH has an influence on many of the parameters, however only limited knowledge is available to be able to express these possible influences. Consequently, a constant pH has been assumed. The inclusion of alkalinity in the model, however, does allow for detection of pH problems.
- No attention has been given to alterations in the composition of the organic matter in specific portions of wastewater (e.g. the readily biodegradable substrate). Therefore, the parameters in the rate expressions have been assumed to have constant values. This means that only concentration changes of the wastewater components can be handled whereas changes in the wastewater character cannot.
- The effects of nutritional constraints (e.g., N and P) on cell development have not been investigated. It is, however, simple to include limiting words in the model if necessary.
- The correction factors for denitrification (η_g and η_h) are stable and constant for a particular wastewater, although their values may vary based on system setup.
- The nitrification parameters are considered to remain constant, taking into account any negative effects that wastewater elements may have on them.
- The heterotrophic biomass remains consistent and does not experience fluctuations in species variety throughout time. This assumption is inherent to the assumption of constant kinetic parameters. This means that any changes in substrate concentration gradients, reactor configuration, etc. on sludge settleability are not considered.
- It is expected that the capture of particle organic materials in the biomass occurs immediately.
- The process of breaking down organic matter and organic nitrogen through hydrolysis happens at the same time and equal speeds.
- The type of electron acceptor present does not impact biomass loss during decay.
- The heterotrophic yield coefficient is unaffected by electron acceptor type.
- ASM1 is designed to simulate municipal wastewater treatment and should not be used in systems with significant industrial contributions.
- ASM1 excludes reactions that occur in the absence of oxygen. Simulating systems that have a significant amount of anaerobic reactor capacity can lead to mistakes.

- ASM1 cannot handle high nitrite concentrations.
- ASM1 is not suitable for activated sludge systems with high loads and short sludge retention time (SRT) (<1 day).

I.5 Simulators for Wastewater Treatment Plants

Different forms of computer software may be used to create mathematical models and then forecast the performance of wastewater treatment plants. These include spreadsheets (useful primarily for steady-state simulations and mass balancing), low level programming languages ((e.g. C++, Fortran, Pascal, Visual Basic, etc.), general-purpose simulators (e.g. MATLAB/Simulink, ACSL, Maple, Mathematica, Stella) and specific WWTP simulator environments (or simulation platforms).

The general-purpose simulators offer great versatility, however, the user must provide the models for a specific WWTP configuration. As a consequence, this kind of software requires a proficient user who possesses a comprehensive understanding of the consequences that result from each line of script in the models [37]. In contrast, The WWTP simulator settings should provide a significant amount of adaptability requiring little modeller instruction along with the need for programming expertise [38].

I.5.1 ASIM (ETH/EAWAG, Switzerland)

ASIM (stands for **A**ctivated Sludge **SIM**ulation Program) is a simulation program, which allows for simulation of different activated sludge systems (Figure 1.9). The program was developed at the Institute for Hydromechanics and Water Resources Management (ETH) in Zurich. Special licenses for research and development can be obtained from ETH/EAWAG (www.asim.eawag.ch). A commercial distributor of the program is the company Holinger AG (www.holinger.com).

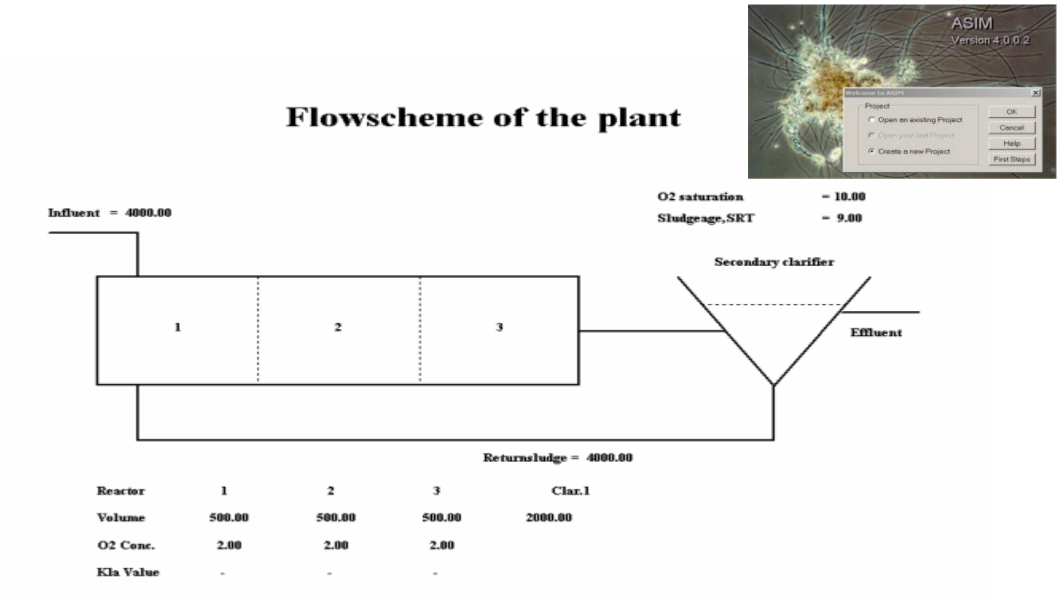


Figure I. 9 The ASIM wastewater treatment process simulator.

The biokinetic models may be freely defined, stored and edited by the user, however, several pre-defined models are available in a model library including ASM1 (adapted), ASM2d and ASM3. The software can also incorporate control loops, which use basic ratio and on/off type controllers.

I.5.2 BioWin (EnviroSim, Canada)

Most types of wastewater treatment systems can be designed in BioWin (Figure I.10) using many process modules including a range of activated sludge bioreactor modules and various clarifier modules (primary, ideal and one dimensional model clarifiers).

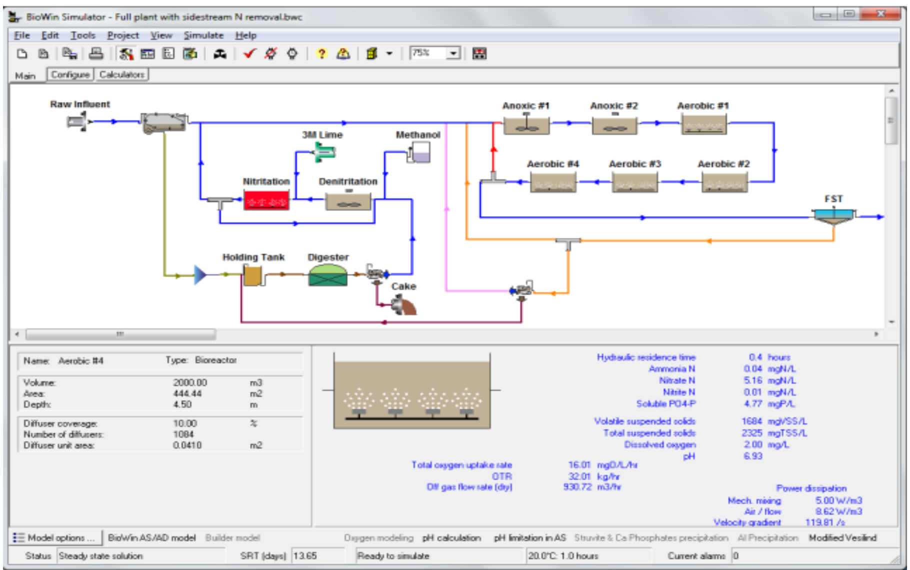


Figure I. 10 The BioWin wastewater treatment process simulator.

Both steady-state and dynamic simulations can be run from the main simulator window. BioWin uses an itinerary that allows to schedule different operational parameters, such as DO set points, air flowrates, and temperature. In order to display simulation results in an integrated form, BioWin incorporates an "Album" for this purpose. The album consists of a series of tabbed pages which may contain any or a combination of the following data display formats: a wide range of chart types, tables and element-specific information displays.

A comprehensive list of the BioWin application references is available at the EnviroSim web page (www.envirosim.com).

I.5.3 SIMBA (IFAK, Germany)

The SIMBA (Figure I.11) simulation platform is based on MATLAB and Simulink and uses the mathematical functionality and the graphical capabilities of both tools. This ensures an open structure and high flexibility of the program (which can be utilized without any prerequisite programming skills). In a SIMBA library, the main components of activated sludge systems are available in the form of blocks [39].

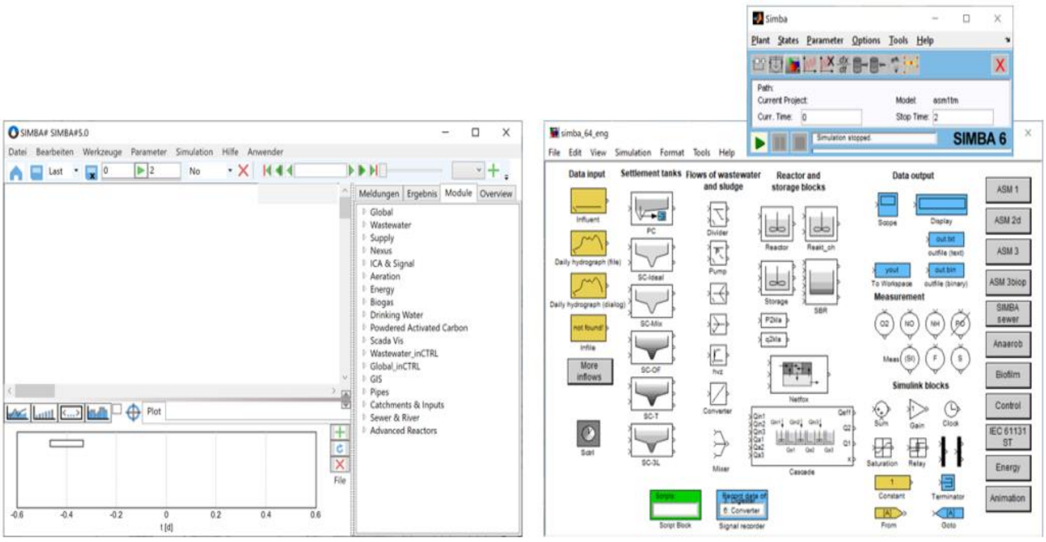


Figure I. 11 SIMBA wastewater treatment process simulator [39].

The model foundations used by SIMBA, e.g. the biokinetic models (ASM1, ASM2d, ASM3), are provided in open format. Additionally, the user has the ability to incorporate new models and functionality. The sensitivity analysis and calibration tool provides an automated model calibration procedure [39].

The SIMBA simulation platform enables comprehensive analysis of the sewage system, wastewater treatment plant, sludge treatment, and waterways [39]. A comprehensive list of the Simba application references is available at the program web page (www.simba.ifak.eu).

I.5.4 STOAT (WRc, UK)

In STOAT (stands for **S**ewage **T**reatment **O**peration **A**nalysis over **T**ime) (Figure I.12), models for all commonly used wastewater treatment processes are available on both the wastewater and sludge treatment sides. The biokinetic models include the standard IWA models ASM1, ASM2d, and ASM3, as well as numerous extensions of these models and the Takaçs model [36] for the clarifier. Specific activated sludge systems, including oxidation ditches and SBRs, can be modelled. The program includes sensitivity analysis, model calibration, and optimization methods, as well as two controller types (PID and ladder logic).

A basic model of the urban environment for studying the sewer-sewage works interaction is included in STOAT, but two external interfaces are also provided - one for the “Open MI” communication protocol and a second for a proprietary, but documented, DHI interface [40]. In addition, the program has support for file exchange with Wallingford Software’s sewer and river models [41].

The technical references concerning the use of STOAT include Stokes et al. [41], Smith et al. [42], Stokes et al. [43] and Ashley et al. [44].

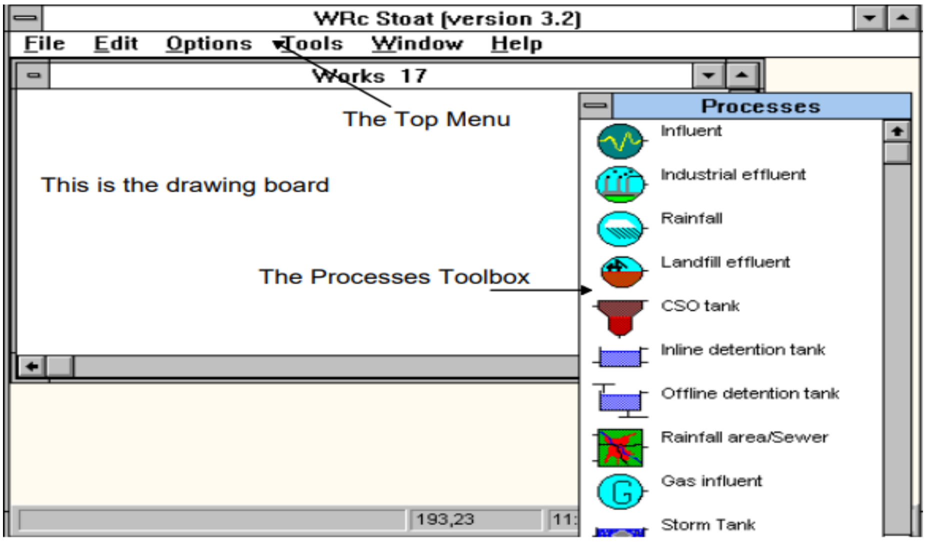


Figure I. 12 STOAT wastewater treatment process simulator [40].

I.5.5 WEST (MOST for WATER, Belgium)

WEST (Figure I.13) provides a framework for dynamic modelling and simulation of wastewater treatment facilities, as well as other water quality systems such rivers, sewers, and urban catchments. The configuration of a researched system (infinite size and complexity) is graphically defined by selecting various elements from a process library. Various control techniques may be applied without further code by selecting and positioning sensor and controller units in the architecture [45].

An extensive model library is available including all the most common models for the activated sludge process and clarifiers. WEST uses the Model Specification Language (MSL), which enables the modeller to adapt and extend the available models or to implement new models [45].

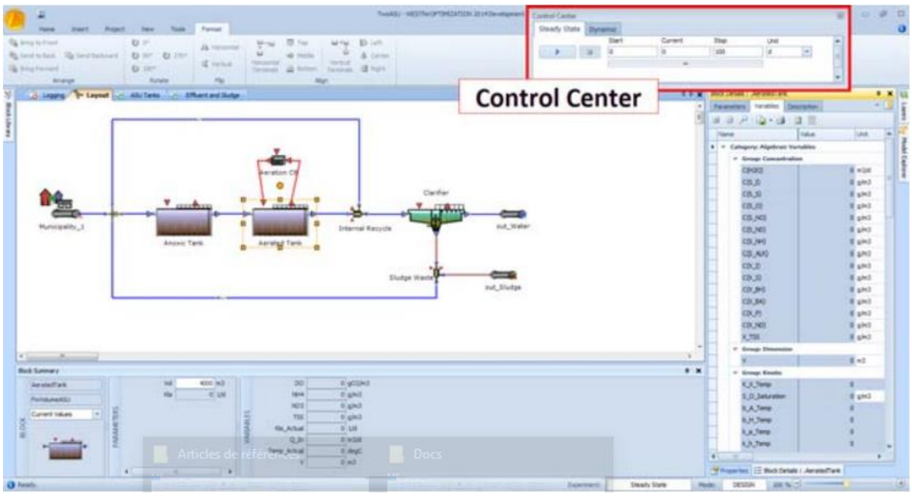


Figure I. 13 WEST wastewater treatment process simulator [45].

I.5.6 GPS-X (Hydromantis, Canada)

In this study, the GPS-X (general-purpose simulator) Module [46] is utilized to simulate the performance of two wastewater treatment plants (WWTPs) employing the ASM1 model. The primary rationale for selecting GPS-X is its extensive usage across various software platforms. Additionally, it offers a free academic license for research purposes, allowing for easy configuration through a user-friendly graphical interface with a wide range of output options. Model libraries are typically provided, further facilitating the simulation process.

GPS-X has a large number of unit processes that may be used to represent a wide range of wastewater treatment plant setups. In activated sludge bioreactors, unlimited number of aerobic, anoxic and anaerobic zone combinations is available. There is also no limit with regard to the number of stages (passes) and internal recycle combinations (including step-feeding) [46].

Standard biokinetic models include temperature dependant versions of ASM1, ASM2d, ASM3, New General, and two-step nitrification (2-step Mantis). The one-dimensional clarifier models can be reactive or non-reactive with the double exponential Takaçs settling function [36]. All GPS-X models are open-code, and available to be edited. Additional model utilities assist in the characterization of influents (Influent Advisor) and edition of the biokinetic models in the Petersen matrix format (Model Developer) [46].

The program provides multiple choices for data input and graphical output, including graphs and data files. It also allows for seamless integration with other programmes such as Excel and MATLAB. The link to MATLAB is used for design and simulation of advanced model based control systems [46].

I.6 Organization of a Simulation Study

An adequate modelling process including model calibration is a key issue for the successful application of these models in practice. This step is usually time consuming and cost intensive since many experiments may be required to determine accurately model parameters [34].

The quality of simulation studies might vary significantly depending on the objectives, skills available, and dollars expended. The study's objectives decide which components and how detailed a plant should be simulated [47]. The objectives will also determine the extent to which a model needs to be calibrated, as the accuracy and dependability of the desired model predictions will be heavily influenced by the quality of model calibration [34]. For typical municipal scenarios with no strong industrial inputs, default parameter choices can typically produce quite accurate descriptions. However, if the tested framework is to be utilized for process efficiency evaluation or optimization, a more exact account of the actual processes will be required [34].

A more standardized use of steady state and dynamic simulations is necessary since a number of model applications for optimization studies and design studies has been growing very rapidly [48]. Independent studies in Belgium by BIOMATH (Petersen et al. [49], Vanrolleghem et al. [45]), in Holland by STOWA (Hulsbeek et al. [48]), in North America by WEFR (Melcer et al. [38]) and in German speaking countries (Germany, Austria and Switzerland) by HSG (Langergraber et al. [47]) have attempted to provide systematic guidelines for calibrating a general model of a WWTP . In recent years, two more protocols were proposed by the Japanese Sewage Works Agency (Itokawa et al. [50]) and an international IWA Task Group (Gillot et al. [51]).

In this section, we outline two protocols. After reviewing each guideline and its applications, our choice was based on the fact that the calibration of our case studies was inspired by several works that applied them. However, we faced a limitation due to insufficient information to fully describe the plant using one of these guidelines.

I.6.1 BIOMATH Calibration Protocol (Belgium)

The protocol developed by (Petersen et al. [49]) was refined by [52] and referred to as the BIOMATH calibration protocol. The protocol is sophisticated and oriented at using scientifically more exact methods, such as the optimal experimental design (OED) technique or sensitivity analysis.

The BIOMATH protocol is consists of four primary stages and 12 modules (Figure I.14). However, the proposed process is not set, but ought to be viewed as adaptable in relation to every individual "case study". The first stage is to define the simulation study's target(s), which is followed by making decisions upon the information given from the researched plant to reach the target(s). The decision is generally made depending on the available time and/or funding for investigation. Some of the eleven modules **(1-11)** may be removed based on the study's objectives, assumptions, and challenges encountered during data collecting. Although each module is considered an independent entity, they are interconnected, and these interactions must be considered when predicting the framework's overall behaviour.

An extension to the BIOMATH calibration protocol was introduced by (Corominas et al. [53]), in their study in Girona, Spain for Sequencing Batch Reactors (SBR) systems. This extension involved a combination of experimental techniques, including lab-scale experimental assays, alongside the application of the biological model ASM1. Over a simulation period of 50 days, dynamic influent conditions were considered to track the evolution of parameters such as (COD), (TN), (TSS), and (VSS). The results of their study demonstrated that by employing this approach, a validated model of high quality could be achieved, thereby enhancing the accuracy and reliability of wastewater treatment plant simulations. In the other hand, Ikumi et al. [54] applied the BIOMATH protocol to guide the calibration of a plant-wide model, incorporating phosphorus, in Cape Town, South Africa (UCT-PW). They utilized the ASM2-3P model along with two global sensitivity analysis methods, Standardized Regression Coefficients (SRC) and

Morris Screening, to simulate biological processes and predict the output of materials such as (COD, Waste Activated Sludge (WAS), and gas composition). While the validation results aligned well with COD removal, they did not match very well for other investigated parameters. Ikumi et al. [54] proposed an extension to the protocol to enhance the calibration process. This would involve creating models of laboratory-scale systems in controlled and well-mixed environments, and then contrasting the projected outcomes of these models to full-scale wastewater treatment plant systems that are integrated into plant-wide configurations.

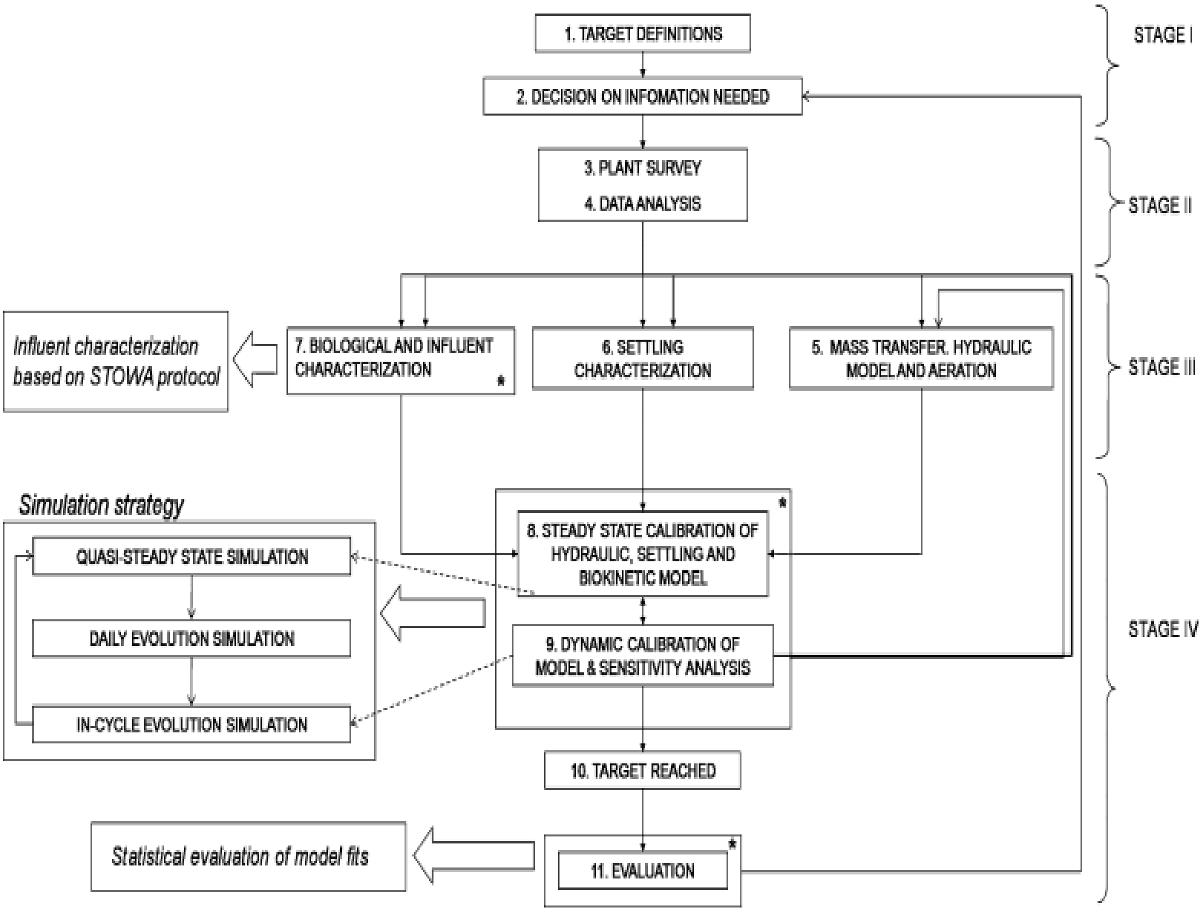


Figure I. 14 The BIOMATH model calibration protocol (modified by (Corominas et al. [53]).

I.6.2 IWA Task Group Protocol

An IWA Task Group on “Good Modelling Practice (GMP): Guidelines for Use of Activated Sludge Models” was published in 2005 in response to the increasing concerns about a proper methodology of overall simulation studies and inter-comparability of the results. The main objective of the group was “to enhance the quality and efficiency of activated sludge (AS) modelling projects, guidelines that include practical protocols on how to use AS models and specific aspects concerning the interaction between modellers and clients are required” [55]. A new protocol was developed (Figure I.15) combining existing guidelines in the field of wastewater treatment field and emphasizing key elements in more general management procedures. The proposed protocol includes the following five main steps which were briefly described by Rieger et al. [55].

Step 1: Project definition. The project objectives are established by considering the requirements and the accessibility of data. In order to establish the project budget, it is necessary to identify the necessary supplementary data. At this stage, expectations for the simulation results (including accuracy) and responsibilities are also defined.

Step 2: Data collection and reconciliation. Existing data are collected from historical records, whereas missing data must be gathered in additional measuring campaigns. The time for data collection and reconciliation should be carefully estimated as this step may consume over 30% of the overall time for a simulation study. Data quality should be validated using data analysis, outlier detection, mass balances (for flows, P, inerts, etc.) and other checks (e.g. typical component ratios). Based on these data, a structure of the plant model should be defined including processes considered, flows and boundaries. This step ends up with an agreement between the modeller and the client concerning the used data and modelled processes.

Step 3: Plant model set-up. This step begins with selection of a simulation platform and sub-models of the general model. Input data, such as volumes, flows, influent concentrations, controllers, etc., are specified. Preliminary simulations with an initially built model are run to verify mass balances, redefine limits, and highlight crucial circumstances. Subsequently, the functional model undergoes testing to ensure the generation of logical outputs. The model adequacy should be confirmed by the client.

Step 4: Calibration and validation. The model parameters are calibrated to achieve concordance between the observed data and what the model predicts. The final accuracy should meet the criteria established in step 1. Expert knowledge and guidance are required to select an appropriate set of parameters that can be “fine-tuned” and how to handle the situations when the measured data and model predictions do not match reasonably. It is necessary to validate the model with the modified parameters using a separate data set.

Step 5: Simulation and result interpretation. Once a verified model is obtained, multiple simulations are conducted to produce scenarios that might be examined in relation to the project objectives established in step 1. Once the client accepts the simulation results, a document containing details of the simulation study is prepared. To ensure comparability, it is necessary to standardise the content of the final report (e.g. for assessing their quality) and provide the adequate information for future model applications.

In the pursuit of reviewing previous research applying (GMP) protocol, Liwarska-Bizukojc et al. [56] investigated the impact of temperature and sludge retention time (SRT) on effluent quality to enhance the predictability and effectiveness of biological wastewater treatment at a full-scale plant in Poland. They applied the Good Modelling Practice protocol to guide the calibration of the ASM1 model under BioWin software. The study revealed that temperature significantly influenced nitrate (NO3-N) concentration in the effluent, and consequently, total Nitrogen (TN) levels. However, as SRT increased, the quality of the effluent declined, particularly in terms of (COD) and total phosphorus. The findings suggested that lower SRT values than those applied in the "Zgierz WWTP" were adequate for the proper removal of nutrients from wastewater. Also, Elawwad et al. [57] conducted a notable study utilizing BioWin models and software (Envirosim, Canada) to assess the performance of a wastewater treatment plant in Cairo, Egypt. They employed the (GMP) protocol under steady-state conditions by adjusting seven stoichiometric and kinetic parameters. According to Elawwad et al., this approach offered a well-organized framework for successfully modelling the "Gabal El-Asfar WWTP". The modelling study demonstrated a successful and accurate correlation with measurements of COD, NH4-N, (NO3-N), and (NO2-N), (TSS), (MLSS), and (MLVSS).

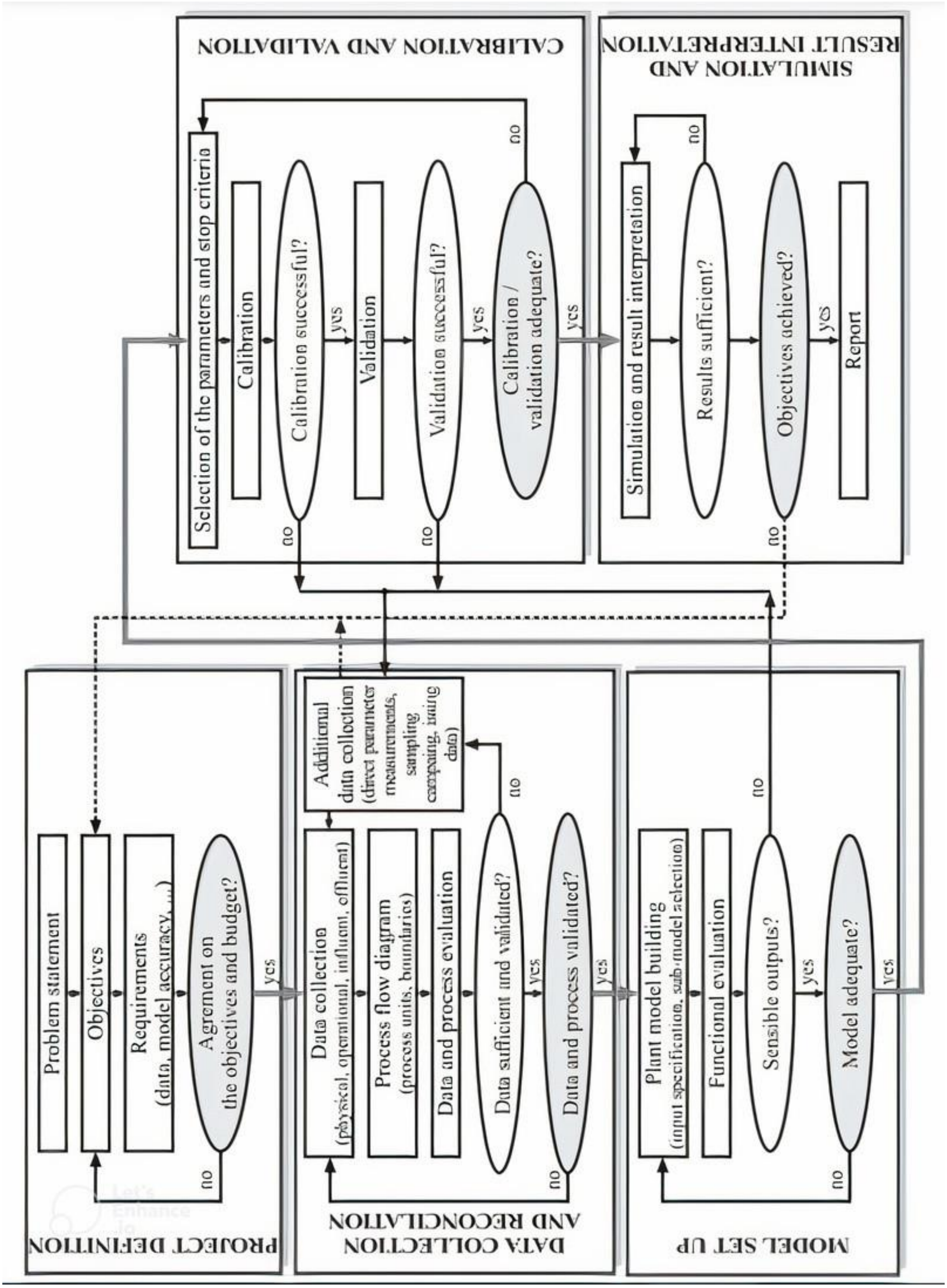


Figure I. 15 Overall procedure of the IWA Task Group protocol (Rieger et al. [55]).

I.6.3 Insights From Independent Explorations

In examining the importance of standardizing modelling protocols, we've surveyed various research papers. While many researchers and practitioners lean towards independent approaches, acknowledging the uniqueness and nuances of activated sludge modelling prompts us to consider the value of drawing inspiration from diverse methodologies. Moreover, while standardized protocols offer benefits like consistency and comparability, their applicability conditions, reliance on lab-scale experiments, and specific measurement requirements can be limiting. Nonetheless, exploring both standardized and solo calibration efforts provides valuable insights into enhancing modelling practices for wastewater treatment and environmental management.

A major sewage treatment plant in the United Arab Emirates was studied by Elshorbagy et al. [58], a dynamic simulation model based on the ASM1 framework was developed for the activated sludge process, utilizing the GPS-X simulation environment. To calibrate the model, they conducted two rounds of field measurements and lab-controlled tests to estimate a range of kinetic and stoichiometric parameters deemed necessary the ASM1 model. Through respirometry techniques, six stoichiometric and kinetic parameters were estimated under steady-state conditions, while manual adjustments were made to COD fractions. The results of the dynamic simulation showed a satisfactory correlation between both observed and generated discharge parameters of COD, TSS, and NH4-N, providing validation for the successful modelling of the plant's processes.

Gao et al. [59] established a mathematical model for simulating a biological nutrient removal (BNR) process for treating wastewater through a cyclic activated sludge system (CASS) reactor (experimental batch with specific microbial communities), an extended ASM1 (E-ASM1) model in (MATLAB 8.4) environment was used in this study with a new calibration approach based on different COD ratios through phylogenetic analysis. The purpose of this study was to determine the impact of microbial population fluctuation on the BNR system's performance. To quantitatively evaluate the model performance, standard deviation (SD) was used to assess the reliability of the E-ASM1 model prediction for effluent COD and biopolymer concentrations. The findings demonstrated that the E-ASM1 model could produce more effective predictions than the ASM1 model in terms of effluent COD, SMP, and EPS ammonia (S_{NH}), soluble microbial products (SMP) and extracellular polymetric substances (EPS) concentrations.

Also, Khalaf et al. [60] studied the impact of operating conditions on the efficacy of two dairy wastewater treatment methods in Egypt: conventional activated sludge (AS) and conventional sequencing batch reactor (SBR) using the (GPS-X) simulator. The model calibration was conducted varying temperature conditions (20°C, 35°C, and 45°C) using COD different concentrations. The dynamic simulation results revealed that the optimal temperature for treatment efficiency was 35°C, with COD removal efficiencies ranging from 93.52% to 97.79% and Nitrate (NO3-N) removal efficiencies ranging from 89.01% to 93.22%. At 45°C, oxygen consumption was highest, and sludge settleability improved with decreasing temperature. Additionally, simulations predicted satisfactory performance of the SBR system, even at high COD concentrations (up to 17500 mg/l).

In their study, Mu'azu et al. [61] aimed to calibrate the activated sludge model one (ASM1) for a WWTP in "Dhahran, Saudi Arabia", using GPS-X. Through systematic simulations, the capacity of the wastewater treatment plant (DWWTP) was assessed under various steady-state operational scenarios, considering influencing parameters. The goal was to ensure compliance with regulatory effluent discharge limits for COD, BOD, (NO2-N + NO3-N), NH4-N, and TN. The approach involved adjusting influent fractionation of COD and nitrogen components using GPS-X influent advisor, conducting variables mass balance, and calibrating the model by adjusting kinetic and stoichiometric parameters to match the model output with actual plant effluent quality data. Simulations under different scenarios were then run for validation. Results indicated a tendency for effluent quality parameters like BOD, and TN to exceed regulatory limits, although plant performance was deemed sufficient for managing even greater amounts of organic waste entering the system (beyond 250 mg/L for COD influent).

I.7 Conclusion

This chapter has provided a comprehensive overview of the activated sludge process, examining its operation and functioning. Through this, we explore the state of the art in biological modelling, with a particular focus on the ASM1 model and its emergence in wastewater treatment. The chapter concludes with an overview of the crucial task of calibration in modelling endeavours, underscoring its significance and highlighting recent advancements in the field.

By laying this groundwork, we have set the stage for the subsequent chapters, where we will delve deeper into our research objectives and methodologies. The insights gained from this chapter will inform our approach to understanding and application of the activated sludge system for efficient wastewater treatment.

CHAPTER II
DATA COLLECTION AND ANALYSIS
(CASE STUDIES)

II.1 Introduction

The meticulous analysis of wastewater treatment plant (WWTP) parameters serves as a cornerstone in evaluating the efficiency and effectiveness of treatment processes. Among these parameters, BOD (Biochemical Oxygen Demand), TSS (Total Suspended Solids), COD (Chemical Oxygen Demand), NH4-N (Ammonium Nitrogen), and temperature play pivotal roles in assessing the overall performance of the treatment station [62]. Understanding the temporal trends and seasonal variations in these parameters provides crucial insights into the dynamic nature of influent and effluent characteristics. In the forthcoming chapters, these parameters will serve as fundamental inputs for our modelling study, facilitating a comprehensive examination of WWTPs behaviour and aiding in the refinement of operational strategies.

This initial investigation highlights the importance of carefully choosing and studying these particular parameters. It sets the stage for a detailed examination of how wastewater treatment plants work and how well they perform.

II.2 Maghnia Wastewater Treatment Plant

II.2.1 Study Area

The area under investigation is the region of Maghnia, a town in the wilaya of Tlemcen, Algeria (Latitude: 34° 51’ 12” North, Longitude: 1° 41’ 21” West) (Figure II.1). It is a semi-arid zone located in the north-western region of Algeria, 26 km west of Tlemcen and about 60 km from the coast. The region is extended over an area of 294 km^2 with a population of 114,634 inhabitants [63]. The lack of rainfall that Algeria experienced in recent decades has had a significant impact on the entire country, with a special focus on its north-western region. The research area, Maghnia, is located within the North-western Oran coastal river basin.

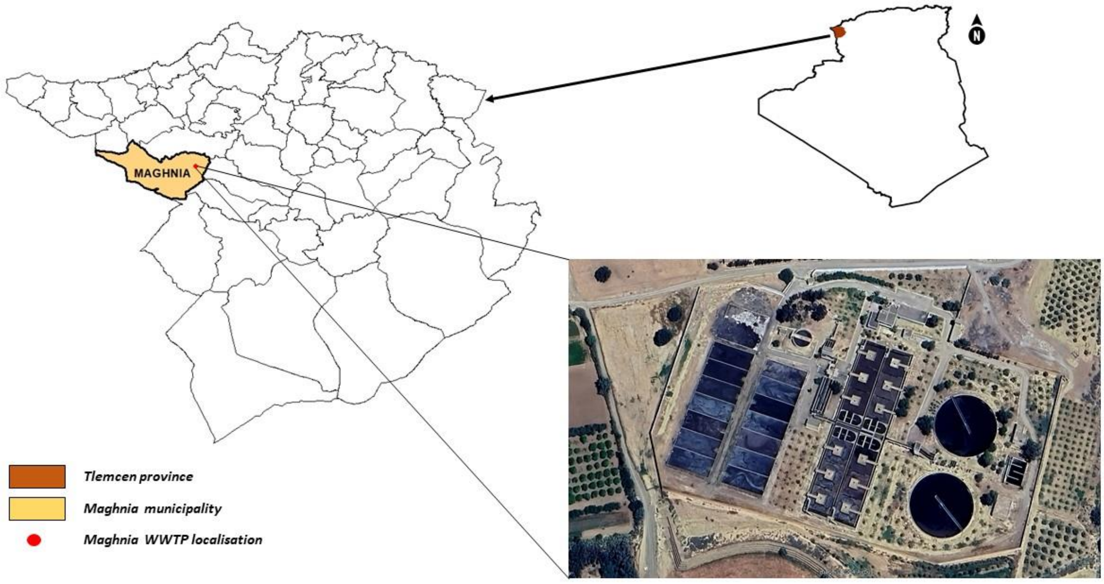


Figure II. 1 Geographic location and an aerial view of the Maghnia City Wastewater Treatment Plant MWWTP.

II.2.2 Description of the Wastewater Treatment Plant (MWWTP)

The Maghnia Wastewater Treatment Plant (MWWTP) was designed to accommodate a flow rate of 30,000 m^3 per day operational since 1999 (Figure II.1), managed by the Algerian National Sanitation Office. It is a low-load activated sludge treatment process facility, which means it operates with a low concentration of suspended biomass and a long solids retention time (SRT). The treatment facility integrates preliminary, secondary, and tertiary treatment systems, as illustrated in (Figure II.2). Screenings and grit removal equipment are used as part of the preliminary treatment. For secondary treatment, an activated sludge method combined with clarity units is used to biologically remove organic and nutrient components from wastewater. The surplus activated sludge is removed from the recycled activated sludge line and sent to sludge drying beds. In the aeration tanks, dissolved oxygen (DO) levels are controlled by an on-off automated controller, and aeration is aided by slow-rotating surface aerators located on walkways [3].The operating conditions of MWWTP are detailed in Table II.1.

Table II. 1 The operating conditions of MWWTP

Parameters	Unit	MWWTP
Population	inhabitants	150,000
Average daily flow rate	$m^3.d^{-1}$	29,400
Flow to discharge in case of rain	m^3/h	30,312
peak flow	m^3/h	3,266
BOD load	$Kg.d^{-1}$	9,614
Suspended Solids	$Kg.d^{-1}$	17,640
Recirculation Flow RAS	m^3/h	1,300

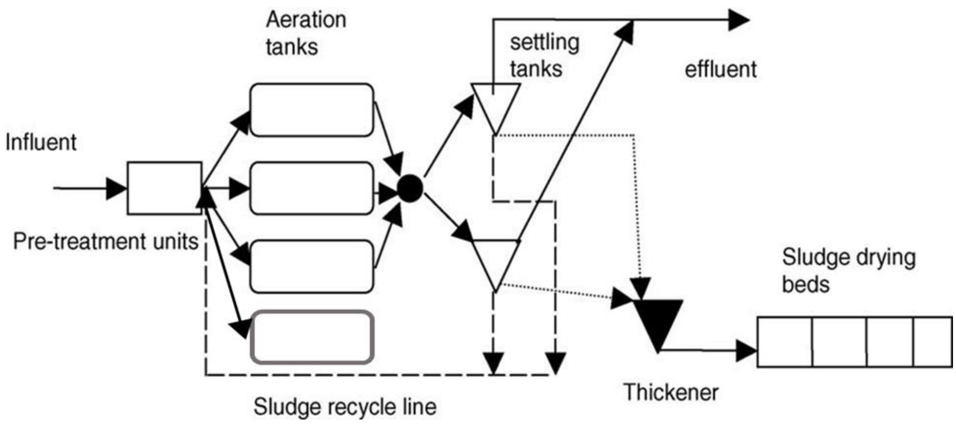


Figure II. 2 Flow sheet of Maghnia WWTP.

II.2.3 Monitored Parameters and Analytical Methods

The laboratory at MWWTP carried out comprehensive analyses to derive the physicochemical parameters essential for the study. A total of 56 samples were collected between July 14, 2021, and January 10, 2023, with monitoring frequencies ranging from 1 to 4 times per month. Collection was performed at a depth of 10 cm below the surface using a Silicon/Teflon water pump to ensure representative sampling.

Twelve key water quality parameters were meticulously measured, including Temperature, pH, (TSS), Dissolved Oxygen (DO), (BOD), (COD), Ammonium Nitrogen (NH4-N), Nitrates (NO3-N), Nitrites (NO2-N), Phosphate (PO4-P), Turbidity, and Chloride. Temperature and pH of surface water were promptly assessed post-collection using HQ40D Portable Multi-Parameter Meters (Hach Company, USA).

Standard methods for water and wastewater analysis were rigorously employed throughout all analytical procedures, ensuring consistency and reliability in the obtained data [64].

II.2.4 Descriptive Data Analysis of Monitored Parameters

Descriptive statistics were employed to determine the features of each measured parameter in terms of: mean, median, standard deviation (SD), minimum (Min), maximum (Max), 1st quartile (Q_1), 3rd quartile (Q_3). Investigating the oscillations in the quality parameter can yield essential insights into the properties of the incoming and outgoing loads, as well as the efficiency of the system in removing contaminants.

The physicochemical parameters derived from analyses were carried out by the laboratory of MWWTP. A total of 56 water samples were gathered between July 14, 2021, and January 10, 2023, to analyse the influent and effluent waters. The purpose was to track daily variations in water quality over time. The statistical descriptions of the analysed parameters for the water samples are presented in Table II.2.

Table II. 2 Statistical results of measured parameters for influent/effluent Wastewater.

Parameter	Unit	Min	Q1	Median	Q3	Max	Mean	SD	Removal efficiency (%)
Influent Values									
TSS	mg/L	76.00	210.00	261.00	335.00	583.00	280.44	123.84	/
BOD	mgO2/L	170.00	360.00	460.00	592.00	850.00	467.52	152.96	/
COD	mgCOD/L	190.00	555.50	653.00	918.00	1403.0	719.04	271.67	/
NH4-N	mgN/L	25.36	49.67	52.00	60.11	79.74	54.31	10.27	/
NO3-N	mgN/L	0.14	0.23	0.32	0.52	2.70	0.51	0.52	/
NO2-N	mgN/L	0.15	0.28	0.40	0.49	0.96	0.40	0.17	/
PO4-P	mg/L	7.30	10.40	11.90	14.90	21.50	12.65	3.28	/
Temp	°C	13.00	20.00	26.50	29.50	32.00	24.85	5.72	/
pH	-	7.05	7.37	7.57	7.95	8.21	7.63	0.33	/
Effluent Values									
TSS	mg/L	13.00	21.00	24.50	28.00	35.00	24.39	5.45	91.30

BOD	mgO2/L	4.00	20.00	23.50	26.50	36.00	22.68	8.40	95.15
COD	mgCOD/L	42.00	61.50	70.00	72.75	90.00	67.71	11.33	90.60
NH4-N	mgN/L	18.50	25.48	32.58	40.03	57.08	33.54	10.12	38.24
NO3-N	mgN/L	0.02	0.03	0.06	0.08	2.40	0.23	0.62	/
NO2-N	mgN/L	0.02	0.04	0.05	0.07	0.57	0.10	0.14	/
PO4-P	mg/L	2.10	5.63	10.05	17.70	34.80	13.03	9.40	/
Temp	°C	13.00	19.38	26.25	29.63	32.00	24.68	5.84	/
pH	-	6.77	7.35	7.69	7.96	8.19	7.62	0.39	/

During the observed period, the average pH value of the influent samples exceeded that of the effluent samples by 1.31%. This variation can be related to the pH elevation caused by the denitrification process [65]. The (TSS) removal efficiency of the MWWTP was calculated as 91.30%, indicating effective removal of solid particles from the wastewater. The temperature differences between the influent and effluent samples remained insignificant, suggesting minimal impact on the treatment process due to temperature fluctuations.

The (BOD) and (COD) treatment performances of the Activated Sludge Process in MWWTP were found to be 95.15% and 90.85%, respectively. These high removal efficiencies indicate the effectiveness of the ASP in degrading organic pollutants in the wastewater. (NH4-N) had an efficiency of 38.24% in the treatment process, while (NO3-N) and (NO2-N) ions had effective removal rates of 55% and 75%, respectively.

Additionally, the average concentration of phosphate (PO4-P) increased by 3% in the influent flow compared to the effluent. This increase is mainly because the plant does not have a phosphorus removal process in place. Although heterotrophic bacteria in the activated sludge process (ASP) do assimilate some phosphorus [66], their contribution alone is not enough to significantly lower the phosphorus concentration.

II.2.5 Temporal Trends and Seasonal Variations

Analysing the temporal fluctuations of various parameters can offer valuable information. As depicted in Figure II.3 and Figure II.4.

The influent BOD, TSS, COD, and NH4-N measurements displayed parallel patterns. In Figure (II.3), the (DO) concentration exhibited an inverse relationship. This contrasting trend suggests that as the available dissolved oxygen increased, the level of contaminants in the incoming wastewater decreased. This phenomena is directly connected to variations in the inflow rate; as the flow rate went up, the availability of dissolved oxygen improved, leading to a drop in pollutant concentration. These findings are compatible with similar studies by [67].

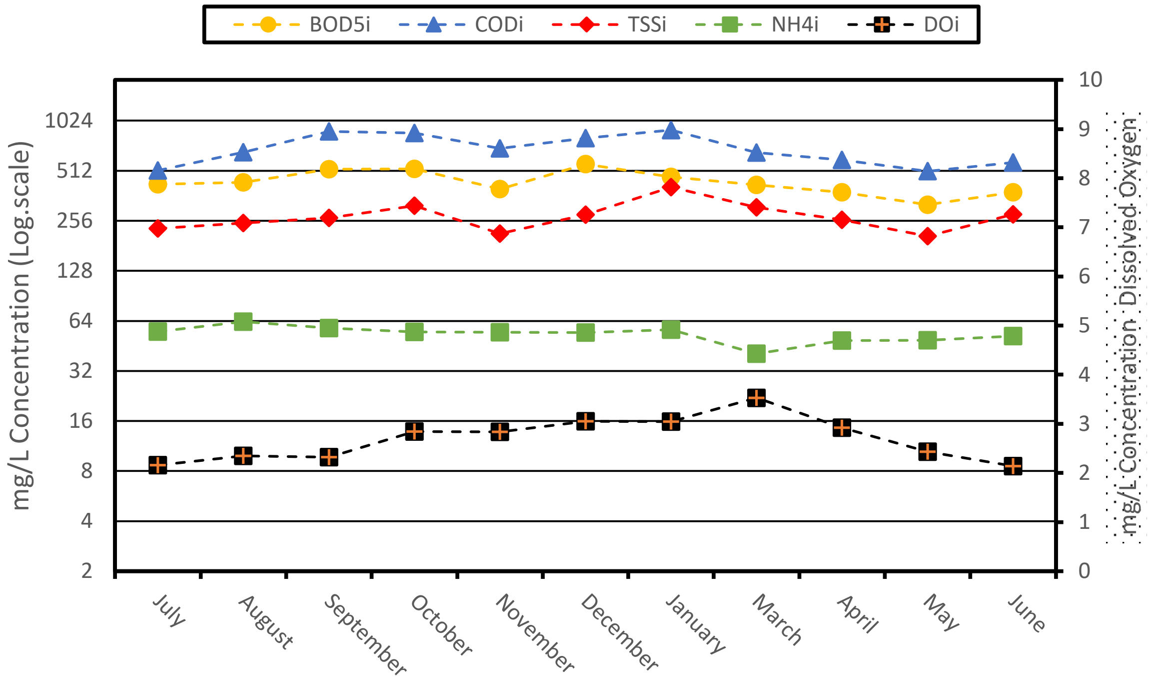


Figure II. 3 Temporal Variation of Average Monthly Influent Parameters.

Regarding effluent quality parameters, it was observed that the variation in dissolved oxygen levels throughout the treatment process influenced the concentration of other quality parameters, particularly TSS and BOD (Figure II.4).

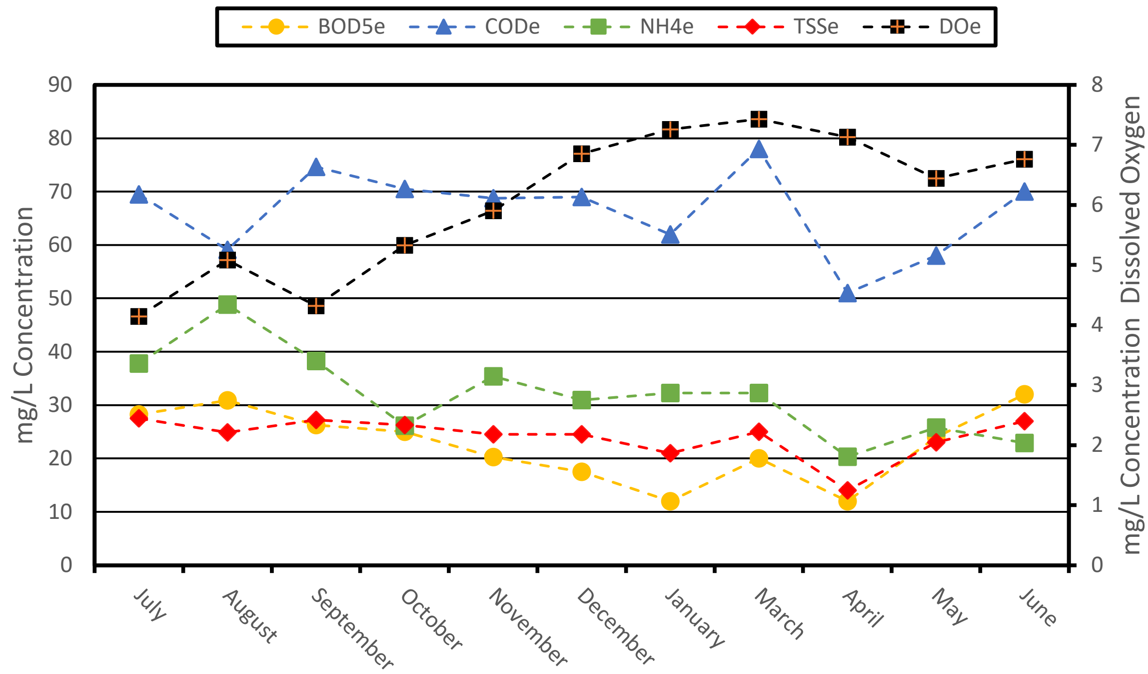


Figure II. 4 Temporal Variation of Average Monthly Effluent Parameters.

An increase in dissolved oxygen levels resulted in higher effluent TSS concentration and a decrease in BOD levels. However, while studying the fluctuations in quality parameters can provide some fundamental insights, it's important to recognize the complex interrelationships among wastewater quality variables. Consequently, relying solely on one parameter or a group of parameters may not sufficiently describe the wastewater stream. Moreover, attempting to analyse fluctuations in variables without a thorough comprehension of the treatment procedures could impede a thorough evaluation of the effectiveness of the treatment system.

II.3 Tlemcen Wastewater Treatment Plant

II.3.1 Study Area

The Wilaya of Tlemcen is situated in the westernmost part of the country. The region is bounded by the Mediterranean Sea to the north, the Wilaya of Sidi Bel Abbas to the east, the Wilaya of Nama to the south, and the Wilaya of Ain Temouchent to the northeast (Latitude: 34° 55’ 24” North, Longitude: 1° 18’ 49” West) (Figure II.5). It covers an area of 9061 km².

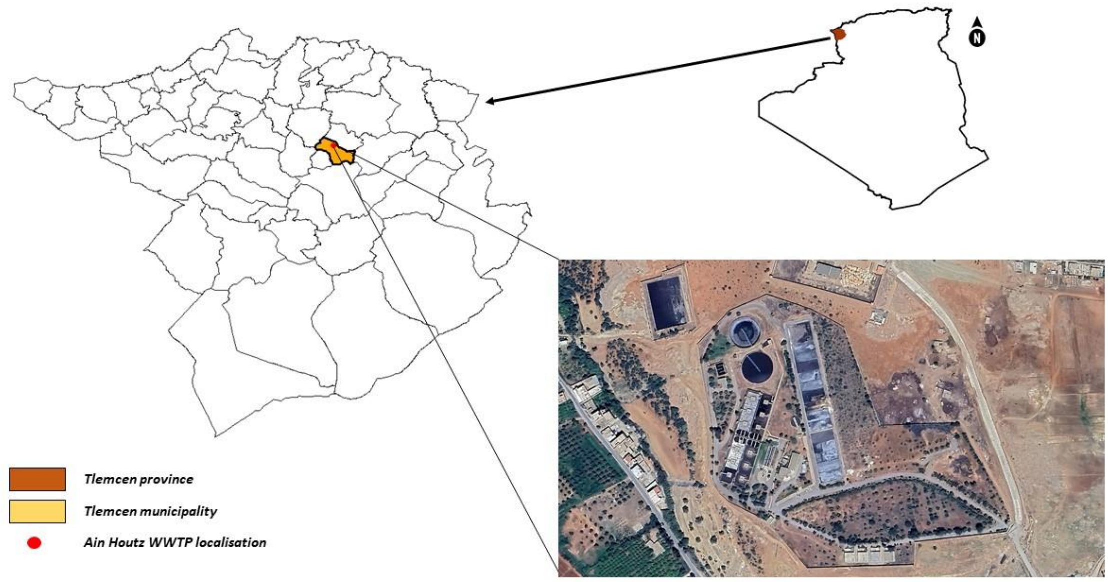


Figure II. 5 Geographic location and an aerial view of the Tlemcen Wastewater Treatment Plant TWWTP.

II.3.2 Description of Tlemcen "Ain Elhoutz" Wastewater Treatment Plant (TWWTP)

Operational since 2005, the TWWTP serves 150,000 population equivalent and processes municipal wastewater at a daily volume of 30,000 m^3, primarily using an activated sludge system Figure II.5. The treatment facility which is a low-load activated sludge treatment process, incorporates preliminary, secondary, and tertiary treatment systems, utilizing the same processes and configuration as the plant in Maghnia. Therefore, Figure II.2 is applicable to both plants, the plant begins with screenings and grit removal units for initial treatment. For the secondary treatment phase, an oxidation ditch process combined with clarification units is implemented to biologically eliminate organic and nutrient components from the wastewater. Following clarification, the treated effluent proceeds to the tertiary treatment phase, involving chlorination and disinfection. The ultimate treated effluent is then released into a stream, the operating conditions of TWWTP are detailed in Table II.3.

Table II. 3 Operating data of the Tlemcen Wastewater treatment plant.

Parameters	Unit	TWWTP
Population	inhabitants	150,000
Average daily flow rate	$m^3.d^{-1}$	30,000
peak flow	m^3/h	3,800
BOD load	$Kg.d^{-1}$	9,300
Suspended Solids	$Kg.d^{-1}$	13,950
Nitrogen	$Kg.d^{-1}$	1,980

II.3.3 Monitored Parameters and Analytical Methods

The physicochemical parameters obtained from the investigations were conducted by the laboratory of the TWWTP. A total of 152 samples were gathered from 01/01/2020 to 31/12/2012 for influent and effluent waters. These samples were obtained on a daily basis to observe any variations in their characteristics over time. Specimens were obtained from a depth of 10 cm beneath the water's surface utilizing a Silicon/Teflon water pump. A total of twelve metrics related to water quality were measured: Temperature and pH, (TSS), (DO), (BOD), (COD), (NH4-N), (NO3-N), (NO2-N), (PO4-P), turbidity and chloride. Temperature, Conductivity and pH of surface water were measured immediately after collection using HQ40D Portable Multi Parameter Meters (Hach Company, USA) [64].

II.3.4 Descriptive Data Analysis of Monitored Parameters

Descriptive statistics were employed to determine the features of each measured parameter in terms of: mean, median, (SD), (Min), (Max), (Q_1), and (Q_3). Studying the variations in the quality parameter can yield essential insights on the properties of the incoming and outgoing loads, as well as the efficiency of the system in removing pollutants, (Table II.4) presents the descriptive statistics of the analysed parameters for the water samples.

Table II. 4 Statistical results of measured parameters for influent/effluent Wastewater.

Parameter	**Unit**	**Min**	**Q1**	**Median**	**Q3**	**Max**	**Mean**	**SD**	**Removal efficiency (%)**
Influent Values									
TSS	mg/L	103	196.5	230.0	261.8	848	231.1	70.7	/
BOD	mgO2/L	72	140.0	185.0	245.0	1 150	211.8	123.3	/
COD	mgCOD/L	120	268.0	340.5	454.8	1 324	385.2	168.2	/
NH4-N	mgN/L	1.69	31.9	40.1	47.6	102	40.8	12.5	/
NO3-N	mgN/L	0.09	0.36	0.81	1.2	3.6	0.9	0.66	/
NO2-N	mgN/L	0.29	1.80	2.80	10.1	16.8	5.5	4.80	/
PO4-P	mg/L	2.06	6.10	7.40	9.0	27.5	8.2	4.26	/
Temp	°C	2.00	18.25	19.00	21.0	27.0	19.6	2.78	/
pH	-	7.32	7.79	7.82	7.87	8.01	7.82	0.08	/
Effluent Values									
TSS	mg/L	11.00	17.00	20.00	23.00	42.00	20.71	5.21	91.20
BOD	mgO2/L	3.00	12.00	16.00	19.00	35.00	16.25	5.88	92.23
COD	mgCOD/L	16.00	28.00	36.00	47.00	79.00	39.00	13.60	90.01
NH4-N	mgN/L	0.32	9.35	13.70	23.51	42.24	16.75	9.53	59.93
NO3-N	mgN/L	0.02	0.16	0.57	0.80	2.10	0.53	0.38	/
NO2-N	mgN/L	0.02	1.20	1.80	6.40	13.20	3.88	3.90	/
PO4-P	mg/L	0.40	3.30	4.80	6.28	27.50	5.62	4.27	/
Temp	°C	9.00	14.38	17.75	21.40	26.50	18.08	4.40	/
pH	-	7.24	7.48	7.51	7.61	8.19	7.54	0.14	/

(TSS) levels in both influent and effluent were notably high, with an impressive removal efficiency of 91.2%, meeting the limit value set by the Algerian government for treated wastewater for irrigation (30 mg/l). Chemical Oxygen Demand (COD) levels, similarly elevated in both influent and effluent, were efficiently reduced by 90%, below the limit of the standard value (90 mg/l).

Biochemical Oxygen Demand (BOD) indicated a substantial presence of organic matter, with an efficient removal rate of 92.2%, although occasional peaks exceeded irrigation standards (35 mg/l). Ammonium Nitrogen (NH_4-N) levels were moderate with effluent values ranging from 0-39 mg/l which is below the FAO's limited value set for irrigation water (5 mg/l), and a removal efficiency of 60%. Nitrate (NO_3-N) concentrations were low ranging between 0 and 13 mg/l, falling within irrigation standards (30 mg/l), while Nitrite-Nitrogen (NO_2-N) levels indicated effective nitrification and denitrification (0 to 2 mg/l), also within regulatory limits (5 mg/l). The average concentration of phosphate (PO_4-P) exhibited a 0.1% increase in the influent flow compared to the effluent, a noteworthy similarity. This resemblance is particularly striking considering the elevated values observed, reaching up to 28 mg/L, mirroring findings from the Maghnia WWTP.

These findings underscore the effectiveness of the treatment processes in removing organic and inorganic pollutants, ensuring compliance with regulatory standards. However, variations in pollutant concentrations and occasional exceedances highlight the need for ongoing monitoring and potential adjustments to optimize treatment efficiency and maintain water quality standards.

II.3.5 Temporal Trends and Seasonal Variations

An examination of the temporal fluctuations in influent parameters such as BOD, TSS, COD, NH_4-N, and temperature at Tlemcen WWTP reveals a consistent pattern (Figure II.6 and Figure II.7).

These parameters exhibit a synchronized trend over consecutive months (Figure II.6), typically rising at the onset of the agricultural year (September) and declining as spring begins (March). Temperature fluctuations follow a predictable cycle, maintaining relative stability for several months around 22°C in June and July during summer, and around 18°C in November, December, and January in winter.

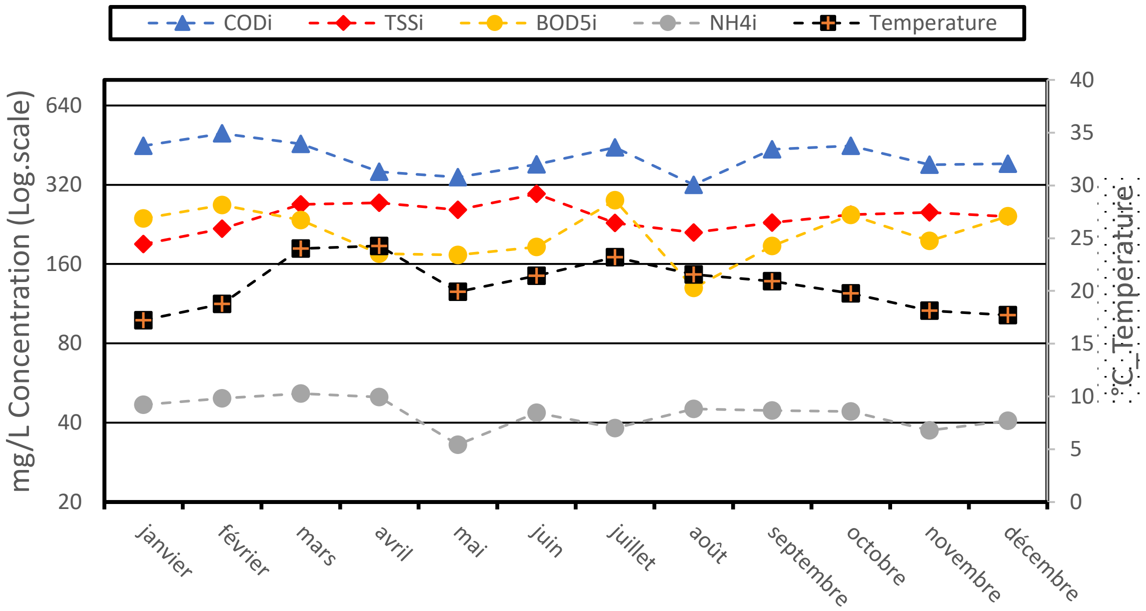


Figure II. 6 Temporal Variation of Average Monthly Influent Parameters.

In contrast, the effluent quality parameters exhibit some irregularities (Figure II.7), particularly notable in COD and NH4-N concentrations, which show pronounced peaks in March (COD=56 mg/L, NH4-N=28.4 mg/L) and May (COD=51 mg/L). However, the fluctuation patterns in other months remain relatively consistent for both BOD and TSS. Notably, the temperature trends in effluent data mirror those observed in influent data, although with a slight decrease apparent in each month's influent-to-effluent transition.

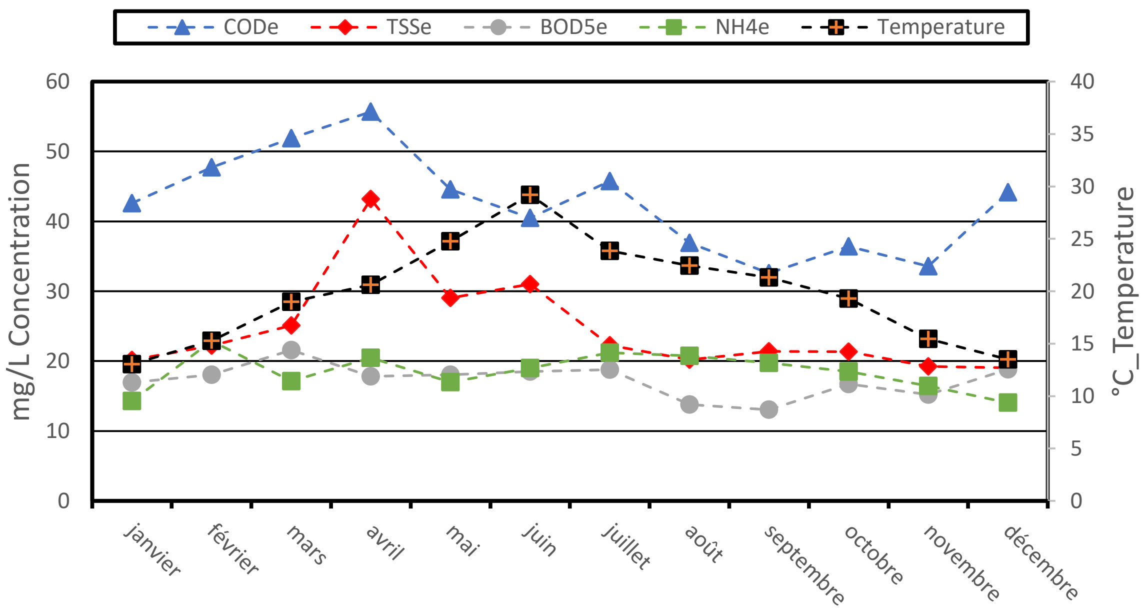


Figure II. 7 Temporal Variation of Average Monthly Effluent Parameters.

II.4 Conclusion

By delving into the fluctuations of these parameters, we gain a deeper understanding of how the treatment processes respond to changing environmental conditions and influent characteristics, ultimately resulting in a wide range of water qualities. It is evident that the available treatments can effectively reduce pollutant concentrations in all their forms to levels that are currently considered non-hazardous. This knowledge serves as a foundation for future chapters, where we will employ modelling techniques to further explore and optimize WWTP performance.

CHAPTER III
ASM1 APPLICATION ON THE MAGHNIA WASTEWATER TREATMENT PLANT

III.1 Introduction

The activated sludge process stands as one of the most prevalent methods employed in medium to large-scale wastewater treatment plants, as noted by [62]. This treatment process comprises two pivotal components: the biological reactor, responsible for decomposing pollutants through biological mechanisms, and the clarifier, designed to separate water from biomass and other particulate matter primarily via physical processes, as described by [68]. Nonetheless, the activated sludge processes often encounter complexity due to their physical characteristics and the variability of pollutant loads in raw wastewater, a point highlighted by [69]. This underscores the critical need for utilizing modelling tools, not only to delineate the diverse phases and processes involved in bacterial culture development but also to facilitate predictive analyses under a spectrum of management scenarios.

This section presents the representation of the tanks configuration and the operating system of the Maghnia wastewater treatment plant in the GPS-X software. The theoretical background of the ASM1 model has been detailed in **CHAPTER I**. Following the model calibration, simulations are conducted to validate and forecast the model's behaviour. The obtained results are then discussed and evaluated.

III.2 Building the Layout

III.2.1 Construction of the WWTP Layout:

GPS-X generates dynamic process models by utilizing graphical representations of unit processes. Consequently, the initial stage involved constructing Maghnia's WWTP in a graphical format. In order to accomplish this, the user selected items, represented by process unit icons, from the process table in GPS-X's unit process library. These objects were then joined together using flow routes to produce the process flow diagram for the WWTP, as depicted below (Figure III.1):

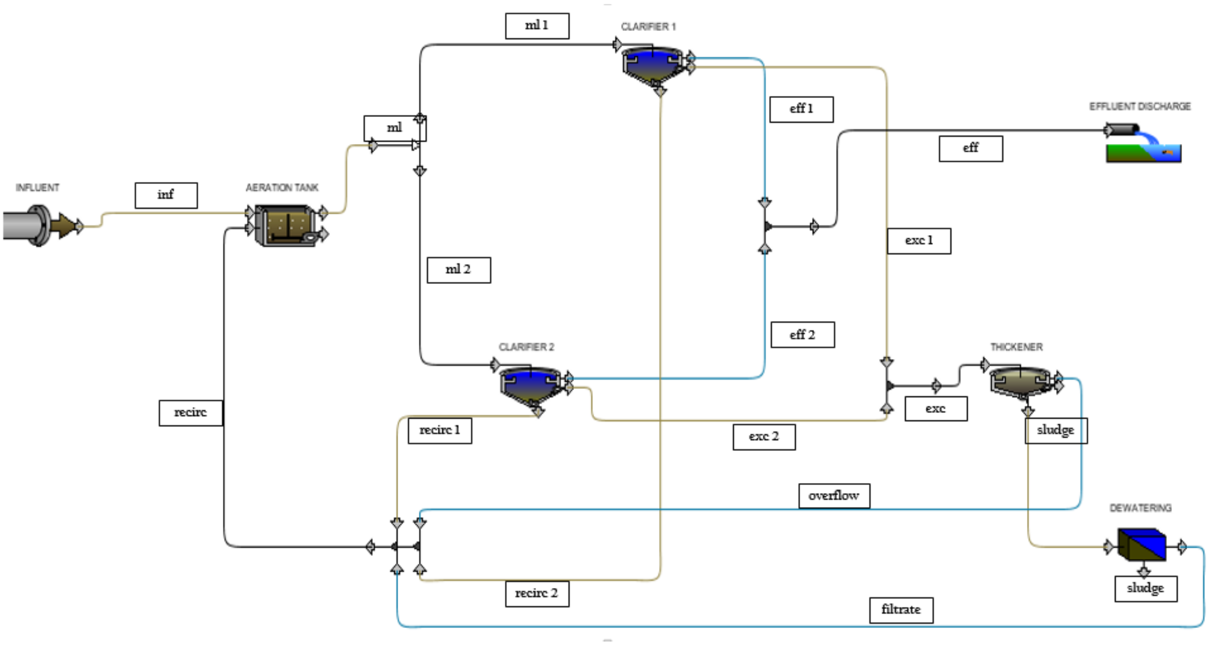


Figure III. 1 Layout of Maghnia's WWTP in GPS-X.

In terms of streams, "inf" refers to the influent (mixed influent). The stream "ml/ml1/ml2" corresponds to the biologically treated effluent exiting the aeration tank. Following the clarification step, the effluent streams ("eff1/eff2") are combined for discharge ("eff"), while the excess sludge streams ("exc/exc1/exc2") are pumped to the thickener. Additionally, recirculation streams from the clarifiers ("recirc1/recirc2") are mixed with the thickener overflow and the filtrate from the filter press to form the recirculation stream ("recirc"), which is then pumped back to the aeration tank. Lastly, the "sludge" stream refers to the concentrated sludge following thickening and dewatering.

III.2.2 Selection of the Library

Prior to conducting the physical assessment of each unit process, it was imperative to choose the library that most appropriately matched the wastewater treatment plant (WWTP). A library is a compilation of various components used in wastewater treatment, each having specific state variables. GPS-X offers six ones, each with default values and expressions for calculating state variables. Given the interest in the ASM1 model, the legacy "Carbon, Nitrogen (cnlib)" library was chosen for this study. This selection enables the later implementation of the IWA Activated Sludge Model No. 1 for the aeration tank.

III.2.3 Selection of the Model for each Process Unit:

For each process unit defined, a collection of models exists to explain the object's behaviour, the choice of model is mostly determined by the available information needed to calculate the state and combination variables based on user inputs.

III.2.3.1 Influent

The characterization of influent wastewater serves as the foundation of the simulated system, given that the influent's properties significantly impact the behaviour of the entire wastewater treatment plant (WWTP). GPS-X provides six different models for influent characterization: "bodbased", "codfractions", codstates, "sludge", "states", and "tsscod". As the ASM1 model relies on COD fractions, the **codstates** model was selected for influent characterization. In this model, the majority of the state variables, which were not provided by the user, were computed as a proportion of the total COD. Although the software provides default values for these COD percentages, users can choose to modify them in order to improve the calibration of the WWTP plant model.

The mathematical representation of the incoming wastewater introduced into the model of the plant is the most crucial aspect of any simulated system. Without thorough analysis of influential characteristics, the plant model will be limited in its ability to predict the dynamic behaviour of the plant [46].

For better understanding of the influent characterization, Hydromantis developed a specialized utility program known as the “Influent Advisor” Figure III.2. This tool assists users in visualizing and balancing influent characterization data. As mentioned in **CHAPTER I**, a mass balance defines the variation in the quantity of a compound by accounting for what is introduced or produced. The “Influent Advisor” automates this process, mitigating errors and ensuring accuracy in influent characterization.

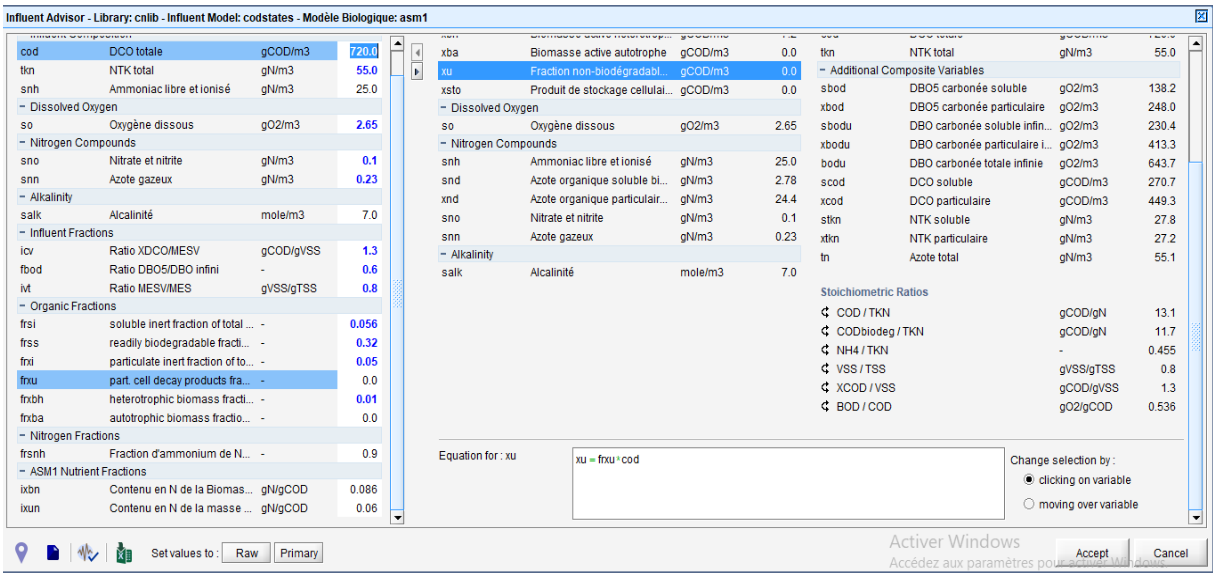


Figure III. 2 Influent Advisor menu.

III.2.3.2 Aeration Tank

As mentioned in **CHAPTER I**, ASM1 was chosen as the model to explain the biological treatment in the aeration tank.

III.2.3.3 Clarifier

As it was referred in **CHAPTER I**, the model chosen to describe the settling dynamics in the two clarifiers was the one-dimensional, nonreactive model known as "simple1d", proposed by Tackaçs [36].

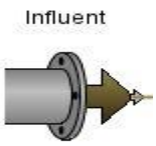
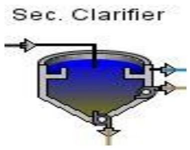
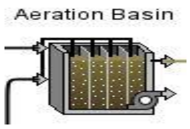
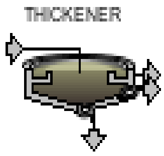
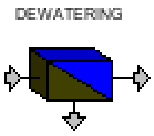
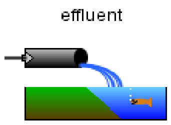
III.2.3.4 Thickener and Dewatering

Because there is a lack of particular data regarding factors such as solids capture efficiency, minimum sludge concentration required for processing, and the organic and nutrient composition of the sludge, an empirical model was chosen to simulate these unit processes. When specified data was not available, default values of certain parameters were used. The model utilizes a mass and flow balance to determine the flow rate and concentrations of the sludge.

III.2.4 Physical and Operational Data:

For the calibration of the physical and operational data of Maghnia WWTP, data of each process unit collected from the Office National de l'Assainissement (ONA) was used as shown in the Table below [3]:

Table III. 1 Physical and operational data.

Process Unit	**Physical Parameter**	**Value**	**Process Unit**	**Physical Parameter**	**Value**
	Influent flow	29400 m^3/d		Clarifier Type	Flat Bottom
	Influent type	Sinusoidal		Surface	1661 m^2
	Model	codstates		Water depth	4 m
	Nbr. of tanks	4		Model	Empiric (Default)
	Tanks Depth	5.6 m		Surface	154 m^2
	Max. Volume	4723 m^3		Water depth	4 m
	Model	Empiric (Default)		Model	Default
	Surface	450 m^2		Effluent limits	Default
	Nbr. of beds	14			

III.3 Model Calibration

A steady state calibration is highly important for determining initial circumstances prior to a dynamic model calibration and initiating the first parameter iteration [70–72,14].

Firstly, we must check the adequacy between the results from the simulations and the measurements carried out on the current station. For this we will run the plant in steady state conditions, by comparing the simulated results with the data collected on the station, we carry out a relative calibration. A validation is then carried out on a set of measured values.

III.3.1 Operational Assumptions

III.3.1.1 Aeration

The simulation was carried out with these hypotheses by adjusting the aeration parameters, on the one hand, the proportionality factor between the transfer of oxygen in the sludge and in the clear water (coefficient α) was taken to 0.8 (default value) [73], the concentration of dissolved oxygen in the reactor was set at a value of (2 mg/l). These two adjustments make it possible to obtain an oxygen requirement per day, necessary for the elimination of carbon and nitrogen pollution, close to the calculation according to the station sizing method [73].

III.3.1.2 Sludge Recirculation

It is proportional to the inlet flow rate, remaining in a range of 40% to 100%. For the steady-state simulation, we choose a maximum recirculation of 100%, which makes it possible to maintain concentrations in the aeration tank.

III.3.1.3 Sludge Extraction

The extraction flow rate is determined to evaluate the sludge production at the station, The method for calculating sludge production as outlined by [74], facilitates the estimation of sludge extraction relative to its production.

Sludge production: 1.02 * (TSS Flow + BOD5 Flow) / 2)

This gives an approximate sludge production of 13899.54 $kg.d^{-1}$.

III.3.2 Methodology

The dynamic modelling of the activated sludge process has become an indispensable tool for the design and management of wastewater treatment plants [31,58]. However, the calibration of these models appears to be a critical issue in their widespread application [75]. The selection of all relevant parameters to achieve accurate predictions using the model is one of the major challenges of activated sludge models (ASMs) during application and calibration [76].

The calibration of the ASM1 model is typically conducted through a step-by-step process, where just a couple of parameters are adjusted manually rather than employing an algorithmic standardisation procedure [34]. This method frequently offers a rather precise depiction, especially for typical municipal wastewater treatment cases

The model relies on COD fractions and various stoichiometric coefficients (such as volatile suspended solids (VSS)/ total suspended solids (TSS) ratio, soluble fraction of total COD, heterotrophic yield coefficient Y_H and autotrophic yield coefficient Y_A). Determining these coefficients is necessary to improve wastewater characterization. To achieve this, the study employed the average observed concentration values of COD, TSS, and NH4-N parameters.

The total COD concentration within the influent of the treatment plant was comprehensively fractionated into separate components: readily biodegradable substrate (S_S), slowly biodegradable substrate (X_S), soluble inert matter (S_I), and particulate inert matter (X_I). (S_I) is commonly estimated using the soluble COD in the effluent or as 90% of the effluent COD, a method supported by research like [77]. The process data from the treatment facility only provides measurements of total COD. Therefore, the influent COD fraction was estimated as 90% of the effluent COD. To characterize the COD influent fraction, the CEMAGRAF protocol was used, following the established practice of using CEMAGREF's default parameters for (S_S) and (X_I) in the adjustment fractionations [22,51,78].

The mean value of the (S_I) fraction was determined to be 0.056, which differs from CEMAGREF's default value of 0.13. For the S_S fraction, a value of 0.32 was chosen based on CEMAGREF's settings. The value for (X_I) was obtained from CEMAGREF settings and has a mean value of 0.05 [48-50]. The remaining 57.4% of COD is classified as biodegradable substrate (X_S). The fraction values are reported in Table III.2:

Table III. 2 Parameters related to the organic matter fractionations COD.

Parameter Fraction	**Symbol**	**Ratio**	**Value g COD/m^3**	**Reference**
Soluble biodegradable substrate	S_S	0.32	230.10	[78,79]
Soluble inert substrate	S_I	0.056	40.26	[77]
Particulate biodegradable substrate	X_S	0.574	412.72	Own Study [X_S=TCOD-(S_S+S_I+X_I)]
Particulate inert substrate	X_I	0.05	35.95	[78,79]

The methodology suggested by [34] was employed for the calibration of the steady-state. The inflow was defined by introducing a constant supply of influent and composition with averaged concentrations of COD, TSS, NO2-N, NO3-N, NH4-N, PH and temperature for 28 samples provided by the plant laboratory over the period July 14, 2021, and January 10, 2023 (Table III.3). The model was fine-tuned to conform to the average effluent concentration data for the specified period and mass balancing was performed regarding COD. As a consequence, the concentrations of all organic components, including biomass, were reported as COD units [4].

Table III. 3 Input values for Steady state simulation.

Parameter	Symbol	Averaged Concentration
Flow rate	Q (m^3/j)	30900
chemical oxygen demand	COD (mg/l)	748
total suspended solids	TSS (mg/l)	276
Nitrites	NO2-N (mg/l)	0.39
Nitrates	NO3-N (mg/l)	0.54
ammonium	NH4-N (mg/l)	55
potential hydrogen	pH	7.60
Temperature	T (°C)	24

At the outset, the default values of stoichiometric, kinetic, and other parameters relating to biochemical and clarifying thickening processes were employed, as indicated by Alex et al. [35] - **Table I.3, CHAPTER I -**. The evaluation of these parameters can be conducted either through experimentation under specific conditions [17] or by computationally calibrating the model using experimental data gathered. The latter approach involves the determination of certain parameters through the comparison of simulated concentrations with measured ones.

Since COD establishes a connection between electron equivalents in the organic substrate, the biomass, and the utilized oxygen [81], the focus was directed towards dynamic variables that influence the output COD value, such as biomass concentration (X_{BH}) and maximum specific growth rate ($\mu_{-max\ H}$).

The key aim of calibrating the model is to produce a more accurate calculation of the saturation constant (K_S), decay coefficient of heterotrophic biomass (b_H), and ($\mu_{-max\ H}$) and one stoichiometric coefficient: heterotrophic yield coefficient (Y_H), which are the most important parameters in predicting dynamic situations [71,72,83].

The Steady-state simulation technique consists of three phases to approximate the simulation line to the experimental data:

• The first step is to improve the clarity of the mathematical reaction to COD output and dynamic factors by employing a range of values for ($\mu_{-max\ H}$) [84], while maintaining the default values of other parameters.

• After determining ($\mu_{-max\ H}$), it's necessary to change factors linked to (X_{BH}), such as (Y_H) and (b_H), for accurate calibration [82].

• Identified discrepancies between anticipated and observed values and adjusted parameter values to achieve accurate match. The goal here is to develop a correlation between the model's prediction and the experimental data.

A simulation program can perform model calibration visually or numerically. However, due to the complexity of the ASM1 model and the absence of precise data necessary for automated calibration, a direct mathematical simulation for actual parameter identification difficulties was not possible [75,85]. Consequently, the decision was made to visually adjust the parameters according to the experimental measurements.

Visual evaluation of the agreement between observed and simulated values was strengthened using a statistical approach. This study used the mean absolute error (MAE) (Equation III.1) to assess and corroborate the model's trustworthiness in reflecting reality.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|r_i| \qquad \text{(III.1)}$$

With:

r_i: Residual = O_i - P_i

O_i: Observed values

P_i: Predicted values

III.3.3 Calibration Results

The calibration of COD primarily involved adjusting the kinetic and stoichiometric parameters of the ASM1. Specifically, two stoichiometric coefficients - Y_H and Y_A - and kinetic parameters - ($\mu_{-max\ H}$), (b_H), and the (K_S) - were modified. Table III.4 presents the calibrated parameters alongside the default ASM1 values. Other parameters were assumed to have minimal impact on the model's outcomes, so their default ASM1 values were retained. The calibrated yield for heterotrophic biomass (Y_H = 0.66 g COD/g COD) was consistent with both the default value and those reported in the literature. Similarly, the autotrophic biomass yield remained at the default value (Y_A = 0.24) as noted in the literature. However, the calibrated rate ($\mu_{-max\ H}$ = 3.2 d^{-1}) and the coefficient (b_H = 0.66 d^{-1}) showed significant deviations from the default values. The half-saturation constant value, however, was unchanged from the default. The calibration of TSS largely depended on the accuracy of wastewater characterization, as the model calculates suspended solids based on the ratio of soluble (S) and particulate (X) to the total COD, emphasizing the importance of accurate total COD fractionation.

Table III. 4 Calibrated and typical values for kinetic and stoichiometric parameters (pH=7).

Parameter	Symbol	Unit	Range	Default Value	Calibrated Value	Reference
Stoichiometric Parameters						
Yield for heterotrophic biomass	Y_H	g COD/g COD	[0.57 - 0.67]	0.67	0.66	[86]
Yield for Autotrophic biomass	Y_A	g COD/g COD	[0.15 - 0.24]	0.24	0.24	[73]
volatile suspended solids/ total suspended solids	VSS /TSS	g VSS/ g TSS	-	0.70	0.80	[86]
particulate COD to total COD	XCOD/VSS	g COD/ g VSS	-	1.48	1.3	[18]
Kinetic Parameters						
Maximum specific growth rate for heterotrophic biomass	$\mu_{-max\ H}$	d^{-1}	[0.6 - 13.2]	6	3.2	[86]
Heterotrophic decay coefficient	b_H	d^{-1}	[0.3 - 1.2]	0.62	0.66	[30]
Half saturation constant	K_S	mg COD/L	[10 - 40]	20	20	[30]

The main goal of steady-state model calibration is to match the values that were modelled for each variable with the corresponding mean values acquired. This approach has been widely used in numerous research projects to assess the efficiency of activated sludge systems in major municipal treatment plants [34,52,87,88].

Figure III.3 demonstrates the ASM1 model's accurate depiction of MWWTP performance. The simulated effluent COD values closely matched the actual measured COD, with a low mean absolute error (MAE) of 3.70% (Table III.5). Since COD is a key parameter in ASM models, significant calibration efforts were focused on adjusting COD parameters. For TSS, the influent average was calibrated using two stoichiometric coefficients: the VSS/TSS ratio was set at 0.80 (g VSS/g TSS), consistent with [89], and XCOD/VSS was adjusted to 1.3 (g COD/g VSS), differing from the default value of 1.48. The model accurately reflected the observed TSS data in (Figure III.4), Nitrifying microorganisms, crucial for the nitrification process, are highly sensitive to environmental factors such as oxygen levels, temperature, pH, increased BOD, and the presence of harmful substances; thus, NH4-N calibration was omitted. All kinetic and stoichiometric parameters related to the nitrification process (Mass N/mass COD in biomass (i_{XB}), Nitrate for denitrifying heterotrophs (K_{NO}), Ammonification rate (K_a) and correction factor for anoxic hydrolysis (η_h)) were set to the default values, this approach aligns with the perspective presented by [90]. The ASM1 model showed less alignment with measured data for NH4-N (Figure III.5), resulting in a mean absolute error of 37% (Table III.5).

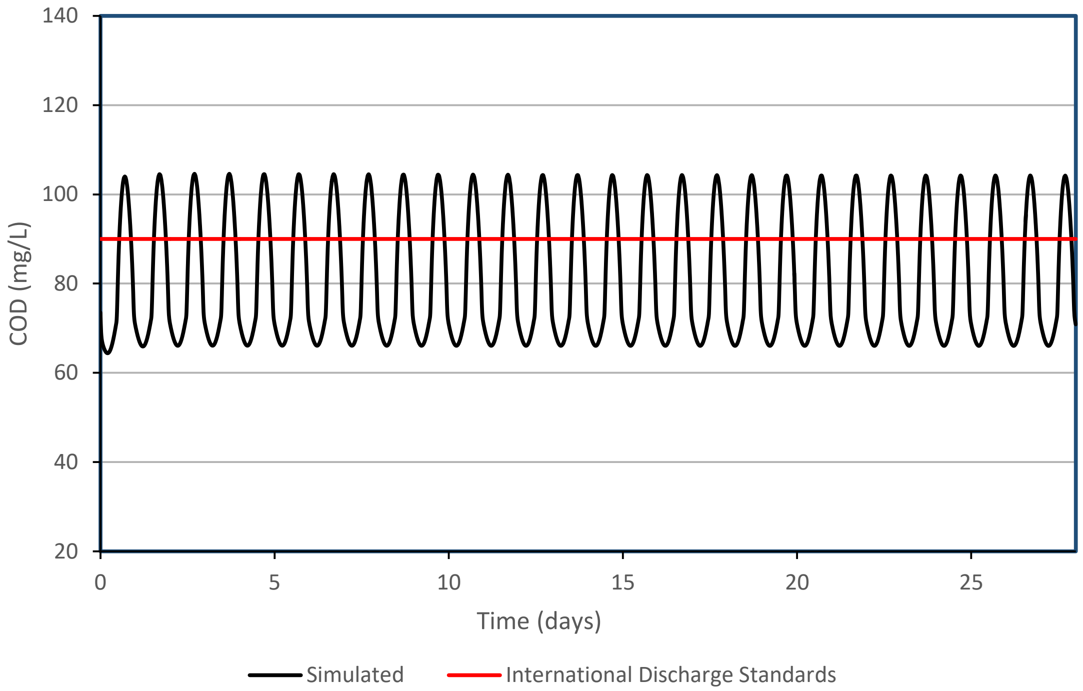


Figure III. 3 Steady State Calibration results for the effluent COD.

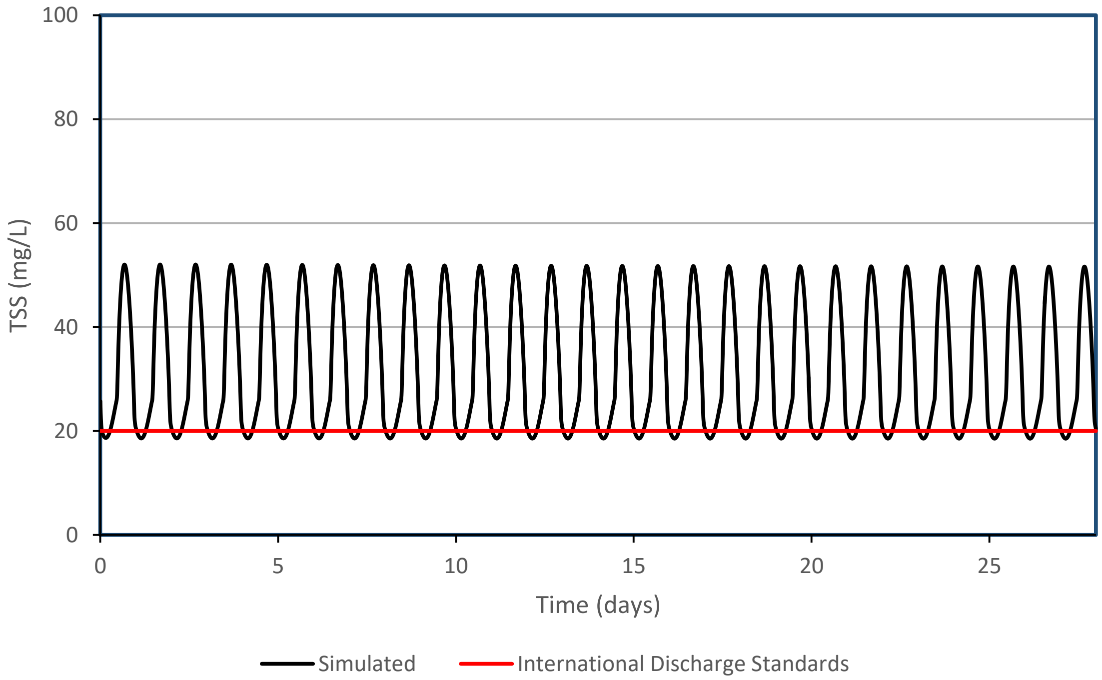


Figure III. 4 Steady State Calibration results for the effluent TSS.

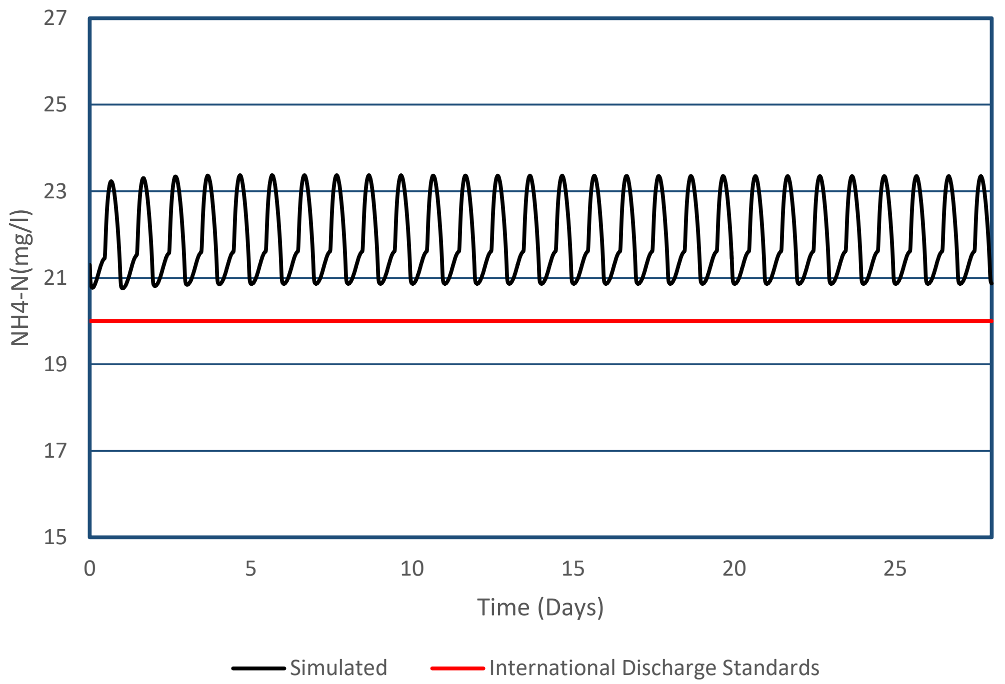


Figure III. 5 Steady State Calibration results for the effluent NH4-N.

Table III. 5 MAE values of different output variables tested for a steady state simulation (COD, TSS and NH4-N).

Parameter	Unit	Measurement	Simulation	MAE
COD	mg/L	67.71	70.25	0.037
TSS	mg/L	24.39	20.23	0.17
NH4-N	mg/L	33.54	21.03	0.37

III.4 Model Validation

The model was validated by simulating long-term influent process data over a 4-month period from July 14, 2021, to November 30, 2021. The simulated results were then compared to the actual effluent process data. The average relative error for the entire year was calculated, with MAE values of 23%, 67%, and 56% for COD, TSS, and NH4-N, respectively (Table III.6).

Table III. 6 MAE values of different output variables tested for a dynamic simulation (COD, TSS and NH4-N).

Parameter	Unit	Measurement	Simulation	MAE
COD	mg/L	66.75	70.44	0.23
TSS	mg/L	8.15	25.06	0.67
NH4-N	mg/L	14.54	32.27	0.56

Figure III.6 illustrates the correlation between the simulated and measured COD concentrations in the plant effluent. The comparison demonstrates a significant agreement for the majority of the simulation period. This agreement can be attributed to the detailed characterization of influent wastewater (S_S, X_S, S_I, and X_I) and the adjustment of the ($\mu_{\text{-max H}}$) value based on insights from [34].

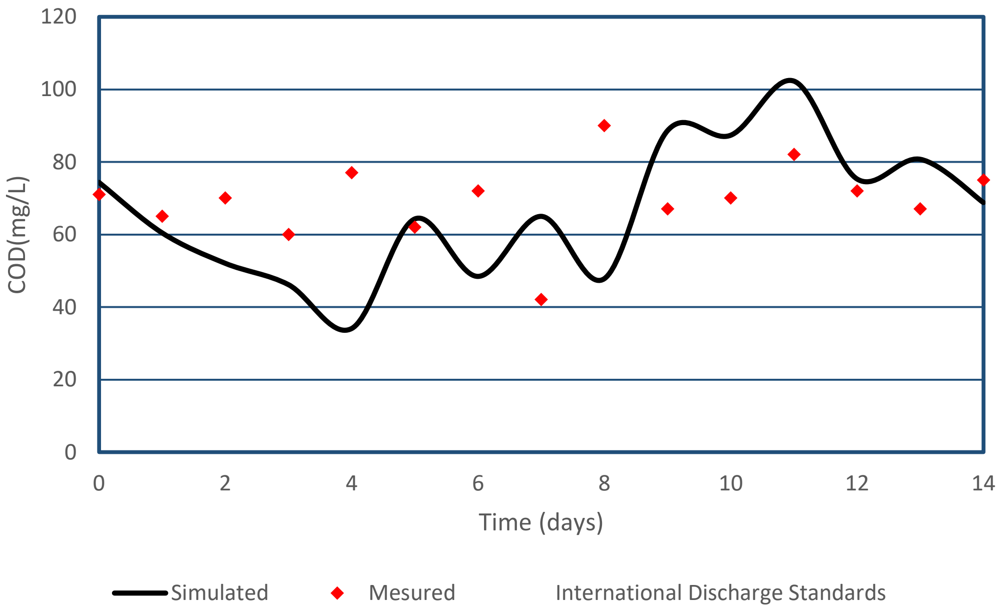


Figure III. 6 Dynamic Simulation results for the effluent COD.

The data shows a lower precision in representing the behaviour of TSS and NH4-N in the effluent (Figures III.7 and III.8). The discrepancies might be due to uncertainties related to the observed TSS flows. It's worth noting that a large portion (86%) of the measured TSS effluent exceeds the 20 mg/L threshold, which is the limit discharge standard according to the World Health Organization (WHO) for wastewater [91]. Additionally, the NH4-N effluent doesn't meet the international discharge standard (<20 mg/L), with 93.33% of NH4-N effluent concentrations exceeding the specified limit. These results align with comparable findings from research conducted on treatment plants in north-eastern Algeria [89] and the United Arab Emirates [58]. For both scenarios, the dynamic simulation results exhibited a notable lack of concurrence with the measured TSS and NH4-N values. Moreover, (Figure III.8) indicates that certain parameters may not be appropriate for autotrophic nitrifiers, such as ammonium-oxidizing bacteria and nitrite-oxidizing bacteria, emphasizing the difficulties in effectively depicting the behaviour of these variables in the dynamic simulation.

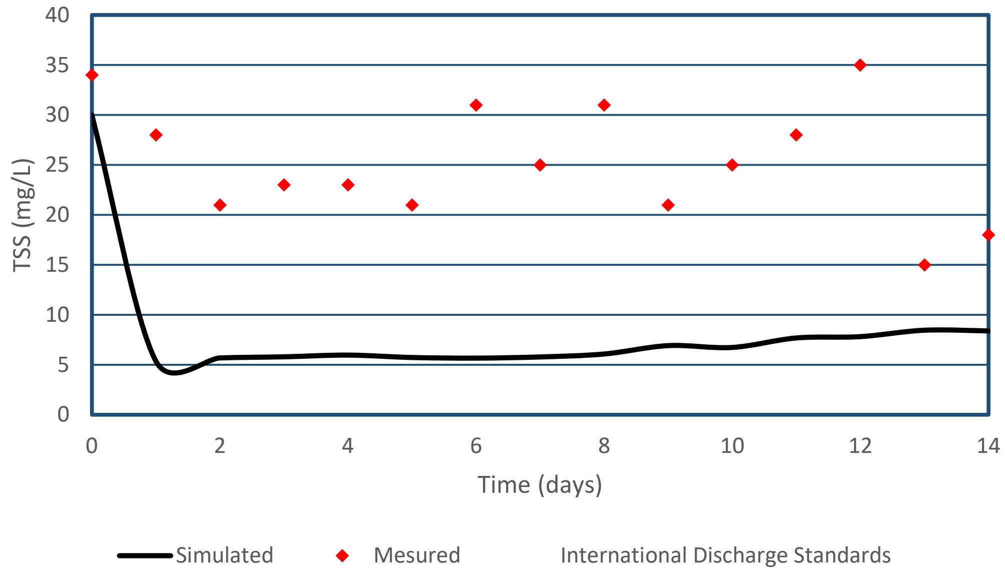


Figure III. 7 Dynamic Simulation results for the effluent TSS.

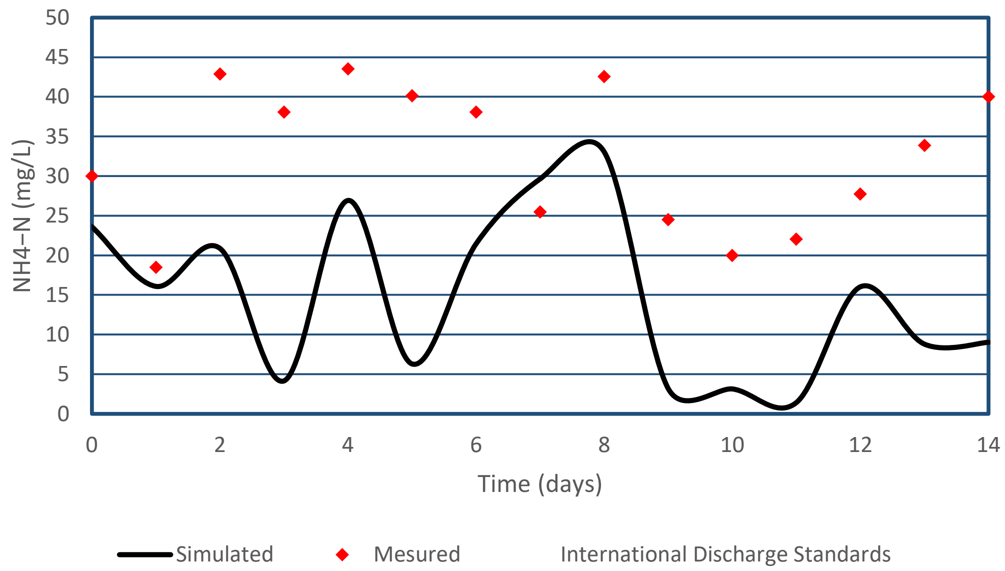


Figure III. 8 Dynamic Simulation results for the effluent NH4-N.

III.5 Conclusion

While the study yielded promising outcomes in predicting COD removal performance (MAE=23%), it also encountered challenges primarily associated with uncertainties in measuring (TSS) and (NH4-N) levels (67, and 56% respectively). These uncertainties underscore the necessity for additional efforts to enhance model validation, particularly focusing on the calibration of parameters related to nitrification/denitrification by anoxic digestion and also settling hypothesis for clarifiers. Addressing these challenges through improved validation processes will not only bolster the reliability and accuracy of the ASM1 model but also strengthen its applicability for wastewater treatment plant management and optimization efforts. Furthermore, these findings highlight the model's ability to test hypotheses and predict outcomes.

CHAPTER IV
SENSITIVITY ANALYSIS APPROACH FOR CALIBRATION OF TLEMCEN WWTP MODEL

IV.1 Introduction

The ASM1 is frequently too sophisticated for making forecasts in real-world wastewater treatment plants. Characterizing wastewater for mathematical modelling using the ASM1 can be a challenging and time-consuming task. In addition, employing an excessive number of parameters for the model may lead to inadequate identification of the parameters [92]. Thus, a sensitivity analysis, which enables you to choose relevant parameters, is a very useful tool in this process. Sensitivity analysis can be categorized into distinct methods: (1) can be swiftly used to find for the most relevant inputs, (2) are based on differential analyses, (3) are based on the sampling process, and (4) are based on variance methods [93].

In this study, within the context of (ASMs), a sensitivity analysis module provided by [46] is employed to identify which parameters require adjustment during model calibration. These analysis are conducted to assess whether the modifications made to these parameters significantly influence the model outputs regarding COD effluent quality.

IV.2 Building the Layout

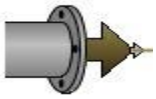
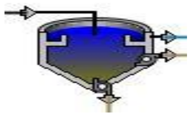
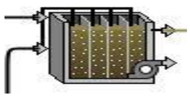
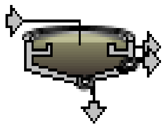
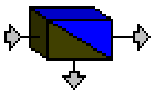
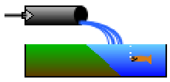
To simulate the wastewater treatment plant of Ain Elhoutz effectively, the modelling process must follow the steps outlined and demonstrated in **CHAPTER III**, ranging from "Building the layout" to "Construction of the WWTP layout" and "Physical and operational data." Both plants share similarities in process type (Low load activated sludge), influent discharge (municipal wastewater), number of tanks for each process, and certain physical parameters. Additionally, they are located in the same region within the Wilaya of Tlemcen.

Given these similarities, particular emphasis will be placed on the part of the modelling process, which is crucial for the biological process, particularly organic removal of COD. This section requires careful configuration, as it serves as a key element in achieving efficient description of the plant.

IV.2.1 Physical and Operational Data

The data for each process unit were collected from the Office National de l'Assainissement (ONA) presented in the following Table [3]:

Table IV. 1 Physical and operational data.

Process Unit	Physical Parameter	Value	Process Unit	Physical Parameter	Value
Influent 	Influent flow	30000 m^3/d	Sec. Clarifier 	Clarifier Type	Flat Bottom
	Influent type	Sinusoidal		Surface	1661 m^2
	Model	codstates		Water depth	4 m
Aeration Basin 	Nbr. of tanks	4	THICKENER 	Model	Empiric (Default)
	Tanks Depth	5.6 m		Surface	154 m^2
	Max. Volume	4723 m^3		Water depth	4 m
DEWATERING 	Model	Empiric (Default)	effluent 	Model	Default
	Surface	450 m^2		Effluent limits	Default
	Nbr. of beds	14			

IV.3 Model Calibration (Sensitivity Analysis)

In the previous chapter, our focus was on describing the ASM1 model's application to the Maghnia WWTP, particularly in matching the behaviour of three key output state variables: COD, TSS, and NH4-N, essential for wastewater treatment plant modelling. We utilized a step-wise simulation procedure to address uncertainties stemming from model inputs and their impact on outputs. However, a challenge arises with manual calibration procedures, particularly during the early stage where it is necessary to determine and describe the uncertainty of model inputs by assigning suitable ranges and manually adjusting them. This step often relies on expert judgment to calibrate parameters and specify the level of certainty regarding observed data values [94,95].

IV.3.1 Operational Assumptions

The following assumptions were derived from the results of Maghnia's WWTP modelling in Chapter III, considering the similarity in processes and the quality of raw water entering.

IV.3.1.1 Aeration Parameters:

The proportionality factor (coefficient α) between the transfer of oxygen in the sludge and in the clear water was set to 0.8, following the default value as suggested by [96]. The concentration of dissolved oxygen in the reactor was fixed at 2 mg/l [97].

IV.3.1.2 Sludge Recirculation:

A maximum recirculation of 100% was selected to maintain concentrations in the aeration tank.

IV.3.1.3 Sludge Extraction:

The software provides control over sludge extraction based on the hydraulic balance of the system, considering the model chosen for the secondary clarifier, the amount of Return Activated Sludge (RAS) (100% recirculation) and the influent flow rate from the aeration tank were factored into the sludge extraction process.

IV.3.2 Methodology

IV.3.2.1 Model Calibration

This study delves into the dynamics of Chemical Oxygen Demand (COD) effluent quality, viewing it as a pivotal measure of plant performance [81]. Our focus aligns with previous research emphasizing COD's significance [98].

The application of ASM1 model in this study was guided by a sensitivity analysis approach, pertinent to the long-standing control and identification issues within the scientific community [21,80,92,99].

Understanding the impact of temperature on wastewater treatment processes, especially within the Activated Sludge Model No. 1 (ASM1) framework is crucial [4]. Temperature significantly influences the kinetics of biochemical reactions and microbial activity in wastewater treatment systems. Within ASM1, temperature variations can alter reaction rates, biomass growth, and substrate utilization efficiency. Moreover, temperature fluctuations can affect the efficiency of organic removal, such as COD [34,100]. Considering this, the consistency of temperatures was assessed across consecutive months, which were expected to be closely aligned. The influent flow was defined by providing daily COD concentrations for a fixed temperature in each simulation. This dataset was compiled from 8 samples provided by the plant laboratory, covering two distinct periods: November 1st, 2022, to December 1st, 2022, for dynamic calibration fixing the temperature amount to (18°C), and June 1st, 2022, to July 30th, 2022, for validation (Temperature= 22°C).

In this study, the influent of the treatment plant was analysed to determine the overall concentration of COD. This concentration was then divided into different components, namely: (S_S), (X_S), (S_I), and (X_I). Notably, the concentration of particulate products originating from biomass decay (X_P) was found to be negligible in the influent. Given the challenge of directly measuring (S_I), it is commonly estimated by either measuring the soluble (COD) in the effluent or by assuming it to be 90% of the effluent COD, an approach backed by studies like [77]. Considering that the process data from the treatment facility under investigation only evaluated the total (COD), the soluble fraction (S_I) was approximated to be 90% of the COD in the effluent. In order to determine the COD influent fraction, adjustment were conducted using CEMAGREF's predefined values for (S_S) and (X_I), which is a widely accepted approach in the field (Table IV.2)

Table IV. 2 Parameters related to the organic matter fractionations COD.

Parameter fraction	Symbol	Ratio	Reference
Soluble biodegradable substrate	S_S	0.32	[78,79]
Soluble inert substrate	S_I	0.056	[77]
Particulate biodegradable substrate	X_S	0.574	Own Study [X_S=TCOD-(S_S+S_I+X_I)]
Particulate inert substrate	X_I	0.05	[78,79]

IV.3.2.1.1 Kinetic & Stoichiometric Adjustments

The calibration parameters that influence short-term dynamics, such as maximum specific growth rate of heterotrophic biomass ($\mu_{max.H}$) and heterotrophic yield coefficient (Y_H), are crucial components that need to be estimated during dynamic calibration [34,56]. On the premise of dynamic data, the focal point of model calibration lies in obtaining a more dependable estimation of key coefficients, including saturation constant (K_S), decay coefficient of heterotrophic biomass (b_H), ($\mu_{max.H}$), and (Y_H) (see Table IV.3). These parameters hold paramount significance in predicting dynamic scenarios for COD effluent dynamism [77].

Table IV. 3 Typical values for kinetic and stoichiometric parameters at neutral pH.

Parameters	Symbol	Unit	Range	Default Values	Reference
Organic Matter Fractions					
Heterotrophic biomass fraction of total COD	X_{BH}	-	[0 – 0.1]	0	[86,101]
Stoichiometric Parameters					
Yield for heterotrophic biomass	Y_H	g COD/g COD	[0.57 - 0.67]	0.67	[86,102]
Kinetic Parameters					
Maximum specific growth rate for heterotrophic biomass	$\mu_{–max\ H}$	d^{-1}	[0.6 - 13.2]	6	[86,90]
Half saturation constant	K_S	mg COD/L	[10 - 40]	20	[68,96]

IV.3.2.1.2 Sensitivity Analysis Optimizer (GPS-X Software)

The sensitivity analysis optimizer is a module that minimizes the value of a user-selected objective function by modifying its free variables. The module employs the Nelder-Mead simplex algorithm [103] for minimization. The method has been changed to support variable boundaries. The simplex technique is a multi-dimensional approach that searches through the multidimensional "surface" using a direct search method in order to identify the objective function's local minimum [46].

To achieve the desired outcome of matching the COD effluent, a Controller Data File was generated on GPS-X. This file includes COD influent concentrations alongside corresponding flow rates (Figure IV.1) to ensure the dynamism of the process for November and December simulations. It's important to note that the temperature was held constant at (18°C) throughout the calibration process.

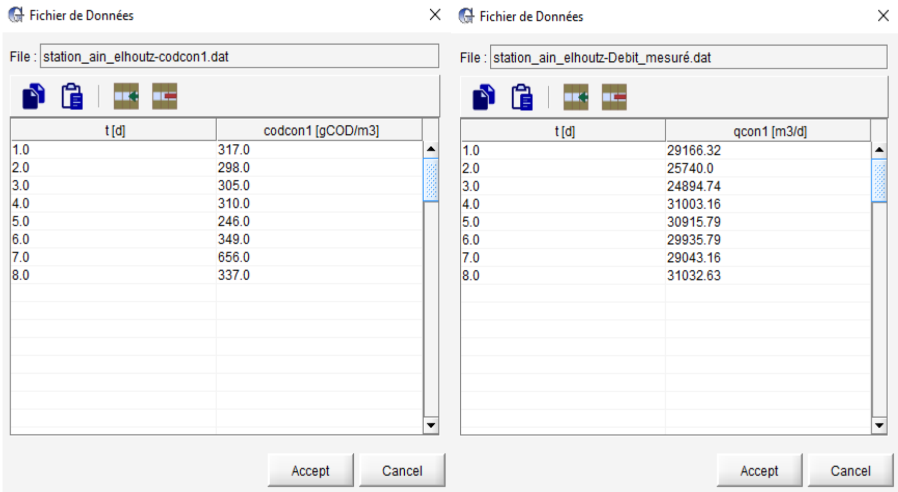


Figure IV. 1 Data File Tool with Values (COD & Flow rate).

Following this, to configure the GPS-X optimizer module, we begin by selecting the target variable as COD effluent outputs. Next, we identify the sensitive parameters requiring adjustment during fitting and specify the optimizer settings (figure IV.2.(a)). The final step entails determining the optimization approach. For this, we will utilize the Fit to Data, Time Series, and Maximum Likelihood methods as objective functions (figure IV.2.(b)). It's essential to note that the initial parameter values utilized in the optimization process of sensitivity analysis are set to the default values.

(a) (b)

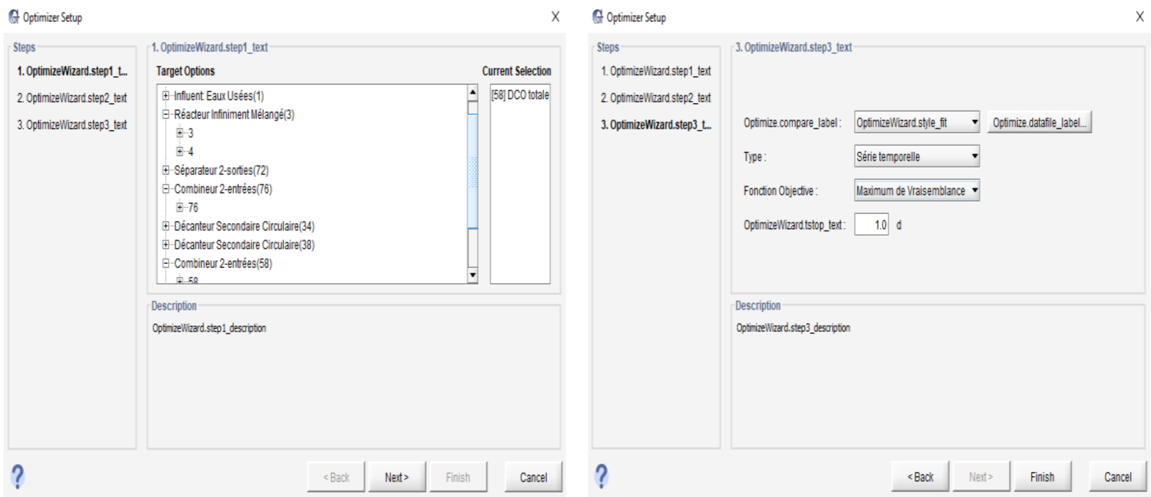


Figure IV. 2 Optimizer Setup Wizard: (a) Optimizer Settings, (b) Optimization Approach.

IV.3.2.1.3 Model Validation

After calibrating the model, another dynamic simulation will be conducted. In this stage, the parameter values identified as sensitive will be implemented as initial conditions for the modelled plant. The same procedure employed in calibration will be followed here.

The influent flow will be described by introducing daily chemical oxygen demand (COD) values at a constant temperature of 22°C. The dataset consists of 8 samples obtained from the plant laboratory between June and July 2022. These samples are carefully selected to cover various conditions characteristic of both summer months.

This study used the linear regression approach for correlation testing [104] to verify the model and confirm its dependability in mirroring reality.

IV.3.2.2 Model Calibration Overview

Figure IV.3 provides a concise summary of the calibration process conducted for the model. It illustrates the key steps involved in adjusting parameters and optimizing the model to accurately reflect observed data. By visually outlining the calibration procedure, this summary offers a clear understanding of the methodologies employed and the outcomes achieved.

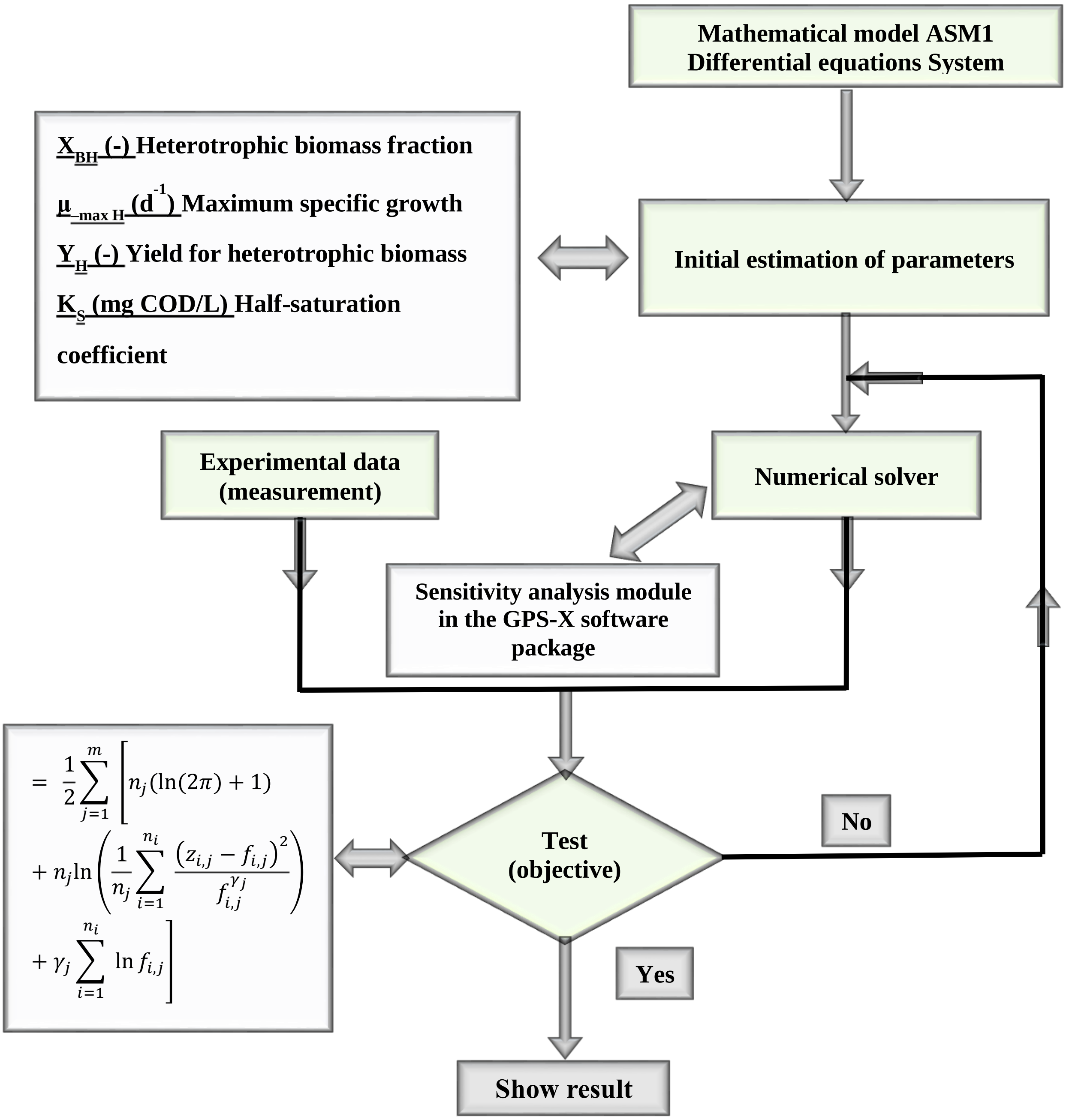


Figure IV. 3 Schematic Overview of different steps in the model calibration protocol.

IV.3.3 Calibration Results

The calibration of COD effluent involved meticulous adjustments of key parameters: the Heterotrophic biomass fraction (X_{BH}), ($\mu_{\max H}$), (Y_H), and the substrate (COD) half saturation (K_S) (Table IV.4), Numerical optimization adjustments were employed to fine-tune the modelled COD effluent.

The application of numerical optimization for model calibration has been demonstrated in previous works [105–107], particularly for various models derived from the ASM family. Considering the complexity of the calibration process, this study opts for the application of dynamic optimization methods, focusing solely on the aerobic growth of heterotrophs for the COD degradation process.

The heterotrophic biomass fraction of total COD underwent a range of adjustments from 0 to 0.1, which aligns with findings from [61], who elevated this parameter to (0.16 d^{-1}). This range concurs with the observations of [101], where the parameter spanned between 0 and 0.1. The ($\mu_{-max\ H}$) rate was fine-tuned within the interval of 6 to 7 (d^{-1}). a range that resonates with [61], who increased the parameter to 6.98 (d^{-1}), and with [90], who noted a wide range of 1 to 8 in the literature, as well as the range [0.6-13.2] according to [96], noting that ($\mu_{-max\ H}$) exhibited high sensitivity to COD fluctuations, decreasing to a value of 3.48 (d^{-1}). The (Y_H) was reduced from 0.67 to 0.57 (g COD/g COD), a modification suggested by [102]. This range adjustment aligns with [96], indicating a span of 0.57 to 0.67 (g COD/g COD). Furthermore, the substrate (COD) half saturation experienced calibration within the range of 10 to 20 (mg COD/L). This falls in line with observations from [68], who set this parameter at 20 (mg COD/L), and is consistent with the insights provided by [34,96], showcasing a parameter range of 10 to 40 (mg COD/L), The default value of (K_S) for COD prediction was uncertain and optimized, ultimately set to 16.17 (mg COD/L), as indicated in Table IV.4.

Table IV. 4 Calibrated values for kinetic and stoichiometric parameters.

Parameters	Symbol	Unit	Range	Calibrated Values
Organic matter fractions				
Heterotrophic biomass fraction of total COD	X_{BH}	-	[0 – 0.1]	0.1
Stoichiometric Parameters				
Yield for heterotrophic biomass	Y_H	g COD/g COD	[0.57 - 0.67]	0.57
Maximum specific growth rate for heterotrophic biomass	$\mu_{max\ H}$	d^{-1}	[0.6 - 13.2]	3.48
Half saturation constant	K_S	mg COD/L	[10 - 40]	16.17

The adaptation of the (X_S), (S_S), (X_I) and (S_I) fractions was balanced by correcting the (X_{BH}) fraction so that the COD mass balance would be respected (Table IV.5).

Table IV. 5 Parameters related to the organic matter fractionations COD after calibration.

Parameter fraction	Symbol	Ratio	Reference
Soluble biodegradable substrate	S_S	0.295	[78,79]
Soluble inert substrate	S_I	0.031	[77]
Particulate biodegradable substrate	X_S	0.549	Own Study [X_S=TCOD-(X_{BH}+S_S+S_I+X_I)]
Particulate inert substrate	X_I	0.025	[78,79]
Heterotrophic Biomass	X_{BH}	0.1	calibrated

Model calibration involves determining the model parameters that best fit a certain set of experimental data obtained from the investigated WWTP. Figure IV.4 demonstrates the successful representation of the sensitivity module for calibration performance. The simulated effluent COD values are very similar to the actual measured COD readings, with accuracy assessed by a linear regression method. As seen in Figure IV.5, the regression coefficient has a value of 0.79, indicating a strong correlation.

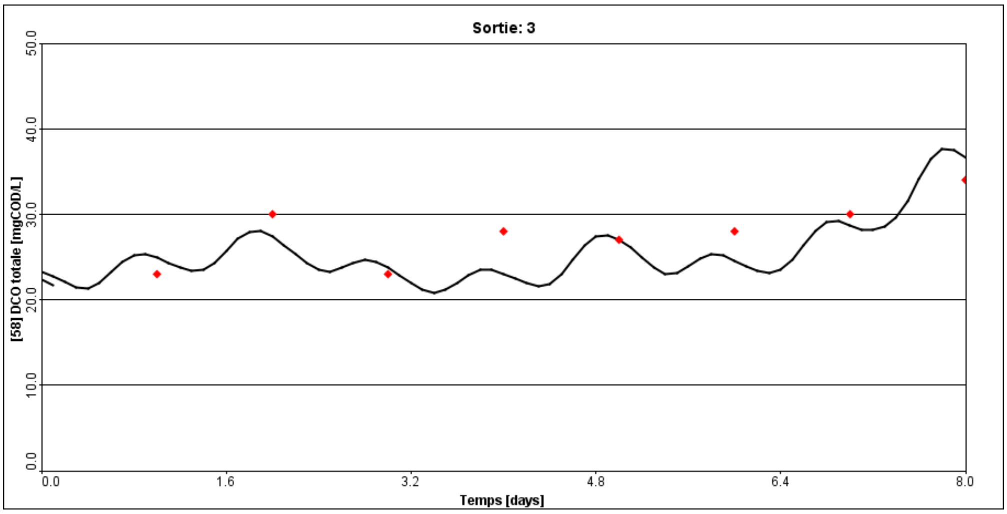


Figure IV. 4 Dynamic Calibration results for the effluent COD.

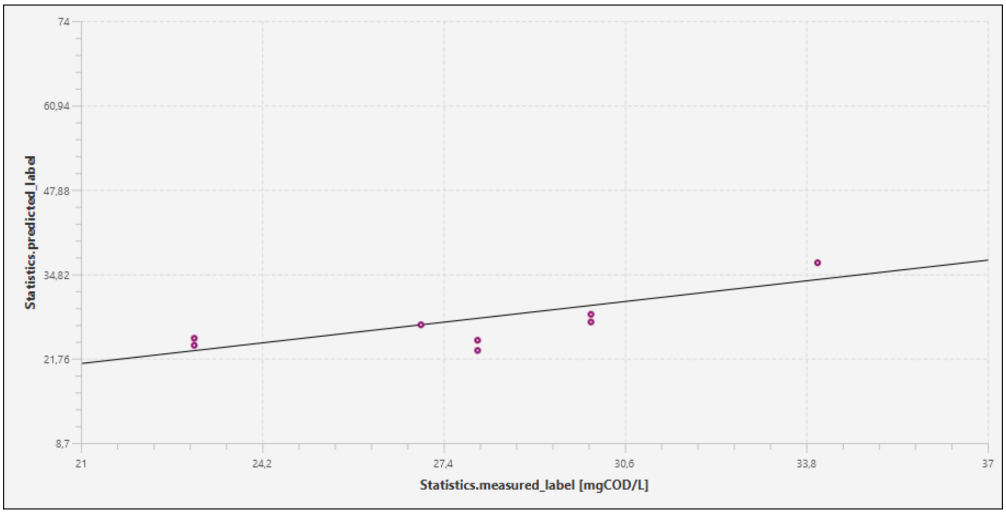


Figure IV. 5 Linear Regression test (measured COD/simulated COD).

IV.4 Model Validation

It is important to highlight that the objective of dynamic calibration is not to forecast precise values for individual output variables, but rather to anticipate the overall trend of their fluctuations. In this regard, the dynamic calibration conducted proved to be entirely effective. Furthermore, experts emphasize that accurately predicting changes in all significant output variables within an acceptable tolerance range holds more significance than achieving precise predictions for only one or two output variables in an ideal scenario [38].

The next phase was validating the model. The model is deemed validated when its predictions align with observed values from an independent dataset [56]. The results of model validation presented in (Figure IV.6 and Figure IV.7), suggest that the calibration was completed correctly, and the model may be considered valid, the correlation (R^2=0.68) appears significant and highly representative of successful calibration efforts. A simulation is considered adequate when there is no substantial statistical divergence between the simulated and measured values of the variable being studied [34].

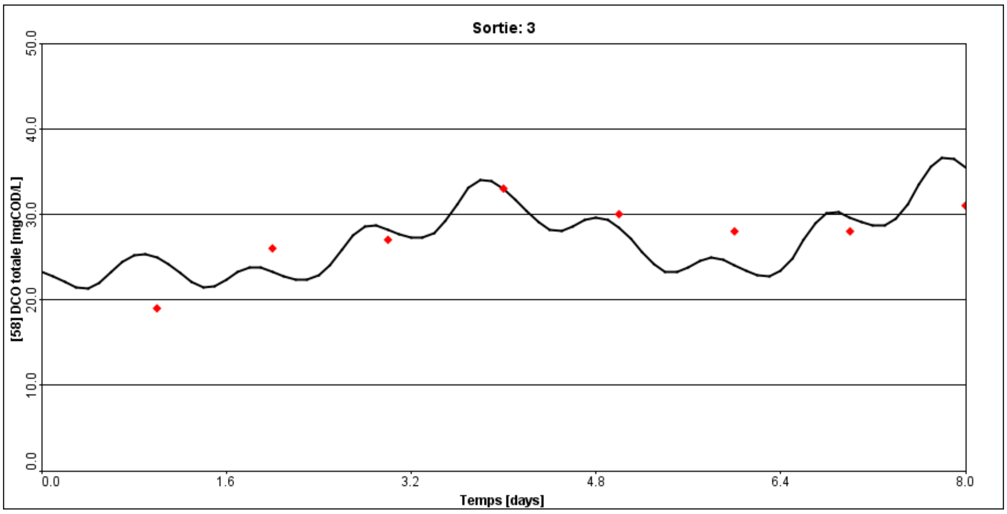


Figure IV. 6 Dynamic Validation results for the effluent COD.

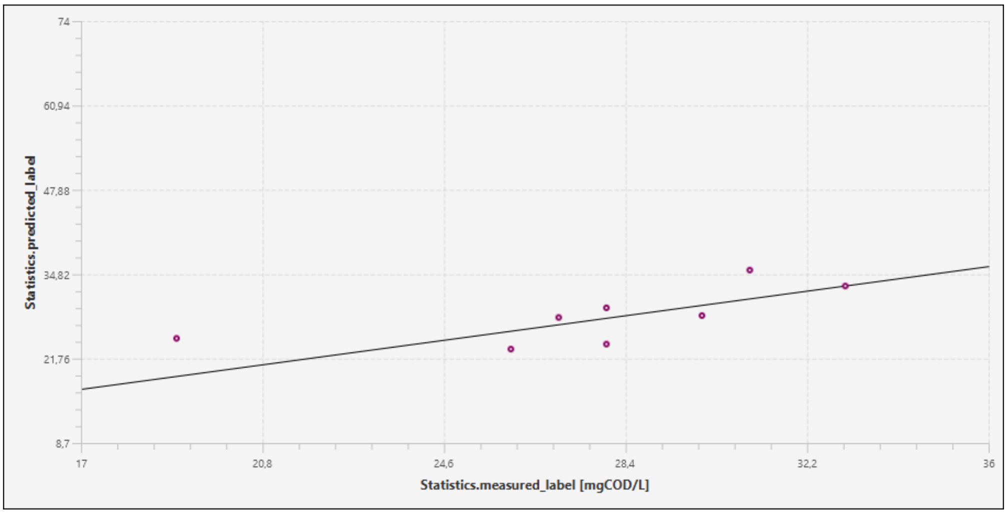


Figure IV. 7 Linear Regression test (measured COD/simulated COD).

IV.5 Conclusion

In this study, we present a straightforward and systematic approach for achieving successful dynamic calibration, entirely implemented within the GPS-X based Activated Sludge Process (ASP) model for real WWTP modelling.

Our objective was to optimize the most pertinent coefficients among the 20 sensitive kinetic and stoichiometric parameters of ASM1 using WWTP monitoring data. By doing so, we aimed to achieve the most accurate representation of the activated sludge process during simulations, thereby minimizing prediction errors across various state variables.

The ASM1 model effectively adapts to and accurately reflects the dynamic fluctuations in COD effluent concentrations, as confirmed by the linear regression approach, resulting in R^2=0.79 and R^2=0.68 for calibration and validation of the model, respectively. These regression coefficients underscore the reliability and precision of the model's predictions. The optimized parameters not only enhance the model's accuracy but also establish it as a valuable tool for WWTP operators and researchers alike.

CONCLUSION AND PERSPECTIVES

1. General Conclusion

In this comprehensive study, we introduce clear and systematic methods aimed at achieving effective dynamic calibration, fully integrated within the GPS-X based Activated Sludge Process (ASP) model for real WWTPs modelling. Our methodology entails a combination of laboratory experiments, historical data from the municipal laboratory, and experimental modelling to create information for the plant model's development and calibration. Through this approach, we aim to provide a robust framework for enhancing the accuracy and reliability of WWTP modelling and optimization processes.

- The first chapter has offered a thorough exploration of the activated sludge process, shedding light on its operation and functionality. Through this examination, we've delved into the forefront of biological modelling, with a specific emphasis on the ASM1 model, the way sludge settles, and previous research on modelling activated sludge treatment plants. We also checked out different computer programs used for modelling.
- For the data collection and analysis section, influent parameters at the Maghnia WWTP, including BOD, TSS, COD, and NH4-N, exhibited similar trends, while dissolved oxygen levels showed an inverse correlation with changes in the inflow rate. Regarding effluent quality parameters, it was noted that the fluctuation in dissolved oxygen levels throughout the treatment process influenced the concentration of other quality parameters, particularly total suspended solids (TSS) and biochemical oxygen demand (BOD).
- Similarly, at the Tlemcen WWTP, influent parameters displayed synchronized trends over consecutive months, temperature fluctuations maintained relative stability for several months around (22°C) in summer, and (18°C) in winter. However, irregularities in effluent quality parameters were noted, with peaks observed in March (COD=56 mg/L, NH4-N=28.4 mg/L) and May (COD=51 mg/L). Despite these fluctuations, other months remain relatively consistent for both BOD, TSS and Temperature.
- The data analysis underscores the importance of monitoring and understanding the dynamics of influent and effluent parameters in wastewater treatment processes. These insights are crucial for optimizing plant operations and ensuring compliance with environmental standards.
- For characterizing the COD influent fraction, we’ve employed the CEMAGRAF protocol conducting adjustment fractionations. Following CEMAGREF defaults, a

fraction of 0.32 was assigned for (S_S). (X_I) was determined with a mean value of 0.05, also adopted from CEMAGREF defaults. The (S_I) fraction was found to have a mean value of 0.056. Consequently, the remaining 57.4% of the COD was categorized as (X_S).

- In the modelling section, the ASM1 application for the Maghnia WWTP underwent a systematic step-wise procedure. This involved adjusting certain stoichiometric and kinetic parameters of the model, representing the calibration process for the model. The modelling results clearly indicate that the Maghnia plant operates without issues under steady-state conditions, with output variables meeting discharge standards. The ASM1 model proved effective in accurately predicting the steady-state behaviour of the WWTP's removal processes for COD, TSS, and NH4-N, with corresponding MAE values of 3.7%, 17%, and 37%, over an 18-month data period.
- After confirming the compatibility of the computer tool with reality under Steady-state conditions, we proceeded to present the results of dynamic model validation. This phase emphasized the effectiveness of plant-wide modelling in predicting COD removal performance, achieving 23% accuracy for COD effluent. This validation highlighted the strong calibration of the model, providing significant insights and assistance for other wastewater treatment plants looking to enhance their operations. However, the study encountered challenges stemming from uncertainties in measuring TSS and NH4-N, resulting in lower accuracy compared to measured values, with mean absolute errors of 67% and 56%, respectively. Addressing these challenges will require additional efforts to enhance the model's validation, particularly regarding nitrogen and suspended solids removal processes.
- Another approach was adopted regarding the ASM1 application for Ain Elhoutz WWTP, in this last part of the study we delved into the dynamics of Chemical Oxygen Demand (COD) effluent quality, recognizing its pivotal role in assessing plant performance. The objective was to pinpoint the most influential coefficients among the 20 sensitive kinetic and stoichiometric parameters of ASM1, utilizing COD data from WWTP monitoring to achieve highly accurate simulations. Adjustments were made to key parameters: the Heterotrophic biomass fraction (X_{BH}) of total COD underwent adjustments, ranging from 0 to 0.1, with a maximum value capped at 10% of the total COD. The ($\mu_{-max\ H}$) exhibited significant sensitivity to COD fluctuations, declining to 3.48 d^{-1}. Likewise, the yield for heterotrophic biomass (Y_H) was fine-tuned from 0.67 to 0.57 (g COD/g COD). Although the substrate (COD) half saturation (K_S) was

optimized and set to 16.17 (mgCOD/L), its uncertainty remained a factor during the optimization process.

- The ASM1 model effectively adapts to and accurately mirrors the dynamic changes in COD effluent concentrations, as evidenced by the linear regression approach, yielding correlation coefficients of (R^2=0.79) for calibration and (R^2=0.68) for validation of the model. These coefficients underscore the reliability and precision of the model's predictions regarding their sensitivity. Moreover, the optimized parameters not only enhance the model's accuracy but also establish it as a valuable tool for WWTP operators and researchers, facilitating improved decision-making and optimization efforts within wastewater treatment processes.

2. Perspectives

The modelling of wastewater treatment plants (WWTPs) presented in this thesis represents a significant step forward in a relatively new field, particularly in Algeria. However, there is still much room for improvement in accurately depicting real-world functioning through numerical models. The outcomes of this study offer promising avenues for future research. Some potential areas for further investigation include:

- Conducting batch tests based on respirometry to accurately estimate the true value of COD fractions. These tests should be carried out at different temperatures to analyse yield and kinetic parameters, providing a deeper understanding of influent and nutrient fractions. Despite their associated effort and cost, batch tests are crucial for validating the calibration process.
- Establishing a robust methodology for calibrating Scenario Analysis and devising effective management strategies. This involves introducing model-based optimization and scenario analysis platforms and evaluating the costs associated with different scenarios.
- Exploring the modelling of WWTPs using alternative models such as “ASM2”, “ASM3”, and “Mantis2” for future development. The objective here would be to identify the model that best characterizes the behaviour of the plants.

Utilizing the findings from these research endeavours as a framework or guideline to aid decision-makers in considering economic and environmental factors when designing civil and environmental infrastructures. These results can serve as valuable tools for informed decision-making processes.

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