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Wastewater treatment simulation modeling software: review

Hagar H. Hassan
Civil engineeringdepartment, faculty of engineering, Alexanderia university, Egypt

ABSTRACT: *Modeling plays a pivotal role across a spectrum of applications, notably in the optimization and design of wastewater treatment plants (WWTPs). This is exemplified in the research by Croll, H.C. et al. in 2023 [1], where modeling, combined with reinforcement learning, is applied for process control optimization in wastewater treatment. The study delves into various approaches, challenges, and the future trajectory of this research. Through modeling, the WWTP's operational costs can be controlled while simultaneously enhancing effluent quality. It is imperative to predict effluent quality using WWTP models, as emphasized in Aghdam, E. et al.'s work in 2023 [2]. These models empower operators to assess the plant's future performance and provide a valuable means to assess and improve operational parameters.*
A multitude of computer simulators are readily available, each harnessing combinations of models to facilitate WWTP design and optimization. Notable examples include AQUA Designer, AQUA Aero, Bio-Win, SIMBA water, STOAT, GPS-X, Capdet Works, West, Toxchem (TM), and Wat pro. For instance, Sakib, F.S. in 2022 [3] focused on the design and modeling of a municipal wastewater treatment plant using GPS-X, showcasing the practicality of these software tools. Furthermore, Callahan, J.L. et al. in 2022 [4] employed BioWin modeling to simulate the treatment of domestic wastewater through anaerobic sludge blanket technology, demonstrating the versatility of simulation and modeling in addressing real-world challenges.
In addition, Bacci di Capaci, R. et al. in 2023 [5] presented a comprehensive approach to sewage sludge hydrothermal carbonization, incorporating simulation, modeling, and a Life Cycle Assessment. This holistic methodology underscores the significance of simulation and modeling tools in tackling complex environmental issues.This review will shed light on the key software packages available and underscore their pivotal role in the design and optimization of WWTPs.

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I. INTRODUCTION

Simulation plays a crucial role in the field of wastewater treatment. While it's possible to conduct experiments on physical models, it's worth noting that the majority of engineering simulations are now computer-based programs, a point emphasized by Croll, H.C. et al. in 2023 [1], and reiterated in the study by Aghdam, E. et al. in 2023 [2]. The primary objective of simulation is to experiment with models, evaluating their applicability in real systems comprehensively and with minimal effort, as discussed in the research by Aghdam, E. et al. in 2023 [2]. When creating a model for a specific experiment, it's essential that the model is both user-friendly and convincingly replicates real-world systems, as highlighted by Aghdam, E. et al. in 2023 [2] and Sakib, F.S. in 2022 [3].

Simulation serves various roles, including acting as a statistical process control chart for facility operations and facilitating design and analysis, as outlined by Croll, H.C. et al. in 2023 [1] and Callahan, J.L. et al. in 2022 [4]. Moreover, simulation is instrumental in solving nonlinear differential equations related to facility processes, as brought to attention in the research by Aghdam, E. et al. in 2023 [2], and aligned with the observations made by Sakib, F.S. in 2022 [3] and Callahan, J.L. et al. in 2022 [4]. Simulation remains the preferred approach for analyzing non-uniform or unknown system behaviours, typically employed after real system experimentation, as evidenced in the study by Selișteanu, D. et al. in 2021 [6]. These researchers developed a software emulator for modeling and controlling an activated sludge process in a wastewater treatment plant.

Most models used in simulation feature a visual interface, simplifying their integration into plant processes. Additionally, these models rely on equations and mathematical approaches that incorporate time-dependent parameters and variables to define the model, with variations from one model to another, as discussed by Al-Obaidi, M., Kara-Zaitri, C., and Mujtaba, I.M. in 2020 [7]. This diversity in mathematical approaches was reaffirmed in the study by Selișteanu, D. et al. in 2021 [6].

Creating a well-estimated model is essential, as it aids in making informed decisions about design substitutions and unit process sizing. This approach not only saves time but also introduces confidence in the design, as articulated in the research by Sakib, F.S. in 2022 [3]. Furthermore, it facilitates the evaluation of various optimization scenarios aimed at reducing operational costs, including energy costs to meet effluent quality requirements, as exemplified in the article by Arif, A. U. A., Sorour, M. T., & Aly, S. A. in 2018 [8]. Precise models are also instrumental in predicting the consequences of shutting down a unit process and measuring improvements for process control, as underscored by Sakib, F.S. in 2022 [3]. These points were further emphasized in the study by Arif, A. U. A., Sorour, M. T., & Aly, S. A. in 2018 [8], which conducted a comparative analysis of different wastewater treatment plant types. simulation and modeling are integral tools in wastewater treatment, offering a comprehensive and efficient means of assessing real-world systems and optimizing processes.

II. The upside and downside of utilizing software packages in wastewater treatment

Advantages of Software Packages:Software packages offer several advantages in wastewater treatment. They enable the evaluation and analysis of costs, as highlighted in the book by Brđanović, D. in 2021 [9]. Additionally, they allow for the assessment of a wastewater treatment plant's response to various perturbations, a topic covered extensively in the book authored by Shah, V., Desai, J., and Shah, M. in 2022 [10]. These packages also facilitate the estimation of scenarios aimed at improving the operation of existing wastewater treatment plants, as demonstrated in the research by Chaplin, B.P. in 2018 [11]. For new wastewater treatment plants, software packages provide valuable design alternatives, a point emphasized by Sakib, F.S. in 2022 [3]. Furthermore, they reduce the scale-up time by enabling the evaluation of different options before constructing a pilot plant, as exemplified in the study conducted by Mu'azu, N.D., Alagha, O., and Anil, I. in 2020 [12], which systematically modeled municipal wastewater activated sludge processes.

Most software packages incorporate Artificial Intelligence (AI) algorithms, enhancing short-term forecasting of wastewater treatment plant performance, as discussed by Wongburi, P. in 2021 [13]. These AI technologies can be integrated into wastewater treatment systems, improving data analysis, prediction, and decision-making. In summary, software packages offer valuable tools for optimizing wastewater treatment processes.

Disadvantages of Software Packages:While software packages have numerous advantages, they also come with certain disadvantages. First, not all programs are readily available for free, as noted in the book "CFD Modelling for Wastewater Treatment Processes" authored by Laurent, J. et al. in 2022 [14]. Additionally, software packages may lack precision in predicting output or effluent in cases where practical examination is required, as discussed in an article by Nemcik, J. et al. in 2022 [15]. Learning to use these programs effectively can also be challenging.

Moreover, creating models to predict scenarios, conduct sensitivity and uncertainty analysis, and estimate parameters can be labor-intensive when done in real life, a challenge highlighted by Molinuevo-Salces, B. et al. in 2019 [16] and further discussed in the book "Trends, Paradigms, and Advances in Mechatronics Engineering" by Mohan, V.G. et al. in 2022 [17]. However, integrating innovative approaches, including simulation and dynamic modeling, can yield significant cost savings, as indicated in Mohan, V.G. et al.'s book [17]. Additionally, remote usage of these models, such as predicting daily COVID-19 case rates from influent concentrations across wastewater treatment plants, has proven beneficial to communities, as described in the article by Kobeyev, S. et al. in 2022 [19] and the research by Wu, F. et al. in 2020 [20]. Given the importance of stability and process safety in wastewater treatment, accurate real-time data is increasingly necessary, a point emphasized by Wu, F. et al.[20] .

To ensure models adapt perfectly to dynamic variations, several adaptive methods are employed. These include Just-In-Time (JIT) and ensemble modeling, discussed by Ewusi, A., Ahenkorah, I., and Aikins, D. in 2021 [21], and moving window (MW) and supervised machine learning, as mentioned by Aldrees, A. et al. in 2023 [22]. However, modeling can be affected by unstable percentages for unlabelled and labeled data, as Lotfi, K. et al. highlighted in their study in 2020 [23]. Nevertheless, there are semi-supervised learning procedures that efficiently use unlabelled data to upgrade the model's accuracy and stability, especially when output variables exhibit a tendency, as explained by Zhou, M. et al. in 2022.[24] , while software packages offer valuable tools for wastewater treatment optimization, it's essential to consider both their advantages and disadvantages when applying them in practice.

III. Software packages origin over the years

Software packages' countries of origin have been a notable aspect of their development over the years. Many commonly used software packages in wastewater treatment include GPS-X, STOAT, SIMBA, and BIO-Win, among others. Interestingly, most of these software packages originate exclusively from Northern America and Europe (Figure 1). For instance, both SIMBA and GPS-X software packages have their headquarters based in Canada, as reported by Alex, J. in 2004 [25] and confirmed by Sakib, F.S. in 2022.[3]

It's worth noting that some developers have created multiple software packages for WWTP simulations and modeling, a prime example being Hydromantis, as indicated in the study by Al-Wardy, A.H., Alquzweenib, S.S., & Al-Saadi, R.J. in 2021 [26]

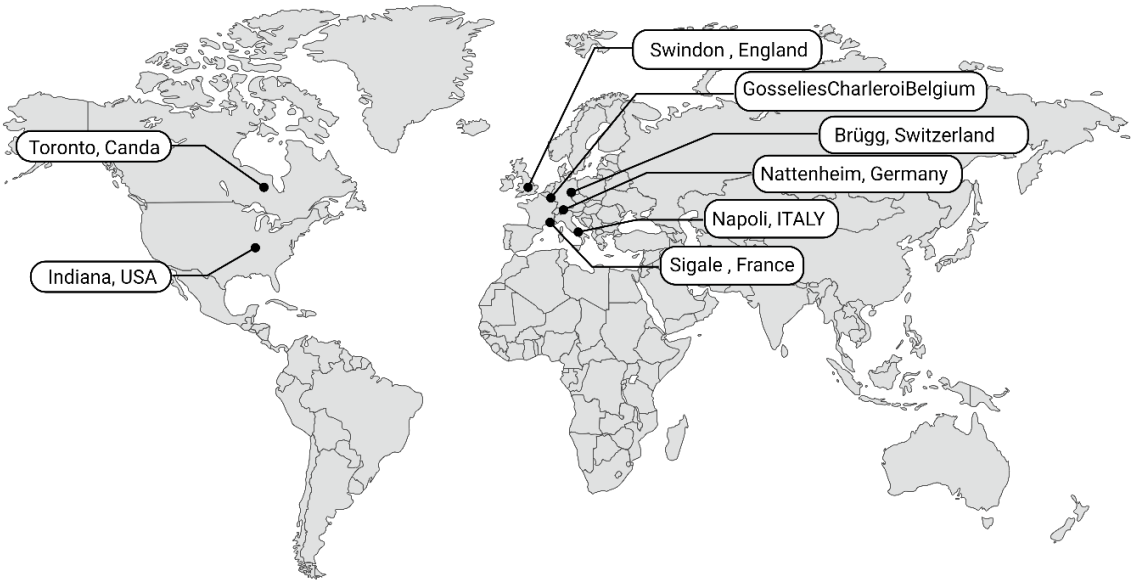

Fig. 1 Locations of most available software packages around the world for wastewater treatment

Over the last decade, a significant number of simulation software packages have been developed, with a notable surge between 1995 and 2010 (Figure 2). Furthermore, most software packages have continuously received updates to keep up with modern requirements. This surge in development and updates can be attributed to the increasing demand for such software and advancements in both software and hardware in recent years, as pointed out by Lotfi, K. et al. in 2020 [23] and Selişteanu, D. et al. in 2021 [6].

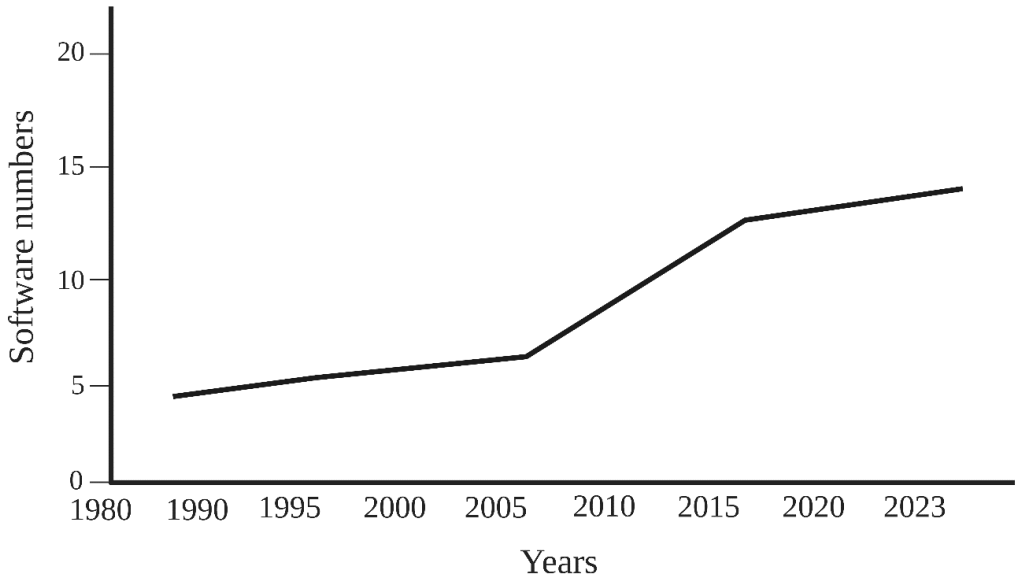

Fig. 2Timeline for more than 10 software packages over the years

IV. Future of modeling WWTPs

Further research will focus on the integration of non-monetary optimization objectives in the performance index, such as plant flexibility or the risk of failure, as reported by Analouei, R., Taheriyoun, M., and Amin, M.T. in 2022 [27]. Their study conducted a dynamic failure risk assessment of a wastewater treatment and reclamation plant. This research aligns with the findings outlined by Lu, J.-Y. et al. in 2019 [29], which highlighted the remaining barriers and future implications in the optimization and operation of wastewater treatment.

Recent advancements have seen artificial intelligence (AI) and machine learning algorithms (MLAs) becoming integral components in cutting-edge software packages. This integration allows these packages to predict the performance of wastewater treatment plants, as emphasized by Bina, B. et al. in 2022 [28], during their investigation into the simulation and modeling of a real combined industrial wastewater biological treatment process.

The incorporation of AI and MLAs promises to significantly enhance the output, reduce time requirements, and enable more efficient WWTP design with minimal effort. These potential improvements in treatment plant modeling were discussed by Aghdam, E. et al. in 2023 [2], and are also explored in the book by Mohan, V.G. et al. in 2022 [17]. Additionally, Qiu, X. in 2023 [30] delved into the application of Artificial Intelligence, specifically Artificial Neural Networks, in wastewater treatment.

AI technologies can be seamlessly integrated into wastewater treatment systems, enhancing their capabilities in data analysis, prediction, and decision-making. Conversely, software packages are purpose-built tools designed to manage and optimize wastewater treatment processes, often incorporating ML and AI techniques to enhance performance and efficiency. These synergistic technologies collectively contribute to improving the overall effectiveness of wastewater treatment operations.

In conclusion, wastewater treatment simulation modeling software plays an essential role in optimizing WWTPs. While these software packages offer numerous advantages, it's important to acknowledge their limitations. As technology continues to advance, the integration of AI and ML holds the promise of further enhancing wastewater treatment processes.

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