TOWARDS SUSTAINABLE WATER MANAGEMENT THROUGH SYSTEMIC MODELLING

E. Karkou[1], G. Arampatzis[1]*

[1]School of Production Engineering and Management, Technical University of Crete, Chania, Greece

(*garampatzis@tuc.gr)

ABSTRACT

Water depletion and generated industrial wastewater indicate the opportunity to recover water through efficient treatment and management of resources, mitigating the pressure on the environment, resulting in added-value products and less waste. Circular economy practices are being adopted in the industrial sector, attempting to close the water loops through recovery, reuse and recycling as well as reincorporating the reclaimed resources and by-products into the value chain. In addition, the exchange of resources among different actors can facilitate the transition to a circular model through synergies and collaborative networks.

This research lies in the investigation and modelling of water and wastewater treatment and management as well as synergies at different levels in the process industry. This study derives from the process industries (Dow, BASF, Solvay, Agricola, Tüpraş) participating in the EU-funded AquaSPICE project, which aims to materialize water use, build resource-efficient industries and implement innovative technological and circular solutions.

The pillars for sustainable water management encompass the reduction of water resources consumption, enhanced industrial processes' performance and exploitation of all generated by-products. Overall, there are four levels to be modelled: **(i)** in-process modelling, **(ii)** in-factory modelling and **(iii)** systemic modelling. The first level includes the development of mathematical models to predict water quality, process performance, energy requirement and chemical consumption. The second level of modelling encompasses a treatment train or a factory (more than one production process) and targets to minimize water losses and optimize water demand and supply through water balance and management models. Systemic modelling refers to the exchange of water and by-products among industries and non-industrial actors, such as the municipality or the local authorities, considering quality, costs, water tariffs and their interdependencies. In conclusion, fit-for-purpose closed-loop approaches are required in the industry.

KEYWORDS: process industry, wastewater treatment, systemic models, sustainability

INTRODUCTION

Freshwater reserves correspond to 2.5 % of the total available water, with a decreasing trend due to population growth and climate change, while industrial water demand increases [1], [2]. The pivotal role of water in industry indicates the utilization of non-conventional water sources coupled with sustainable and more efficient technologies. To this end, the potential of exploiting the wastewater generated by the industry emerges [3]. Industrial wastewater treatment may comprise a bridge-building tool in EU for achieving a zero-pollution environment by 2050. Conventional and advanced water/wastewater treatment technologies have been studied, including aerobic granular sludge [4], [5], adsorption [6], [7], membrane bioreactor [8], [9], advanced oxidation processes [10]–[12], ion exchange [13], membrane-based processes (reverse osmosis [14]–[16] and ultrafiltration [17], [18]) and coagulation/flocculation [19].

The simulation and prediction of the performance of one or a series of such processes throughout an industrial production chain is achieved by mathematical modelling, taking into account the effect of industrial contaminants and operating conditions (flow rate, pressure, viscosity, porosity, resin, etc.). However, ineffective management of water and wastewater streams across a production chain can result in leakages and losses [20]. For this reason, water balance and management tools seem promising within a complex industrial network comprised of several stages. Last but not least, in case an industry participates in a consortium, into which by-products of a partner are exchanged to be utilized as raw materials by another partner, the complexity increases and systemic modelling should be applied. This way, circular economy practices and beneficial symbiotic relationships become a significant aspect that needs to be modelled [21]–[24]. Under any circumstance, water reuse quality requirements must be met in order to exploit reclaimed water as an alternative water resource within the industry [3].

The aim of this study is the fit-for-purpose modelling of water management strategies in the industrial sector with the aspiration of reusing water derived from alternative sources. A three-layered approach was followed and implemented for six industrial partners within the context of the EU-funded AquaSPICE project (GA No 958396).

METHODOLOGY

Based on a literature review, a methodology has been developed aspiring to select the suitable level of modelling and the required steps to be followed for each use case, as shown in Figure 1. It consists of four phases, each of which entails specific steps to be followed. The fundamental objective is to define thoroughly the system to be modelled and simulated along with its requirements. The case studies to which the methodology is applied encompass the chemical industry of Dow in Terneuzen and Böhlen, the Solvay chemical plant, BASF, Agricola's slaughterhouse plant and the Tüpraş petroleum refinery, which are described in short.

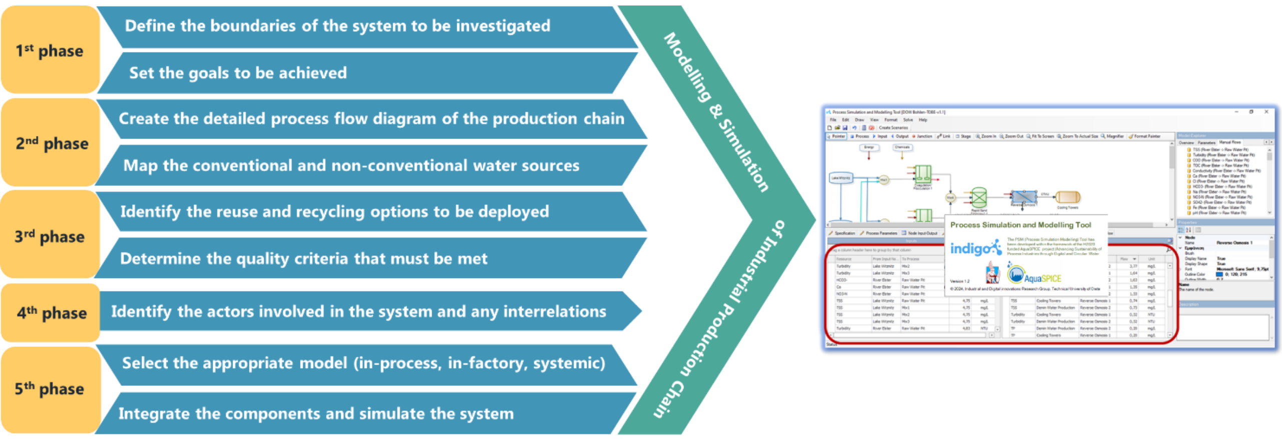

Figure 1. *Overview of the methodology for the selection of the appropriate modelling level.*

Chemical plant, Dow, Netherlands and Germany: Dow operates in the sector of chemicals and is located in a coastal area with limited availability of freshwater. For this reason, lake and river water and treated industrial effluents, including the cooling tower blowdown, are investigated as alternative water sources for reuse purposes.

Chemical plant, Solvay, Italy: The Rosignano Solvay plant produces a variety of products, including plastic materials and hydrogen peroxide. The industrial wastewater from the peroxide and peracetic production plant is treated, with the intention to adopt reuse practices. In addition, the industry is part of the Consortium Aretusa and exchanges wastewater and water between the municipality and a water utility company. Thus, the optimal allocation of resources is a pivotal matter.

Chemical plant, BASF, Belgium: Water is abstracted from the docks of the Antwerp port for the BASF production plant. Energy-intensive activities require the use of water as carrier for the thermal transfer and also brackish water is exchanged between production plants and cooling towers as cooling water. The potential of utilizing the cooling tower blow down as make-up water for the cooling towers and the reverse osmosis concentrate as reuse stream due to its high salinity level within the industry has widened the sustainable water management practices.

Slaughterhouse plant, Agricola, Romania: Agricola International SA is a private meat group company, which produces approximately 150 tons of meat per day. Taking into consideration that the production of 1 kg of meat requires the consumption of 6 L of freshwater, it is clear that wastewater generation is an important issue for the industry. The high content of slaughterhouse wastewater in BOD, COD, TSS, nitrogen and phosphorus requires treatment with innovative technologies in order to make feasible the reuse and recycling of reclaimed water.

Oil refinery, Tüpraş, Turkey: Tüpraş oil refinery's production capacity reaches 30 million tons of crude oil annually, consuming huge amounts of freshwater for various purposes, such as cooling water, demineralized water, firefighting water or steam production. To reduce the freshwater consumption and wastewater discharge to the sea, the generated wastewater is treated with advanced technologies to be reused within the industry, considering that the reclaimed water meets the legislated water quality reuse requirements.

RESULTS AND DISCUSSION

Figure 2 illustrates the different modelling levels across the value chain, as emanated from the case studies of the AquaSPICE project and their requirements.

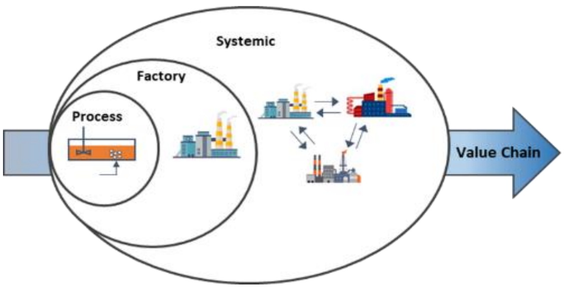

Figure 2. *Schematic representation of the different modelling levels.*

The first modelling level refers to processes for water and wastewater treatment, which result in water recovery and contribute to reduced wastewater production and decreased freshwater intake. This level entails the development of first principle mathematical models to predict their performance (removal efficiency of industrial contaminants, effluent quality, chemical consumption and energy requirements), taking into account process-specific parameters, and is called in-process modelling.

Several process models have been formulated for, among others, cooling tower, membrane bioreactor technology, granular activate carbon filtration, reverse osmosis and an advanced oxidation process. Figure 3 gives an overview of the developed process models per case study. All process models have been simulated in the non-commercial Process Simulation and Modelling (PSM) Tool, which has been developed in .NET framework utilizing Visual Basic and C#. Overall, the PSM Tool is a stand-alone tool, which allows the simulation of the whole transformation process, from the raw materials (freshwater, wastewater, chemicals, energy, etc.) to the products and/or by-products (reclaimed water, brine, sludge, etc.).

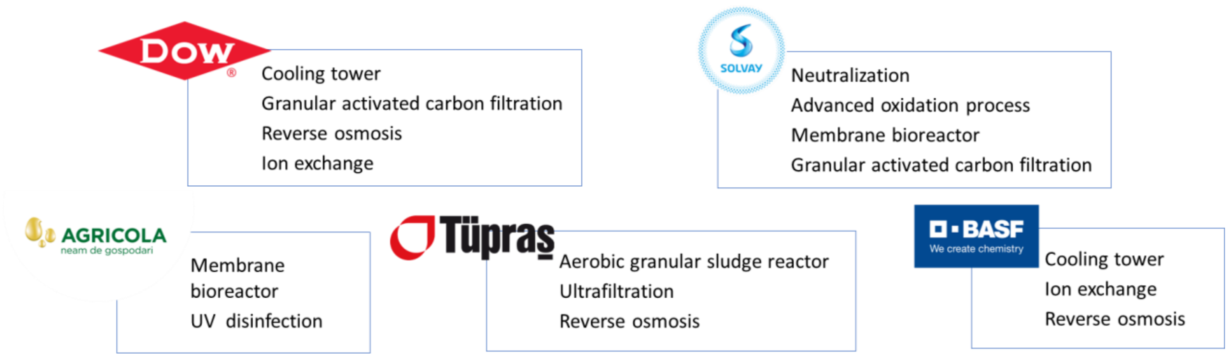

Figure 3. *In-process modelling: Processes for which first principle models have been developed.*

In case a series of processes are to be studied and modelled within an industrial value chain, such as a wastewater treatment plant (WWTP), in-factory modelling level is applied. The objective is the leakages and water losses detection across the value chain, e.g., due to evaporation or sludge production. This way, the water resources management can be improved through water balance tools. This modelling level applies to the condensate grid of Dow, Netherlands, based on flow rates, Q (L/h), and the relevant concentration, C (mg/L). The generic equation is the following:

$$Q_{in} \cdot C_{in} - Q_{out} \cdot C_{out} - Q_{loss} \cdot C_{loss} = 0 \quad (1)$$

The subscript "in" refers to the input, "out" to the output and "loss" to the water loss.

Finally, the third modelling level, systemic level, applies to any process industry that participates in a consortium for water and wastewater sharing. This model-based tool considers as parameters the water/wastewater quality, demand and supply, water tariffs and reuse quality requirements. The potential consortium partners (process industry, private and public companies and authorities) exchange freshwater, wastewater and/or other resources instead of discharging them into the environment, lowering their environmental impact, adding value to their by-products and possible increasing the revenues. A scenario-building approach is followed to investigate and find the feasible and sustainable solution related to the activities taken place in Solvay plant, in Italy, which exchanges its industrial wastewater with the municipality and a water utility company that has the wastewater reclamation plant (WWRP) of Aretusa, with the intention to reclaim water and reuse it within the industry for cooling and other purposes. Overall, the three closed-loop scenarios are the following:

- **Option 1:** The industrial wastewater from the peroxide and peracetic production plant of Solvay is treated within the pilot-scale WWTP of Solvay, then is sent to the municipality's WWTP for secondary treatment and finally to Aretusa's WWRP for tertiary treatment.

- **Option 2:** The industrial wastewater of Solvay is treated within the pilot-scale WWTP of Solvay and then is sent to the Aretusa's WWRP for tertiary treatment.

- **Option 3:** The industrial wastewater from the peroxide and peracetic production plant of Solvay is treated within the pilot-scale WWTP of Solvay and then the effluent is mixed with water from Aretusa, in a variable ratio based on wastewater composition.

Figure 4 illustrates the interrelations among the three actors within the consortium, the exchanging of resources and the fundamental criteria of the model. The systemic model indicates the feasible option, calculates the water composition and supply at each stage and also at the final product that is sent to the industry for reuse as well as the total cost for water/wastewater sharing among the partners.

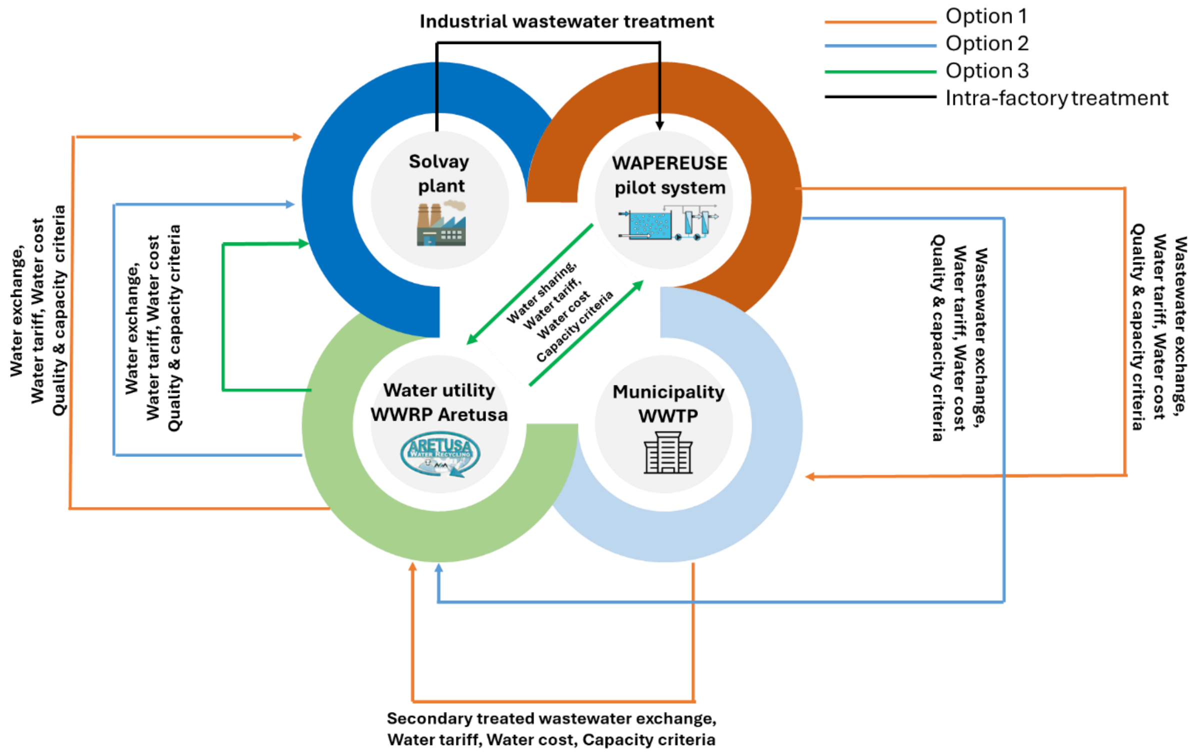

Figure 4. *Systemic level modelling and the interdependencies among the involved actors.*

ACKNOWLEDGMENTS

The research methodology and proposed solutions presented in this article arise from the project "AquaSPICE - Advancing Sustainability of Process Industries through Digital and Circular Water Use Innovations", a collaborative research project that has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No 958396. The responsibility for the content of this publication lies with the authors.

REFERENCES

[1] G. Meran, M. Siehlow, and C. von Hirschhausen, *The Economics of Water*, vol. 18, no. 4. Springer, 2021.

[2] I. V. Muralikrishna and V. Manickam, "Life Cycle Assessment," in *Environmental Management*, vol. 1, no. 2, Elsevier Inc., 2017, pp. 57–75.

[3] C. K. Davis and E. Rosenblum, *Sustainable Industrial Water Use: Perspectives, Incentives, and Tools*. IWA Publishing, 2021.

[4] Y. Hou, C. Gan, R. Chen, Y. Chen, S. Yuan, and Y. Chen, "Structural characteristics of aerobic granular sludge and factors that influence its stability: A mini review," *Water*, vol. 13, no. 2726, 2021, doi: 10.3390/w13192726.

[5] E. J. H. van Dijk, M. Pronk, and M. C. M. van Loosdrecht, "A settling model for full-scale aerobic granular sludge," *Water Res.*, vol. 186, p. 116135, 2020, doi: 10.1016/j.watres.2020.116135.

[6] B. Sizirici and I. Yildiz, "Simultaneous removal of organics and metals in fixed bed using gravel and iron oxide coated gravel," *Results Eng.*, vol. 5, p. 100093, 2020, doi: 10.1016/j.rineng.2019.100093.

[7] M. Mozaffari Majd, V. Kordzadeh-Kermani, V. Ghalandari, A. Askari, and M. Sillanpää, "Adsorption isotherm models: A comprehensive and systematic review (2010−2020)," *Sci. Total Environ.*, vol. 812, p. 151334, 2022, doi: 10.1016/j.scitotenv.2021.151334.

[8] S. Al-Asheh, M. Bagheri, and A. Aidan, "Membrane bioreactor for wastewater treatment: A review," *Case Stud. Chem. Environ. Eng.*, vol. 4, p. 100109, 2021, doi: 10.1016/j.cscee.2021.100109.

[9] S. A. Deowan *et al.*, "Design and testing of a pilot-scale submerged membrane bioreactor (MBR) for

textile wastewater treatment," *Appl. Water Sci.*, vol. 9, no. 59, 2019, doi: 10.1007/s13201-019-0934-8.

[10] C. Y. Hu *et al.*, "Kinetics and model development of iohexol degradation during UV/H2O2 and UV/S2O82− oxidation," *Chemosphere*, vol. 229, pp. 602–610, 2019, doi: 10.1016/j.chemosphere.2019.05.012.

[11] A. Rubio-Clemente, E. Chica, and G. A. Peñuela, "Kinetic Modeling of the UV/H2O2 Process: Determining the Effective Hydroxyl Radical Concentration," in *Physico-Chemical Wastewater Treatment and Resource Recovery*, 2017, pp. 19–37.

[12] P. K. Pandis *et al.*, "Key Points of Advanced Oxidation Processes (AOPs) for Wastewater, Organic Pollutants and Pharmaceutical Waste Treatment: A Mini Review," *ChemEngineering*, vol. 6, no. 8, 2022, doi: 10.3390/chemengineering6010008.

[13] F. Hashemi, H. Hashemi, M. Shahbazi, M. Dehghani, M. Hoseini, and A. Shafeie, "Reclamation of real oil refinery effluent as makeup water in cooling towers using ultrafiltration, ion exchange and multioxidant disinfectant," *Water Resour. Ind.*, vol. 23, p. 100123, 2020, doi: 10.1016/j.wri.2019.100123.

[14] I. A. Tałałaj, "Performance of integrated sequencing batch reactor (SBR) and reverse osmosis (RO) process for leachate treatment: effect of pH," *J. Environ. Heal. Sci. Eng.*, vol. 20, pp. 419–429, 2022, doi: 10.1007/s40201-022-00788-0.

[15] B. Liberman, L. Eshed, and G. Greenberg, "Pulse Flow RO - The new RO technology for waste and brackish water applications," *Desalination*, vol. 479, p. 114336, 2020, doi: 10.1016/j.desal.2020.114336.

[16] D. Gaublomme *et al.*, "A generic reverse osmosis model for full-scale operation," *Desalination*, vol. 490, p. 114509, 2020, doi: 10.1016/j.desal.2020.114509.

[17] R. W. Field and J. J. Wu, "Permeate Flux in Ultrafiltration Processes—Understandings and Misunderstandings," *Membranes (Basel).*, vol. 12, no. 2, pp. 1–18, 2022, doi: 10.3390/membranes12020187.

[18] F. Yang, Z. Huang, J. Huang, C. Wu, R. Zhou, and Y. Jin, "Tanning wastewater treatment by ultrafiltration: Process efficiency and fouling behavior," *Membranes (Basel).*, vol. 11, no. 7, pp. 1–17, 2021, doi: 10.3390/membranes11070461.

[19] M. Ehteshami, S. Maghsoodi, and E. Yaghoobnia, "Optimum turbidity removal by coagulation/flocculation methods from wastewaters of natural stone processing," *Desalin. Water Treat.*, 2015, doi: 10.1080/19443994.2015.1110725.

[20] A. Rupiper, J. Weill, E. Bruno, K. Jessoe, and F. Loge, "Untapped potential: Leak reduction is the most cost-effective urban water management tool," *Environ. Res. Lett.*, vol. 17, no. 034021, 2022, doi: 10.1088/1748-9326/ac54cb.

[21] T. M. Mbavarira and C. Grimm, "A systemic view on circular economy in the water industry: Learnings from a belgian and dutch case," *Sustainability*, vol. 13, no. 3313, Mar. 2021, doi: 10.3390/su13063313.

[22] L. Huang, L. Zhen, and L. Yin, "Waste material recycling and exchanging decisions for industrial symbiosis network optimization," *J. Clean. Prod.*, vol. 276, p. 124073, 2020, doi: 10.1016/j.jclepro.2020.124073.

[23] K. B. Aviso, A. Laddaran, and J. S. Ngo, "Modelling Stakeholder Goals in Industrial Symbiosis," *Process Integr. Optim. Sustain.*, vol. 6, pp. 543–558, 2022, doi: 10.1007/s41660-022-00226-6.

[24] W. S. Ashton, M. R. Chertow, and S. Althaf, "Industrial Symbiosis: Novel Supply Networks for the Circular Economy," in *Circular Economy Supply Chains: From Chains to Systems*, 2022, pp. 29–48.