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N E W S

PROCESS SIMULATION — DIGITAL TWINS OF WATER TREATMENT PLANTS

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INTRODUCTION

Pure water does not naturally exist on this planet, as all water resources are mixtures of water with other substances. The mixtures range from almost pure water in rain or ice caps to water containing high loads of salts, biogenic, and industrial matter. Clean and pure water; however, is not only vital as a primary source of life but has an impact on nearly every sustainability goal and development target of a society.

Traditionally, different approaches and parameters are used to characterise the composition of water mixtures in the potable, sewage, or industrial sectors. However, due to the pollution of the natural sources as well as the increasing demand for water reuse, a common language and denomination must be found. This common language supports the characterisation and comparison of different water types and its use/reuse

across the industries.

“Process simulation is a model-based representation of chemical, physical, biological, and other technical processes and unit operations in software. Basic prerequisites for the model are chemical and physical properties of pure components and mixtures, of reactions, and of mathematical models which, in combination, allow the calculation of process properties by the software” (Wikipedia contributors, 2021).

In plant design, process simulation is used to model the treatment process and to calculate the relevant mass end energy balances. Based on these balances, the process can be evaluated in terms of the energy and chemical consumption as well as the by- product and waste flows. Those balances also form the basis of the treatment plant’s Total Cost of Ownership (TCO) and the plant’s ecological footprint.

Lately, such model-based representation is also referred to as a digital twin (Wikipedia contributors, 2022), which can contribute to the entire lifecycle of a treatment plant.

Considering the fact that wastewater treatment plants alone consume between 1-3% of the total energy consumption globally, the consideration of the lifecycle impact of plants is of key essence (Circular Economy: Tapping the Power of Wastewater, n.d.).

In general — in light of recent energy price increases as well as the necessity to reduce the energy consumption in terms of externally supplied energy (vs. energy recovery and sustainable energy components in situ), these concepts have increased in importance.

However, whereas commercial software tools are available for process simulation in selected industries. e.g. the petrochemical or power industry or municipal wastewater treatment, there is still demand for such tools for water engineering in general. Here, one main bottleneck is the missing universal model for the composition of water mixtures, as mentioned above.

DEVELOPMENT OF A NEW PROCESS SIMULATION TOOL

UNIHA provides water treatment solutions for all sectors and industries. Our mission is to provide our customers with solutions that are optimised for their individual case.

Process simulation enables us to create those solutions and, together with the simulation specialists from SIMTECH (https: //www.simtechnology.com/cms/), we have developed a relevant software tool.

In the first step, we have defined a model for the composition of water mixtures. Water mixtures are composed of pure water (H2O) and non-water matter. This matter can comprise of almost all of the chemical elements as well as inorganic and organic molecules and aggregates:

- Inorganic ions, e.g. Na, Cl, HCO3, CO3, Ca, Mg...
- Inorganic gases, e.g. O02, CO2, NH3, H2S...
- Inorganic solids, e.g. CaCO3, SiO2, metal hydroxides...
- Organic molecules, e.g. methane, phenol, cyanide, pesticides, hormones...
- Organic macromolecules, e.g. carbohydrates, nucleic acids, proteins, lipids, mineral oil...
- Microorganisms, e.g. virus, bacteria, phytoplankton...
- Aggregates/Macroparticles: seaweed, plastic, hair...

It is impractical to balance all of the distinct elements for a treatment process, hence sum parameters are being used. We propose to define the composition by chemistry (inorganic/organic) and physical appearance (dissolved /suspended). This leads to the following composition matrix for the non-water matter (all variables in mg/kg of water):

	inorganic	organic	total
dissolved	IM_d	OM_d	W_d
suspended	IM_s	OML_s	W_s

In the second step, we have developed a model for the mixture mass density (p, kg/ m^3) and heat capacity (c_P J/kg/K) as a function of the composition model above. Both properties are required to describe the mass and energy balances.

Furthermore, we have investigated how to correlate the composition model with commonly used parameters such as Total Dissolved Solids (TDS), Dissolved Inorganic Carbon (DIC), Dissolved/Total Organic Carbon (DOC/TOC), Chemical Oxygen Demand (COD) and the elemental composition of Carbon-Nitrogen-Oxygen. These correlations allow for the input of field data from water analysis to the process simulation.

The third step was the modelling of the unit operations, i.e. the single treatment steps used for water treatment. For the first software version, we implemented the mass and energy balances for the following unit operations:

- Sedimentation
- Flotation
- Chemical and biological reactors
- Membrane and bed filtration
- Adsorption and ion exchange
- Reverse osmosis
- Sludge thickening and dewatering
- Heating/cooling
- Tanks, pumps, mixer/splitter

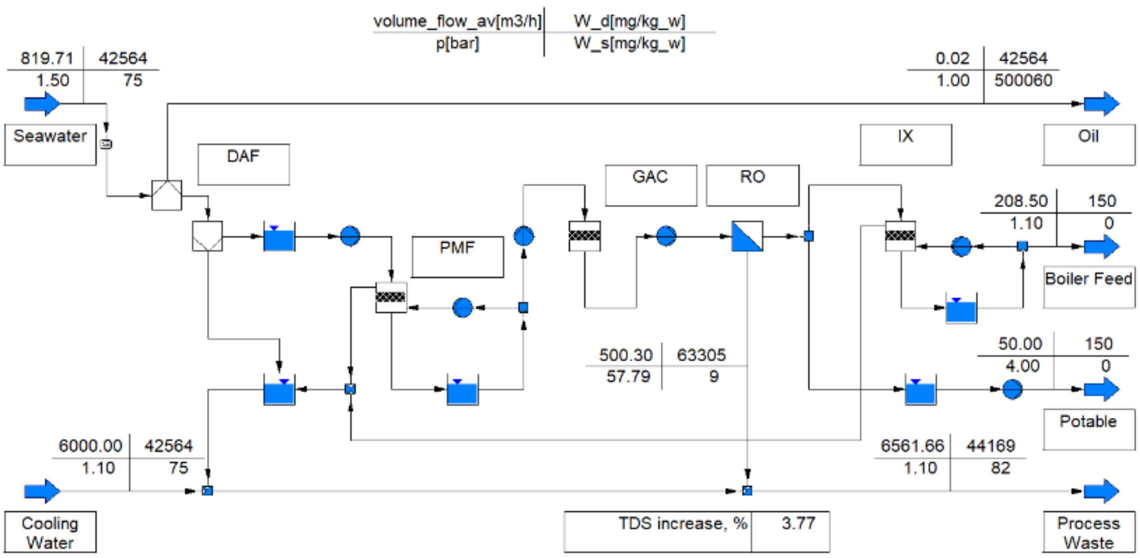


Figure 1: conversion of seawater to boiler feed and potable water; unit operations: dissolved air flotation (DAF), pressure media filter (PMF) with backwash, granular activated carbon filter (GAC), reverse osmosis (RQ), ion exchange (IX), buffer tanks, pumping

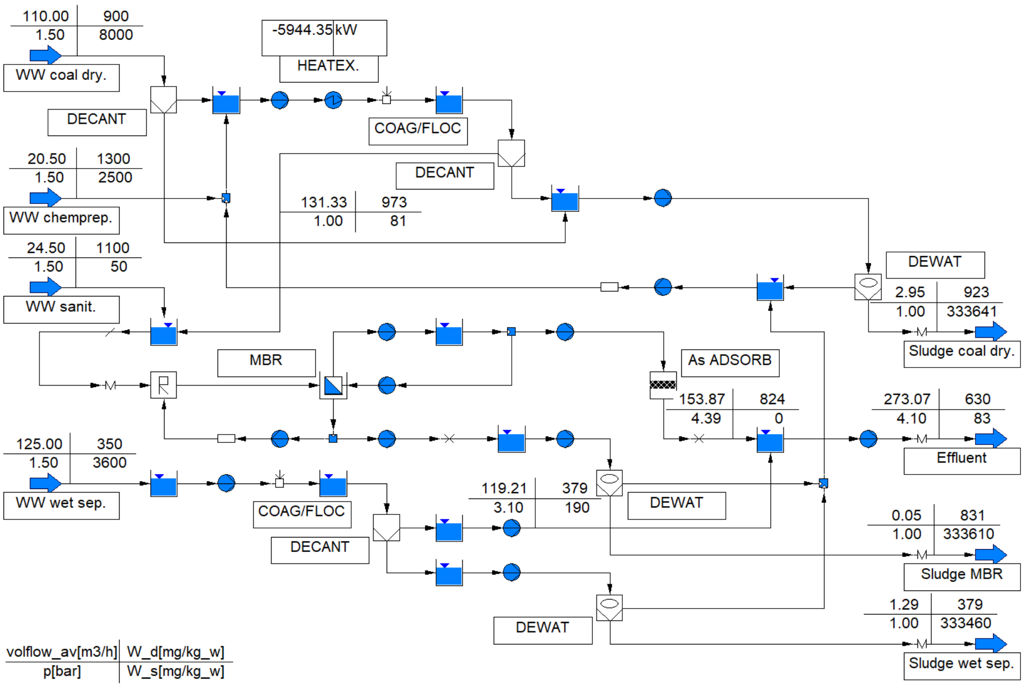


Figure 2: conversion of coal processing waste water for reuse or river discharge; unit operations: cooling (HEATEX), coagulation/flocculation (COAG/FLOC), sedimentation (DECANT), membrane bioreactor (MBR) with backwash, arsenic adsorber (As ADSORB), sludge dewatering (DEWAT), buffer tanks, pumping

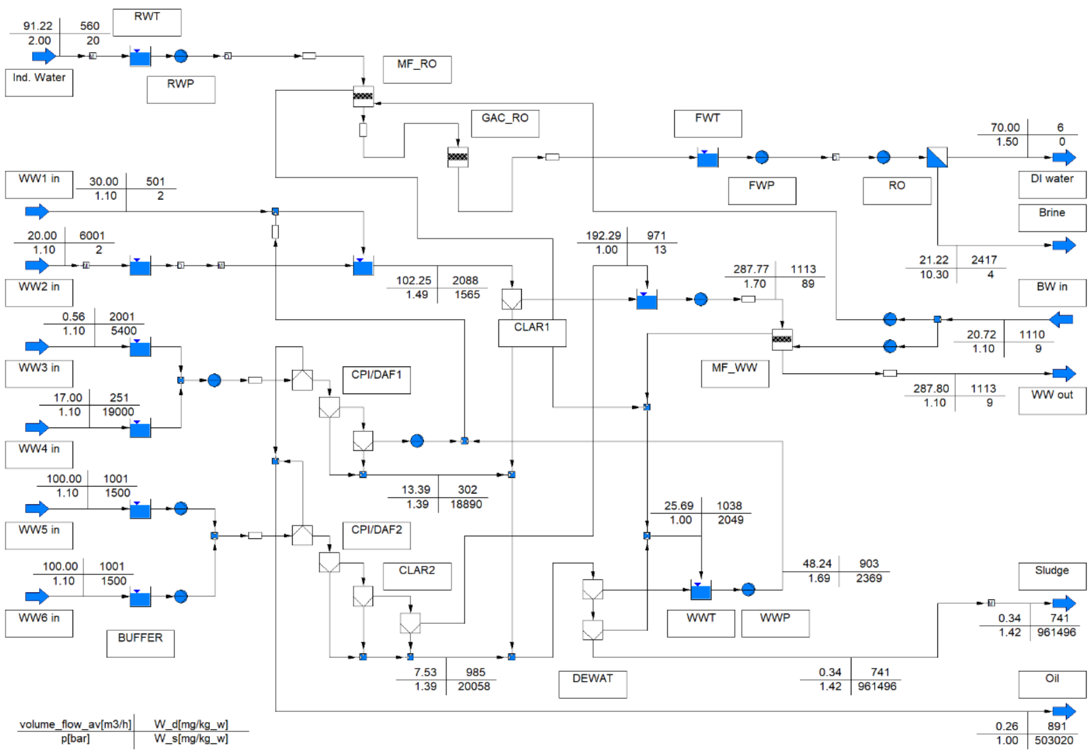
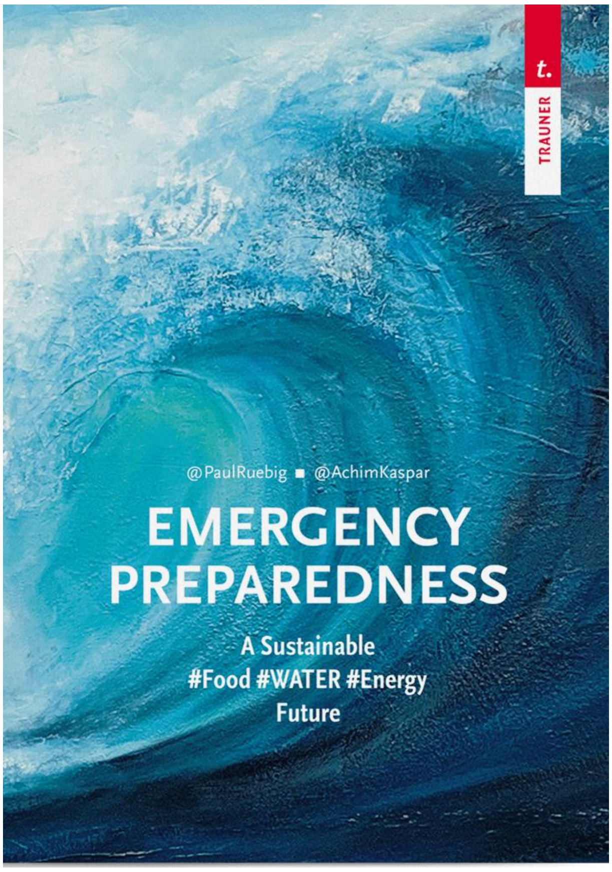


Figure 3: conversion of steel mill waste water for river discharge and conversion of river water to cooling system makeup; unit operations: oil separation (CPI), dissolved air flotation (DAF), pressure media filter (MF) with backwash, granular activated carbon filter (GAC), reverse osmosis (RO), sedimentation (CLAR), dewatering (DEWAT), buffer tanks, pumping

The resulting tool allows for the prediction of the mass and energy balances for every type of water treatment process; hence it forms the process digital twin: First, the process is built graphically by arranging icons resembling the unit operations and connecting them by lines resembling the streams of matter. Next, the user needs to enter the basic settings such as composition, pressure, and temperature of the incoming streams or performance parameters for the unit operations. In the last step, the underlying equation system is solved and the simulation results are displayed.

We presented selected UNIHA cases where the tool was used to identify the optimum treatment scheme and to provide the required data to design the plant equipment.



CONCLUSION AND OUTLOOK

The process simulation tool we have developed allows us to create better solutions for our clients and to move and act quicker. This gives us a clear competitive advantage and serves as a unique selling point. On a meta-level, our simulation tool also allows for a better understanding of mass-energy balances and, hence, quickly gives a base information which can serve to develop energy efficiency strategies, touchpoints for circular economy approaches, and holistic concepts for water resource management.

In light of a growing demand for clean water as well as possible add-on-usages forby-products from water treatment, such holistic concepts also gain more and more importance in an economic and business sphere. These add-on and re-use scenarios, e.g. brine mining for lithium, could yield business models which not only consider water treatment as such but also alternative options for the exploitation of by-products and,hence, a better Total Cost of Ownership balance of the total water treatment facility.

The future might also see a commercially available version of the simulation tool as well as the further integration of the process digital twins in the control and operation of UNIHA plants, e.g. the validation of field data with process simulation results.

SOURCES

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