Servitized cloud-based simulation of evaporation plants: model-based design tools supporting circular bioeconomy

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Abstract. Continuous industrial processes will play a key role for the sustainable transition worldwide. Different flows of matter and energy must be recovered through these systems and integrated in a Circular Economy fashion. To foster in such a virtuous trend the involvement of companies, mostly SMEs (often lacking critical assets, funds, technologies or knowledge), the continuous processes should be packaged, servitized and marketed as plants-as-a-service. Model-based design (MBD) tools can provide test before invest and decision support in the feasibility and procurement phases, as well as optimization and self-diagnosing during operation, in a cyber-physical system (CPS) setting. To ease their provision, a cloud-based collaboration platform, enabling providers to deploy tools in a sandbox, has been developed by the HUBCAP project. The purpose of this paper is to introduce the web application tool built for the evaporation process simulation, validated against real-world performance data for the reference evaporation plant, and deployed to the HUBCAP platform. To structure it, data collection, filtration, processing, and reporting have been performed on the full-scale pilot plant (the EVAPOSIM experiment), a triple-effect evaporator operating in counterflow and vacuum condition. To explore the sustainability of their plant, companies can use this MBD tool through the sandbox of the HUBCAP platform under a servitized (use- or result-oriented) business model (software as a service).

Keywords: bioeconomy, circular economy, model-based design, evaporation plant, digital platform, sandbox, product-service systems, software as a service.

1 Introduction

Continuous industrial processes (e.g., biogas upgrading (Vo *et al.*, 2018), hydrogen as energy carrier (Turner, 2004), industrial wastewater recovery (Gherghel, Teodosiu and De Gisi, 2019) can play a key role for the sustainable transition worldwide. Different flows of matters and energy are indeed intended to be recovered through these systems under a Circular Economy (CE) and Bioeconomy fashion (D'Adamo *et al.*, 2022). To foster in such a virtuous trend the involvement of companies, mostly SMEs (often lacking critical assets, funds, technologies or knowledge) and push the transitioning of manufacturing plants into a cyber-physical system (CPS) setting, it becomes essential to provide test before investing tools (Macedo *et al.*, 2021). Enriched with digital model-based design (MBD) tools (Larsen *et al.*, 2020), such tools can provide decision support and can help to find the most suitable set-points to optimally use the infrastructure under analysis in multiple domains (e.g., energy management (Badicu *et al.*, 2021), manufacturing process (Weiß *et al.*, 2021), real-time optimization (Greppi, Bosio and Arato, 2008)). To ease their provision, a cloud-based collaboration platform, enabling tool providers (companies, research organizations, and Digital Innovation Hubs (DIHs)) to deploy tools in a sandbox (Larsen *et al.*, 2020), has been developed by the HUBCAP project (*HUBCAP project*, 2020). For example, concerning evaporation process, once the plant has been designed and implemented, the main issue is to understand how to make it run efficiently, through a decision-making system to look at daily operation in real time able (Krämer and Engell, 2018). However, even simpler solutions are still needed and also a visualization interface able to easily show results to the human operators needs to be developed to involve them into the decision-making process. In addition, such a tool has not been tested on-line. Therefore, the purpose of this paper is to introduce EVAPOSIM, web application tools built for the evaporation/electrolysis process simulation, validated against real-world performance data for a reference evaporation plant, and deployed to the HUBCAP platform. To explore the sustainability of their plant, companies can use this MBD tool through the sandbox of the HUBCAP platform under a servitized (use- or result-oriented) business model (software-as-a-service (SaaS)). The paper is structured as follows. Section 2 introduces the concept of (bio-) economy in the evaporation plants context and the servitized digital platform deploying MBD to develop CPS. Section 3 presents the research methodology, detailing how the tool has been built based on data collection from a real case. Section 4 presents the tool and Section 5 discusses its functionalities. Finally, Section 6 concludes the paper.

2 Research context

2.1 Evaporation plants and Circular Economy

Industrial wastewaters and landfill leachates are among the most polluted water steams produced by human activity. They can be treated with a combination of several processes (membrane separation, electrochemical and physicochemical processes), to recover a concentrated solution to be disposed of and a purified water stream. Evaporation is one of those treatment processes, whereby a more concentrated solution is obtained from a more dilute solution by evaporation of the solvent, i.e. in the case of wastewater treatment the water. In this sense, the terms evaporation and concentration are often used synonymously. The input is the diluted solution, the output is the evaporated solvent and, as a residue, the concentrated solution. The concentration of the final solution depends on the amount of evaporated solvent. Evaporation requires large amounts of low-thermal-level heat, required to boil off the solvent and then remove it as vapor from the solution that is gradually becoming concentrated. The relevance for the CE of evaporation applied to the treatment of landfill leachates is twofold. From one hand the purified water can be reused following the CE principles, in relation to its specification preferably as a feedstock or auxiliary in industrial processes or on the landfill site itself. On the other hand, the low-thermal-level heat can be obtained by recovering thermal wastes elsewhere on the site, for example the thermal exhaust from a cogeneration plant fed with the locally produced landfill gas.

2.2 Servitized Digital platforms: Model-based Design models and tools

The HUBCAP project developed a collaboration platform, based on the DIHIWARE collaboration platform (a web portal offering several social collaboration features already used in previous European funded projects), under the shape of a web-portal offering portfolios of services and MBD assets (models and tools) to be adopted in the CPSs' development. These services and assets are offered for experimentation in a test before invest approach through a sandbox enabling users to access them in a ready to use way. The platform aims at attracting end-users interested in adopting MBD assets, aggregating them in a community composed of DIHs, providers of MBD assets and developers of CPS solutions. Through its platform, HUBCAP is providing several streams of funding to lower entry barriers for European SMEs interested in adopting MBD in the development process of their CPSs. However, in the future, the use of the HUBCAP platform will be open to a wider worldwide user base community of MBD asset providers and consumers, offering assets according to a SaaS business model.

3 Research Methodology

To develop the tool, data collection, filtration, processing, and reporting have been performed on the full-scale pilot plant (the EVAPOSIM experiment), a triple-effect evaporator operating in counterflow and vacuum condition. Over 40 sensors, distributed throughout the whole process, collect data and load them into the plant supervisor system and can be easily retrieved by plant operator and manager. The evaporation plant is installed close to a landfill that collects municipal solid waste and non-hazardous special waste. The flow scheme of the plant and its top view are shown in Figure 1 and 2.

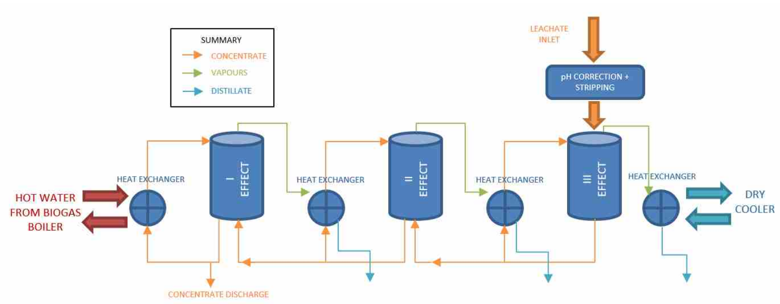


Fig. 1. Flow scheme of the evaporation plant in object [credits: NBT Bulgaria EOOD]

Fig. 1. Evaporation plant: top view [credits: NBT Bulgaria EOOD]

The landfill produces approximately 280 t/day of leachate characterized by high concentrations of chemical oxygen demand, ammonia, heavy metals, perfluoroalkyl substances and chlorides. The leachate is first treated with a reverse osmosis plant, producing about 208 t/day of permeate with characteristics suitable for discharge into surface waters and 72 t/ day of retentate which is sent to the evaporation plant with a dry matter concentration of about 3.5%. The quantity of distillate produced is approximately 60 t/ day, while the final quantity of concentrate with a Dry Matter (DM) concentration of approximately 20% is 12 t/ day. The distillate in this case is recirculated to the head of the osmosis plant, but could be reused after conditioning in the industrial processes.

3.1 Data selection and criteria

The evaporator plant has installed a set of sensors and instruments that are fundamental to control the evaporation process and help to analyse its status. All the plant works on functional logics that control its automatism: these logics are written into the Programmable Logic Controller (PLC) control system. The Supervisory Control And Data Acquisition (SCADA) system is the interface between the operator and the control systems PLC. The plant operator works on SCADA pages, the human-machine interface able to control the plant process to change some set points and to take the data necessary for work. The data recorded by the system are temperatures, flow rates, density, electrical conductivity, pressures, and other parameters. All these data are stored in the SCADA and are graphed for immediate viewing at the operator panel or with remote access to the plant. The data used for the EVAPOSIM experiment refer to the year 2020, during which the plant was in the start-up and commissioning phase and different plant operating modes were possible (making data collection accurate and verified on site).

3.2 Data extraction preparation, filtering and range definition

The data collected by SCADA are saved into external storage unit that can be taken directly from operator panel, or, for a more specific analysis, extracted from storage unit and copied to a PC into a .csv file (containing max. 500k records). When the file unit is full, a new one is created by SCADA and new data are saved. Given the large amount of data to be processed, it was decided to process these files in spreadsheets. It is also essential to choose which measuring instruments are of interest for the model validation. The purpose of data selection was to find data that can be assumed acceptable for the EVAPOSIM project. Data preparation and filtering is an important step prior to processing and involves reformatting data, making corrections to data and the combining of data sets. The selected data are:

- Temperature, to understand the heating status of the plant, the heat exchange efficiency in the heat exchangers, the operating temperature of effects.
- Pressure, regulating the evaporation process, connected with temperature of all the system (with lower pressure value the effect needs less temperature to evaporate).
- Volume of inlet and outlet, to define the evaporator concentration performance.
- Density of concentrate, controlling the discharge set point of concentrate and it is connected to the %DM.
- Electric conductivity of distillate, showing the “quality” of distillate, the amount of salts inside the distillate and so the purity of the evaporate.

It is possible to look at the different modes of operations where specific days and precise times were chosen to analyse the functionality of the plant. During these periods there was a precise control of the plant by specialised technicians, who were able to validate the accuracy of the instrumental measurements and plant operativity. In addition, the evaporator was performing adequately without any anomalies and the data was in line with the design performance. All these indications allowed to validate the parameters recorded in different operating conditions. To make useful the chosen modes of operations for software development, operating windows during the designated running day were identified, choosing working windows as steady state of the plant.

4 Results

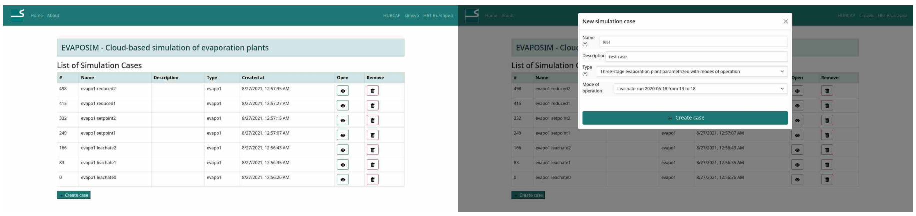
The EVAPOSIM experiment was run to enable the cloud-based simulation of evaporation plants and deliver the related web-app. The simulation approach used is:

- first-principle-based: the behaviour of the physical system is described a-priori using fundamental laws (e.g., mass and energy conservation) and empirical engineering correlations from textbooks and literature (e.g., reaction kinetics),
- steady-state: the process is assumed in steady operation, i.e. all intensive variables and the fluxes of extensive properties are constant in time (so unsuitable for transients processes, control system design, or processes inherently unsteadily operating),
- concentrated-parameters: it is assumed that each unit can be represented as a homogeneous portion of matter (this drastic simplification is widely employed in process engineering, most in the Continuously Stirred Tank Reactor (CSTR)),
- process simulation: the scope of the simulation is an entire process or plant unit (not a single device), accepting coarse-grained, less detailed results in exchange.

The application of this simulation approach to continuous evaporation plants is well-established and gives accurate results. In a previous project, the LIBPF™ process simulation technology was successfully used to model a triple-effect evaporator operating in counterflow and vacuum conditions during the design phase. This process model was the starting point of this work and was validated against real-world performance data (collected, filtered, and pre-processed from a reference evaporation plant in operation).

4.1 Web applications

The EVAPOSIM and ELYSIM web-apps are simple-to-use, customized web applications for the cloud-based simulation of the evaporation plant and the demo process respectively. They make the process models more accessible so that non-experts can prioritize and optimize decisions in the proposal and design phases of new plants. Both are based on pretty much the same code base and work in a similar way. The users can configure simulation cases (full load, partial load, high concentration …), run simulations, and graphically examine results. Figure 3 reports screenshots of the web-app.



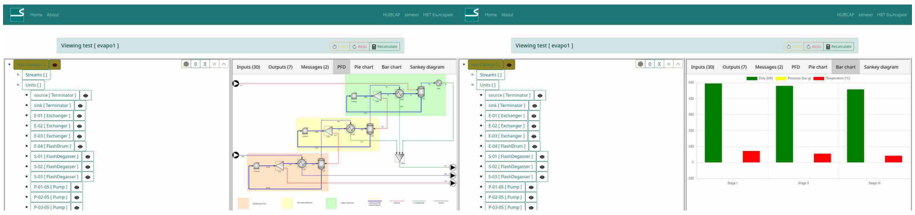


Fig. 1. Top-left: start page of the EVAPOSIM web-app; Top-right: new case creation form of the EVAPOSIM web-app; Bottom-left: case detail page of the EVAPOSIM web-app with PFD view; Bottom-right: case detail page of the EVAPOSIM web-app with bar chart view.

4.2 Demo process model

The demo process model has been deployed to the HUBCAP platform a demo instance of the web application so that new adopters can test it and evaluate its suitability for their customized applications. Three requirements for the demo process model have been defined (1. it should be relevant to perspective adopters; 2. It should be non-confidential and validated against publicly available data; 3. It should be easy to grasp).

Based on a screening of the continuous industrial processes in relation to the CE, renewable hydrogen electrolysers have been identified as most relevant. Electrolysis is an electrochemical process that uses direct electric current to drive an otherwise non-spontaneous chemical reaction, such as the decomposition of water in hydrogen and oxygen. Alkaline water electrolysis employs Nickel-based electrodes separated by a diaphragm (to make sure the product gases are separated), and immersed in a concentrated alkaline solution of potassium hydroxide as electrolyte, and does not require the costly and rare precious metals as catalyzers. Alkaline water electrolysis plants are operated under pressure (typically 30 bar) and at mild temperature (around 60 – 90 °C). Currently, this is the most mature electrolysis technology and it is commercially available up to the range of 10-MW plants. Therefore, the alkaline water electrolysis was implemented as demo process and validated (Sánchez *et al.*, 2020).

5 Discussion and Conclusions

This paper reports the work conducted to develop EVAPOSIM/ELYSIM, the cloud-based simulation tools of evaporation/electrolysis plants into a cloud-based platform. It enables the cloud-based process simulation of evaporation and alkaline water electrolysis plants via a simple-to-use, customized web application, making the process model more accessible so that non-experts can prioritize and optimize decisions in the proposal and design phases of new plants. The process model can be used in all phases of a project: in the feasibility phase to estimate plant size and capital costs; in the proposal phase to estimate operating costs (mainly electrical and thermal energy consumptions) and key performance parameters (conversion efficiency and hydrogen production); in the design phase to guide the equipment sizing and selection; in the operator training phase, to help bring up to speed the operators on the new technology; during operation for on-line monitoring to troubleshoot and optimize the plant. The development of the tool started taking as reference an evaporation plant installed into a landfill that collects municipal solid waste and nonhazardous special waste. The tool will be provided in a cloud asset (the HUBCAP platform), to impel its function of testing before invest for a wide range of evaporation plants. Its use should facilitate users to realize the actual effects of CE and Bioeconomy, giving evidence of which could be the flows of materials and energy related to a specific setting of the plant and of the wastes adopted. Indeed, the main outcome for the users will be the very fast evaluation of the economic and environmental sustainability of the plant analyzed before investing in a specific technology. On the other side, the usage of this tool in a cloud-based environment concurs at facilitating and impelling the provision of such MBD simulation tools through a PSS business model. Indeed, the tool provider can offer the SaaS, obtaining revenues based on its use or result. In addition, the paper aims at facilitating the adoption of other tools and at attracting other models and tools interested in finding new partners and applications in the energy domain. The main future work could be the implementation of the functionality of collecting real-time data from the sensors, obtaining a digital twin of the plant. This could first support the internal measurement of the circular flows going through the plant and second trigger a more effective alignment of the plant resources with its external stakeholders, paving the way towards a Circular Bioeconomy community (D'adamo and Sassanelli, 2022) . Finally, the two main issues to be faced to exploit these tools are the need of dedicated company divisions to … and the necessity to transfer the knowledge and experience of the experts operating on the plants to feed its automated system. Therefore, a new business model is needed where software providers became the integrator of those advanced systems. In this context, a big contrast is raised between SMEs (typically flexible) and big companies (instead rigid).

Acknowledgments

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