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Digital Shadow of a Pilot Scale Packed Batch Distillation Column for Real-Time Operator Training- and Support

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ABSTRACT

Digital twins and digital shadows are frequently used terms by industry and academia to describe data-centric models that accurately depict a physical system intended for process monitoring and control. Processes restricted by a low degree of automation rely greatly on operator competencies in key decision-making; a digital shadow can here assist as a guidance tool [1-4]. This work presents a practical implementation of a digital shadow to support operators running a pilot scale-packed batch distillation column at the Technical University of Denmark (DTU) primarily used in education and teaching activities [5]. This operation is selected due to inherent unsteady process dynamics that are controlled by a set of manual valves, which the student operator must continuously balance to meet purity constraints without disrupting the operation. This realisation employ a modular software architecture, separated into four distinct modules compiled into Docker images and independently deployed. These facilitate real-time connection with the equipment via OPC-UA endpoints, process model analysis via HTTP/HTTPS requests, and a dashboard UI presenting the data accessible through any web browser. The final module is realised as a Python package that stores thermodynamic models and is published on the internal GitLab registry for more straightforward utilisation across multiple projects. The advantages of this implementation strategy are flexibility and speed, allowing for continuously updating process models and directly employing them in various projects.

Keywords: Digital Shadow, Industry 4.0, Operator Support, Pilot Scale, Packed Batch Distillation

INTRODUCTION

Today, digitalisation and Industry 4.0 are terms used prolifically in chemical- and biochemical engineering research. It describes various activities that ultimately focus on expanding automation and optimisation in different aspects of manufacturing and research processes. Enhancing data contextualisation and application of data-driven methods in process development and regular operation are both activities associated with digitalisation [1]. Today, the most common and significant barriers to implementation of digitalisation concepts relates to an immature digital infrastructure, data security concerns and complex systems integration. This makes data consolidation and utilisation across various sources challenging and restrict the compliance with the Internet of Things (IoT) and Big Data architectures [2]. Since the digital twin and digital shadow concepts rely heavily on these enabling technologies in practice, most chemical and biochemical manufacturers are generally committed to improving or expanding their respective digital infrastructure [1]. However, there is still an overall challenge in correctly scoping and quantifying the cost/benefit of these digitalisation projects which limit widespread adoption [1-4]. For systems of a lower automation level that rely heavily on employing operators in crucial operation steps, there is an increased focus on developing methods and tools that assist the operator in decision-making during operation [5]. In this work such example is developed for a digital shadow that is intended as support for student operators in an education setting for a pilot scale batch distillation process. Batch distillation is an old and proven volatility-based separation technology that is most frequently employed today in alcoholic beverage production and in the recovery of aromatic compounds and solvents [6]. These processes exhibit a

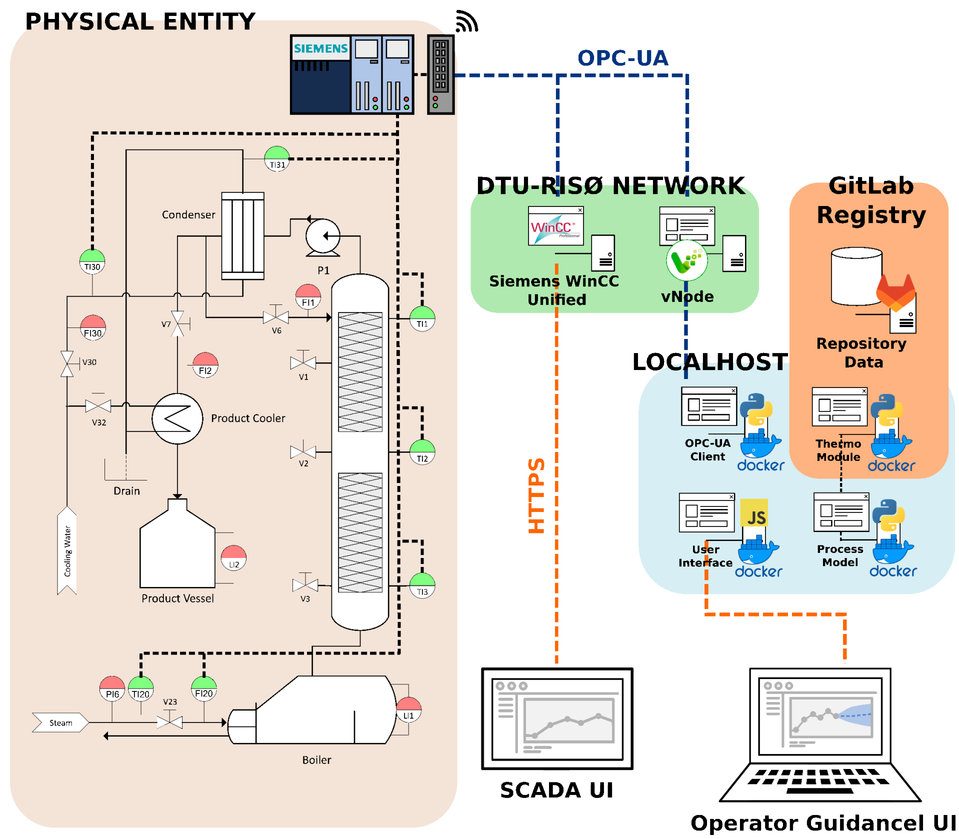

Figure 1: The P&ID of the packed batch distillation column at DTU-KT. The connection to the central digital infrastructure is also displayed, and all digital signals are denoted with dashed lines. The digital shadow modular architecture is also depicted with the installable module dependency connected to the central GitLab registry.

continuous transient behaviour as the product is extracted from the otherwise closed system. While most processes have automated flow control and duty utilisation, the central operation is dictated by the operators who specify desired reflux ratios. The Department of Chemical Engineering at the Technical University of Denmark (DTU-KT) manages a manually operated pilot scale packed batch distillation column primarily employed for education purposes and solvent recovery. The unit is included in the digital retrofitting activities described by Jones et al. in 2022 [7].

MATERIAL AND METHODS

The pilot scale packed batch distillation column at DTU-KT separates a well-documented water-ethanol binary system that forms a high-boiling azeotrope at approximately 92 mol% ethanol. The exercise aims to teach engineers about managing flow rates, reflux ratios, and heating/cooling duty to collect an ethanol product of sufficient purity. The pilot scale equipment consists of a 100L steam-heated boiler (T1) connected to a glass column with an inner diameter of 10 cm. The column is fitted with Mellapak™250Y for a total height of 1.68 m. Atop the column sits a total condenser connected to a pump (P1) that returns the condensate to the column as reflux or to a product tank (T2). The unit is augmented with a total of 13 sensors, of which 6 x temperature (TI) sensors and 1 x flow meter (FI) are logged online with an additional 3 x flowmeters, 2 x level indicators (LI) and 1 x pressure sensor (PI) are read by operators offline. The simplified PI&D for the setup is presented in Figure 1. The initial boiler contains a mixture of approximately 80L 30w% Ethanol. The operator is responsible for manipulating the reflux ratio and the steam- and cooling duty to maximise the recovery and purity of ethanol over an operation period of approximately 2 hours at atmospheric pressure. The digital infrastructure is addressed in a later section.

MATHEMATICAL MODELS

Even though the unit operation is operated frequently at DTU-KT, the collected data is of limited usability for unit characterisation and model development. This is primarily due to vital analogue information pertaining to flow rates, liquid levels and liquid composition being omitted from the digitally stored data. Therefore, reconstructing mass- and energy balances is challenging and requires several simplifying assumptions regarding the process operation characteristics. As a result, this caveat limits the applicability of data-driven and hybrid methods due to a lack of data volume. Furthermore, since the operators are instructed to select a specific reflux ratio and keep this constant, it produces a dynamic profile that becomes very similar across experimental runs. The lack of variability in the dataset ultimately limits the effectiveness of using supervised learning methods such as neural networks to derive the operational characteristics, even if a sufficient data volume is available. This work puts emphasises on delivering mathematical models for the given process. Therefore, simple equilibrium-based models have been employed and deemed sufficiently accurate for the application. The future prospect of employing data-centric models is discussed later.

Separation of the water-ethanol binary at atmospheric pressure can confidently be modelled as an ideal vapour phase and non-ideal liquid phase using the modified Raoult's law. The mixture's vapour-liquid phase equilibrium (VLE), Antoine parameters and binary interaction coefficients are presented by Kamihama et al. [8]. The component heat capacities, densities, and latent heat of vaporisation are modelled using fitted 3rd-order polynomial functions with respect to a reduced temperature. The polynomial function is depicted in equation 1. Coefficients are fitted using saturated temperature data from CRC 101st ed.

$$f(T_r) = A + BT_r + CT_r^2 + DT_r^3 \quad (1)$$

The separation efficiency of structured packaging material Mellapak™ 250Y [9] depends on a flow number (F) calculated based on the vapour flow rate in an empty column and the vapour density shown in equation 2.

$$F = \omega \cdot \left(\frac{g}{A_c}\right) \sqrt{\frac{T}{P \cdot M_{w,g}}} \quad (2)$$

$$\text{HETP} = a \cdot \log\left[1 + F\right] \cdot \left[\frac{F}{s}\right]^p + x_0 \quad (3)$$

This is a function on the vapour flow rate in an empty column, $\omega \cdot (g/A_c)$, and the vapour's molar weight, $M_{w,g}$. The flow number takes a value in the interval 0.5 – 3.5, corresponding to packaging material attaining an equilibrium tray equivalent height (HETP) of 0.32/m – 0.45/m. This results in an expected number of equilibrium trays (NETP) between 3.73 and 5.25 for a packed column height of 1.68m. A surrogate model is fitted to the HETP curve provided by Sulzer in Figure 2. to readily determine the packaging material's separation efficiency from estimating the boil-up ratio and vapour composition. Here, the F values refer to a flow number, while the coefficients a, p, s, and x_0 are coefficients that are determined by fitting equation 3. to the data presented in the Sulzer data sheet for Mellapak 250Y packing at 960 mbar [9]. The fitted expression is presented in equation 4.

$$\text{HETP} = 0.0634 \cdot \log\left[1 + F\right] \cdot \left[\frac{F}{313}\right]^{30.3} + 0.315 \quad (4)$$

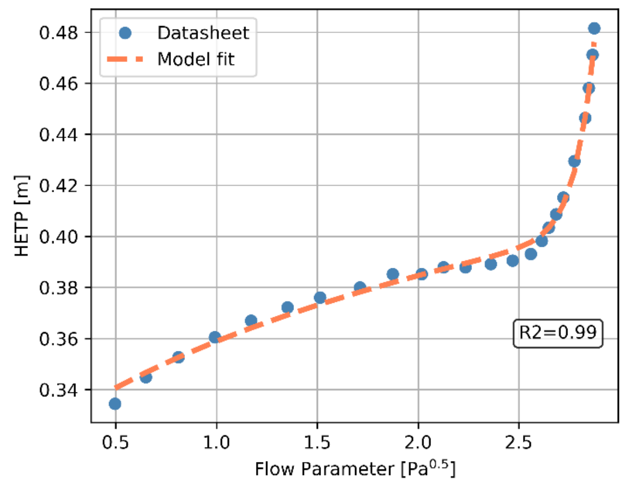

Figure 2. Reported Mellapak 250Y separation as a function of the characteristic flow number.

Currently, the operator is guessing the condensate's total volumetric flow rate and perform incremental adjustments from a visual inspection of the condenser hold-up to balance the flows. Approximating the volumetric condensate flow rate can alleviate this task while simultaneously predicting changes from boiler duty or reflux ratio modifications. This can give rise to more accurate control adjustments that allow for possibly operating at variable reflux ratios, improving the process's energy efficiency. If the steam condensation supplies only heat to evaporate the boiler mixture, the estimated vapour flow rate leaving the boiler can be readily estimated from online sensors with equation 5.

$$V_{est.} = \frac{\Delta H_{vap}^{steam} \cdot FI_{20}}{\Delta H_{vap}^{boiler}} \quad (5$$

From the vapour flow rate and estimated vapour composition, the flow number and NETP can be readily determined from the online sensor readings. In combination with user inputs regarding the reflux ratio and estimation of the condensate composition, it is possible to construct a McCabe-Thiele diagram for the operation, as depicted in Figure 4. In addition, the cooling duty in the condenser is employed to estimate energy efficiency η. It is also employed to estimate the product's composition and thereby track an estimate of the recovered liquid's purity and the remaining amount of ethanol to purify.

RESULTS AND IMPLEMENTATION

Digital shadows and digital twins are frequently attributed as flexible model realisations that satisfy multiple stakeholders across research and manufacturing and

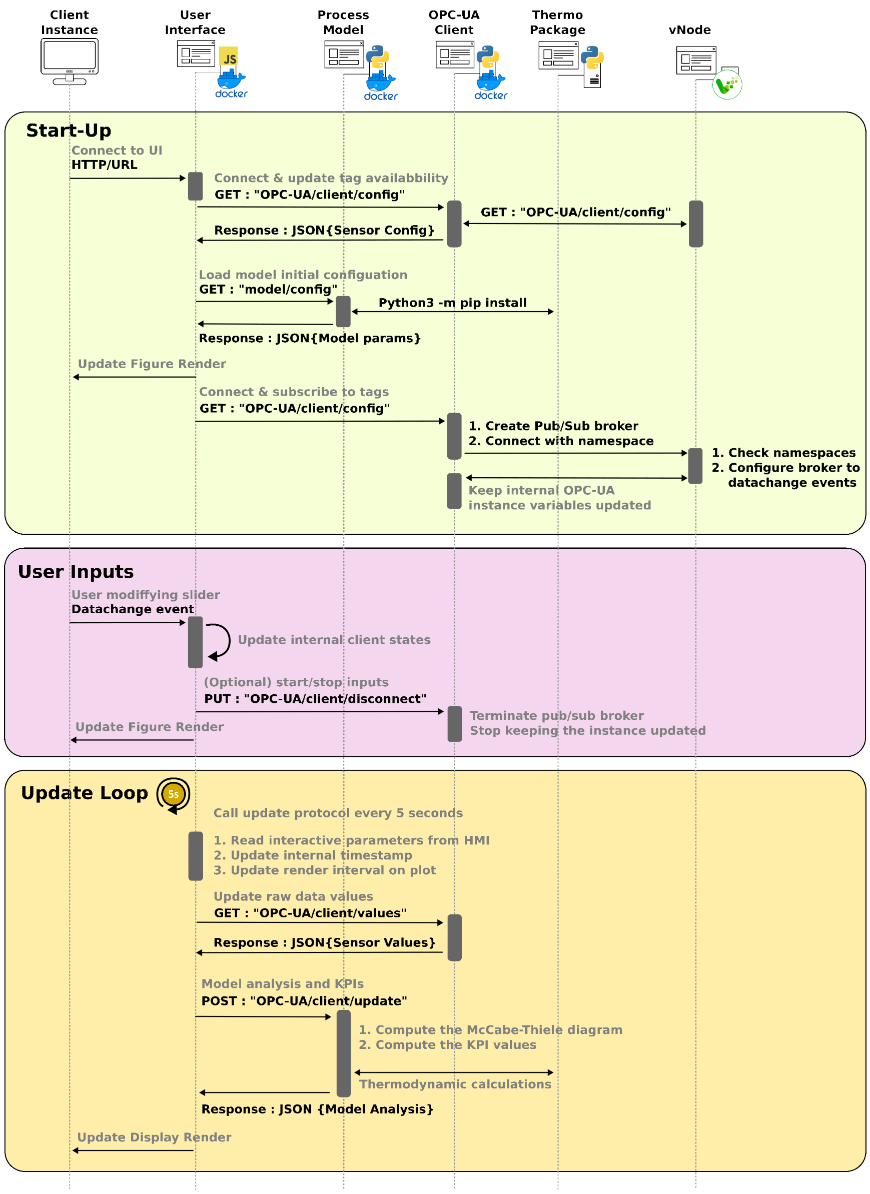

Figure 3: A summarised sequence diagram for the packed batch distillation column core functionality. Here, the various resources are depicted in a column format, with the interactions depicted as prompted connections.

interface easily with physical equipment [2,4]. Consensus is that the best approach is to follow a standardised implementation paradigm that link multiple smaller model realisations and software resources together in a central environment. This work adopts a microservice-oriented approach to realising the software implementation. In addition, the workflow adopts the DevOps development paradigm often utilised in conventional software development [10]. The various modules/services developed in this project are version-controlled using git (v2.36.1) and distributed through GitLab with continuous integration and continuous delivery (CI/CD) pipeline compiling Docker images and package installables. The software is structured into four modules, as depicted in Figure 1. Each module functionality is compartmentalised individually using Docker (v24.0.6) except the thermodynamic module, which is configured as a Python installable dependency. The Docker images are configured as a collection using Docker Compose (v2.22.0). This results in a software collection where each module can deploy independently but allows communication between modules in the collection, as depicted in Figure 3. The UI is developed using Next.js (v13.5.0) with Redux (v4.2.1) state management, Materials-UI library components and D3.js (v7.8.5) visual rendering. The connection, storage and model backend is developed in Python (v3.10.15) and deployed using the FastAPI (v0.103.2) and Uvicorn (v0.18.3) libraries. The connection manager is a general-purpose

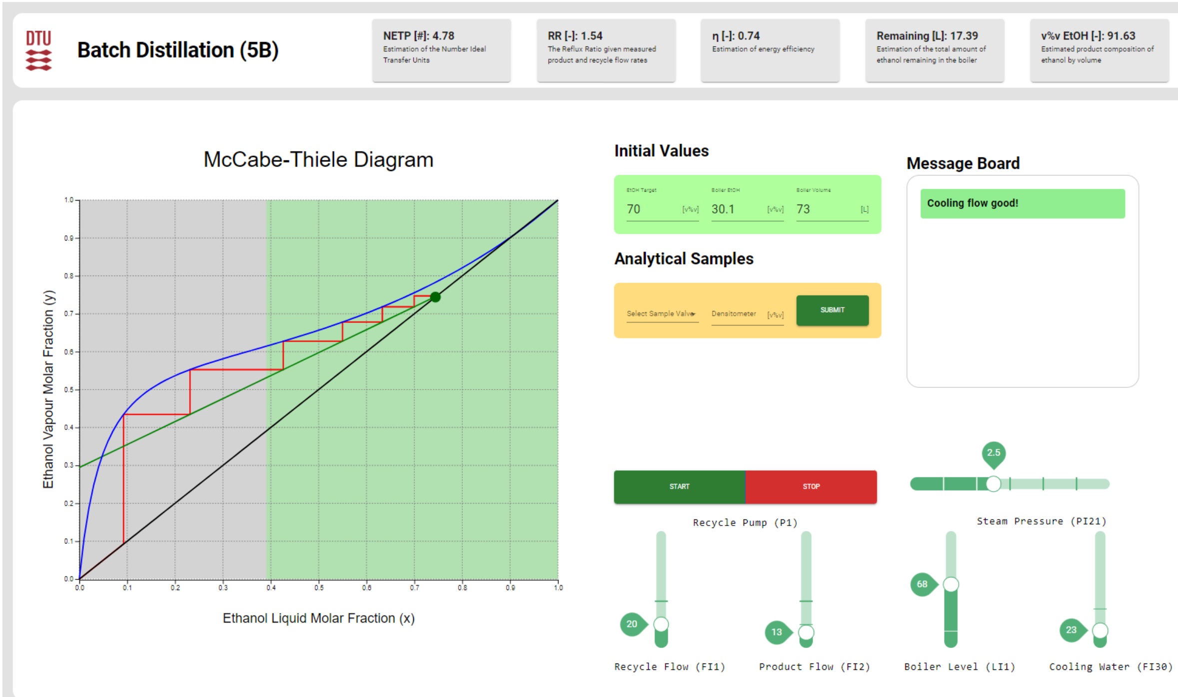

Figure 4: Screen capture of the UI for the pilot scale packed batch distillation column. This cas depicts an operation with an initial boiler content of 73 L and approximately 30 vol% ethanol.

OPC-UA client developed in Python and designed to integrate specifically with DTU-KT pilot equipment connected to the vNode intermediary [7]. The operator accesses the UI dashboard through a web browser on a device connected to the secure network. The UI then manages calls to the various API that establish connection and process model functionalities based on the operator interactions through the UI. All logic concerning model prediction and estimation is compartmentalised with Docker, and all functionality is exposed to the software architecture by a REST API construction. The UI updates the relevant elements based on user interaction and automated update loops. The operator interacts with the logic through the UI abstraction. This interface includes a graphical rendering of the current operational state with a summary of key performance indicators as a McCabe-Thiele diagram, depicted in Figure 4. A series of sliders and buttons are also presented to the operator, which she can use to update the offline sensor values quickly. The UI detects the change in slider position and sends the information to the database, where it is stored next to raw sensor inputs and model analysis. The updated user inputs are used in the succeeding API calls to provide updated trajectories on the McCabe-Thiele diagram. From the online temperature sensor measurements, the molar vapour and liquid compositions are determined for the boiler (TI04), middle column (TI02), and top of the column (TI01), assuming phase equilibrium. The online steam flow rate (FI20) and saturated steam temperature (TI20) also provide an online estimate of the applied heat duty. Combined, it is possible to estimate the boil-up rate and flow number readily. Thus, it is possible to provide an estimation of the HETP and NETP from the Sulzer reference sheet [9]. The operator can update the value of the three offline liquid flow meters depicting reflux (FI1), product (FI2) and cooling water (FI30), respectively, with a slider-based input system on the UI. Also, the boiler (LI1) and product tank (LI2) level indicators are updated with a slider input block. Additional performance metrics such as the condenser duty, reflux ratio (RR), and material balance can then be computed and displayed with the online and offline sensor measurements.

DISCUSSION

This work achieves a practical realisation of a digital shadow for a pilot scale packed batch distillation using a modular implementation approach akin to a microservice architecture which follow a modular architecture suggested in recently published literature [4,7]. In the current configuration, the thermodynamics models are implemented in parallel to the system models and separated into a dedicated thermodynamic installable package. This allows for better utilisation of these models and data across multiple projects for different processes. In this case study, the central objective is not the effectiveness and usability of the final software solution. Instead, focus is placed on the development and delivery process, evaluating the relative ease of modification and expansion to the presented proof-of-concept. With the modular implementation, updating or substituting the first-principles model, in this case, will be more straightforward if implemented as an API resource accessible with communication protocols such as HTTP/HTTPS. As data is collected throughout multiple runs and analytical data is properly contextualised and stored next to the online measurements in a digital and easy-to-query environment, complete or partial data-driven methods in state estimation will be possible in the future. The OPC-UA connection module is sufficiently generic, which has significantly streamlined integrating connection and delivery of other projects at DTU-KT. The selection of the KPIs employed in this work is based entirely on the authors' perceptions. It is important to include the users in the development loop to effectively continue the development of a digital shadow such as the one presented in this case study. Following the DevOps cycle, the next steps are operations and performance evaluation. Operator support and guidance tools do not have to be overly complicated to be effective. Since this exercise is also leveraged in chemical engineering education, the aim is equally to enhance the learning outcome of the exercise. Ideally, the more complex UI can allow the engineer to experience theoretical material employed on real systems in real-time and observe how the dynamic operation affects the various KPIs. Here, the results are largely qualitative, focusing mostly on delivering a platform that leverages the model-based and domain competencies in a format that generates value. With the infrastructure in place, a succeeding project can more easily implement new metrics or compare against future data for a quantitative assessment of the model accuracy, KPI usefulness, etc. Most of the cases explored in this area are centred on bio-based manufacturing. However, this case illustrates a modular approach to developing digitalisation tools, which can arguably be leveraged for other process types as well.

CONCLUSION

It is possible to develop and implement a digital shadow for real process equipment using the micro-service software architecture. The case study delivers a proof-of-concept digital shadow that is of an appropriate- and feasible scope given the process description. The application employs a rudimentary model that could offer some model-based support for operators running the packed batch distillation column at DTU-KT. This guidance system focuses on lowering the barrier for operators to report offline sensor values, providing the operator with enhanced insight into the operation state, and improving offline data collection. Future developments will focus on collaborating with the operators to drive the next development steps in a direction that best suits the use-case of this digitalisation tool.

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