

From Sugar to Bioethanol – Simulation, Optimization, and Process Technology in One Module

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ABSTRACT

This work gives a detailed description of the models, methods, and equipment used in a bachelor's degree lab course. The connections between simulation results and real-world data are highlighted and tools for making the models useful for process design tasks are portrayed. The models cover the production chain for fuel-grade bioethanol, starting from the fermentation of sugar with yeast. In only one semester (14 weeks with 180 minutes per week) the students achieve to produce high-purity ethanol. Some exemplary results of the process designs and their comparison to the realized intermediate and final products are given together with production cost data.

Keywords: Batch Process, Ethanol, Education, Batch Distillation, Biofuels, Data Reconciliation

INTRODUCTION

The Green Processes Lab module, part of the Green Engineering study program at Berlin University of Applied Science (BHT), trains students to simulate, optimize, and implement an industrially relevant sustainable process within a single semester. The selected process is a fuel-grade bioethanol production, with a minimum purity of 99.8 wt.%, using readily available supermarket feedstocks: sugar and yeast.

In earlier modules of the program, students engage with fundamental unit operations, including vessel reactor (fermentation), batch distillation, batch rectification, filtration, centrifugation, dryer, and adsorber. These operations are extensively covered in theoretical lectures, mathematical modeling, and predefined experiments, ensuring a solid understanding of their behavior. Working in teams, students design their processes in five steps with minimal restrictions, aside from safety regulations and two key constraints: They must use only existing equipment, and each process step is limited to a duration of 180 minutes, including the 30-minute set-up, shutdown and cleaning phase. The groups compete to develop the most cost-effective process maximizing bioethanol yield while minimizing resource consumption—specifically sugar, yeast, and electricity. The time constraint adds complexity, demanding meticulous simulation and

process planning.

To tackle this challenge, students utilize the commercial flowsheet simulator CHEMCAD. This software offers fundamental unit operation models and a robust thermodynamic engine for calculating physical properties of pure substances and mixtures. However, the models require parametrization based on the available equipment. Students achieve this through reaction rate regression and data reconciliation, leveraging data from previous experiments and a limited number of newly designed trials.

The parametrized models serve as the foundation for optimizing the economic objective function. Given the stepwise nature of the process, optimizing all process parameters simultaneously is extremely difficult. Instead, teams integrate different optimization strategies refining individual steps while maintaining overall process coherence. This encourages strong intra-group communication, as each member is responsible for a specific process stage. The course can be carried out with four groups, five participants each. Thus, one student is responsible for one process step.

By the end of the semester, each group successfully produced a measurable quantity of bioethanol while tracking the resource consumption. Utility consumption was recorded at each step enabling a precise calculation of specific product costs, facilitating comparisons among

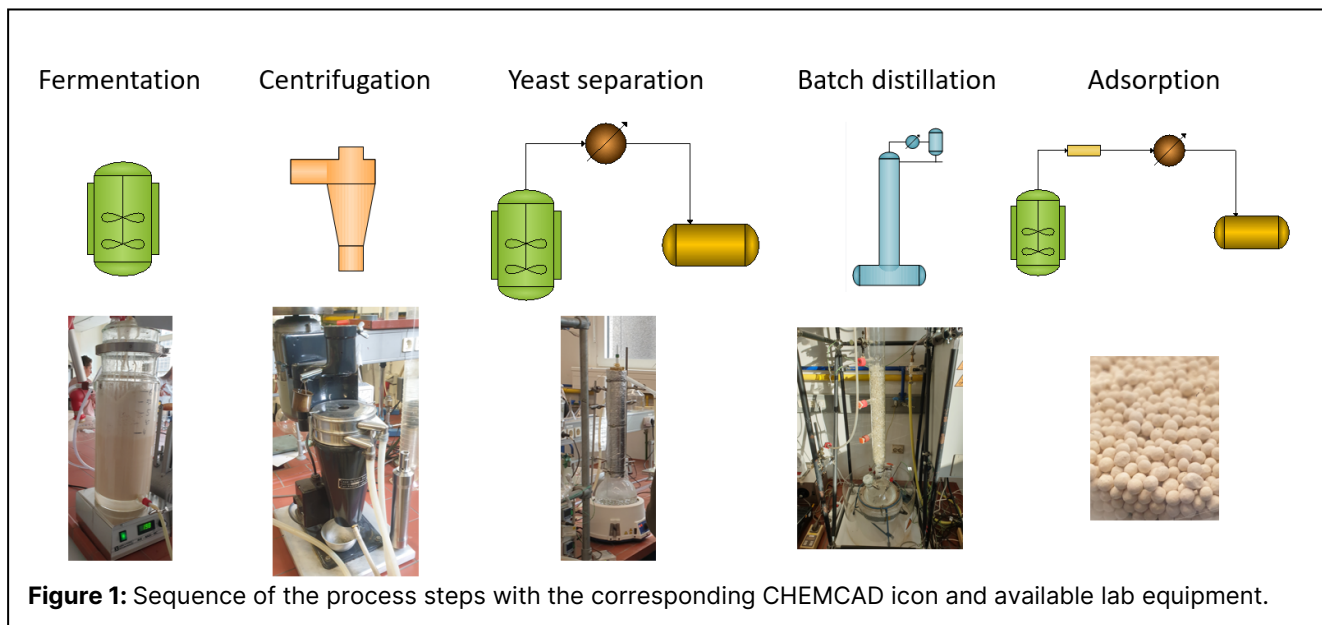


Figure 1: Sequence of the process steps with the corresponding CHEMCAD icon and available lab equipment.

groups and against commercially available bioethanol.

PROCESS EQUIPMENT

Figure 1 illustrates the sequence of process steps alongside the corresponding CHEMCAD icons, which represent the utilized model and the available laboratory equipment. This section provides a summary of the key equipment parameters.

Vessel reactor with temperature control

The fermentation takes place in a cylindrical glass vessel with a usable volume of six liters. Temperature control is achieved through a double-jacketed system, where water circulates via a thermostat. The water temperature is maintained at 30°C, closely matching fermenter temperature. A magnetic stirrer ensures thorough mixing. The vessel remains sealed, besides a tube that directs the produced gas through a gas meter to the atmosphere.

Liquid samples can be collected from the bottom of the vessel for analysis. Glucose and dry matter are measured using optical measurement methods, while the ethanol content is later determined by gas chromatography. However, an estimate for the current ethanol concentration can be approximated from the gas production rate.

At the end of the fermentation step the reactor contents are harvested and frozen to prevent further glucose conversion. The energy required for freezing and un-freezing is not accounted for in the analysis.

Tubular centrifuge

The bulk amount of yeast is separated in a tubular centrifuge. The tube has an inlet diameter d_i of 14.5 mm, an inner diameter d_o of 43.5 mm, a length L of 188 mm, and can rotate at speeds up to $n = 25,000$ revolutions per

minute (RPM). The dry matter content of the feed and the products can be analysed with a high accuracy evaporation scale. At this point the ethanol in the separated centrifugate is replaced by taxed ethanol in compliance with German customs regulations.

Heated glass bulb with condenser

The intermediate product is purified from yeast and glucose in a single stage distillation conducted in a heated glass bulb with a condenser. Two glass bulbs, each with a volume of three liters and a 500 W heating device are available for the process. To prevent foam from entering the water-cooled condenser, an empty glass column is placed on top of the bulb.

The ethanol content of the distillate is measured by analyzing the refractive index of the liquid. At the end of this step, a sample of the distillate is analyzed in a gas chromatograph to detect and quantify any contamination with methanol or other alcohols.

Packed batch column

The plant used to increase the ethanol content consists of a four-liter pot, a column with an internal diameter of 50 mm and a height of 1,200 mm, a condenser with integrated reflux control by a magnetic valve, a guard condenser, a product cooler, and three receiver tanks, which can be connected by a magnetic valve. The column was packed with Raschig rings up to a height of 1,000 mm. The pot can be heated with a maximum duty of 1,800 W, although flooding in the condenser occurs earlier, at around 600 W.

Labview™ is used to control the plant and to visualize the measured temperature profiles, the volume rate and the temperature increase of the cooling water, and the added heat duty. The Labview™ screen and a sketch of the column are depicted in Figure 2.

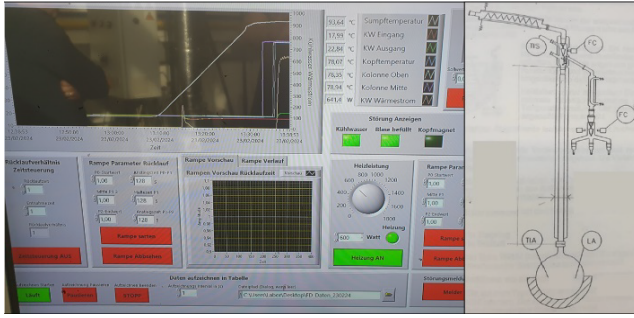


Figure 2. Automated batch distillation plant.

Adsorption plant

The remaining water is adsorbed on the molecular sieve KÖSTROLITH® 3AK. 120g of this zeolite are allocated in the heated glass column of the adsorption plant.

The ethanol-water mixture is transported by a gear pump to a bulb, where it is evaporated using heat from a thermal oil which is maintained at 180°C by a thermostat. The temperature profile in the column is monitored to detect the breakthrough of water. The vapor from the top of the column is condensed and the liquid product is collected in another bulb. The purity of the product is quantified by a high accuracy density measurement.

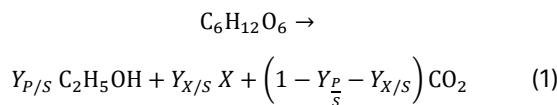
The zeolite is regenerated in a drying cabinet, where it is completely regenerated over around six hours at 230°C until no more water is adsorbed on it.

PROCESS MODELS

Rigorous process models are used to design the process steps and to assess their performance after execution. The models are based on mass and energy balances and on phase equilibrium calculation when applicable.

Fermentation

The fermenter is modelled as a perfectly mixed reactor. The species carbon dioxide CO_2 , ethanol $\text{C}_2\text{H}_5\text{OH}$, water H_2O , alpha-D-glucose $\text{C}_6\text{H}_{12}\text{O}_6$, and biomass X are considered in the material balances. Only one reaction is taken into account, the growth of biomass with the simultaneous production of ethanol. The mass-based stoichiometry is given in equation (1) using the yield coefficients for ethanol production $Y_{P/S}$ and for biomass production $Y_{X/S}$.



The structure of the reaction rate, given in equation (2), is taken from Fogler [1]. The rate uses the mass-based concentrations c_i .

$$\dot{r}_1 = \mu_{max} \left(1 - \frac{c_{\text{C}_2\text{H}_5\text{OH}}}{c_{\text{C}_2\text{H}_5\text{OH}}^{\text{tox}}}\right)^{0.52} \frac{c_X c_{\text{C}_6\text{H}_{12}\text{O}_6}}{K_S + c_{\text{C}_6\text{H}_{12}\text{O}_6}} \quad (2)$$

The reaction rate is implemented in the vessel reactor model in CHEMCAD.

Centrifugation

The separation efficiency of the centrifuge is estimated by balancing centrifugal force, lifting force and drag force. This leads to equation (3) for the separation grain diameter d_T .

$$d_T = \frac{1}{2\pi n} \cdot \sqrt{\frac{18\eta}{\Delta\rho} \cdot \frac{4\dot{V}}{\pi d_0^2 L} \cdot \frac{d_0}{d_i}} \quad (3)$$

Evaporation

The MESH equations (material balances M, equilibrium conditions E, sum equations S and heat balance H) are used to model the evaporation of ethanol and water in the heated glass bulb. The five components mentioned in the Fermenter section are balanced. The caloric properties of the biomass are estimated with the properties of water. The phase equilibrium (K-values / K_i) is calculated with the non-random two liquid model (NRTL) from Renon and Prausnitz [2]. In the equations 4 – 10 x_i refers to the molar liquid fraction, y_i to the molar vapor fraction, M to the molar hold-up, \dot{Q} to the heat duty added or removed, U to the inner energy h to the enthalpy, and V to the vapor flow. The indices L and V refer to liquid and vapor.

$$M: \frac{d(x_i M_L)}{dt} = -y_i V \quad (4)$$

$$E: y_i = K_i x_i \quad (5)$$

$$T_V = T_L \quad (6)$$

$$P_V = P_L \quad (7)$$

$$S: 1 = \sum_{i=1}^{NC} x_i \quad (8)$$

$$1 = \sum_{i=1}^{NC} y_i \quad (9)$$

$$H: \frac{dU_L}{dt} = \dot{Q} - h_V V \quad (10)$$

The MESH equations are solved in CHEMCAD using the vessel reactor unit operation.

Packed batch column

The batch column is modelled by solving a set of the MESH equations, with a number of MESH sets equal to the number of theoretical plates. Therefore, the equations 4 and 10 are modified by adding a vapor flow from the lower plate, a liquid flow from the upper plate and by subtracting the liquid flow to the lower plate. The resulting differential-algebraic equation system is solved in the CHEMCAD unit operation batch column. To include non-integer values for the number of theoretical plates Murphree tray efficiencies are used. Heat losses over the column are estimated for each stage with equation (11), where k is the heat transfer coefficient. At the last stage the reboiler duty is added, at the first stage the

condenser duty is removed.

$$\dot{Q}_{\text{HeatLoss}} = k \cdot A_{\text{Stage}} \cdot (T_{\text{Ambient}} - T_{\text{Stage}}) \quad (11)$$

Adsorption

The adsorption of water on the zeolite is modelled by assuming a water free adsorbent as initial condition, spherical particles of equal size, and a linear adsorption isotherm. The approximated solution to the partial differential equation system proposed by Rosen is used to calculate the dynamic behaviour of the gas phase concentrations. For further details, see Sattler's textbook [3].

PROCESS STEPS

Each process step can only be performed once, making detailed planning of the entire process essential. Process models are developed, fitted to data from preliminary experiments, and used to design the individual process steps.

Feedstock and product requirements

The sugar alpha-D-glucose monohydrate is used as feedstock, because its concentration in an aqueous mixture with ethanol is easier to measure compared to other sugars. Besides water, the only other feedstock is fresh yeast with a dry matter content of around 30% by weight.

The ethanol concentration in the fuel-grade bioethanol product must exceed 98.7% by weight [4].

Preliminary experiments

Preliminary experiments are performed to determine missing model parameters. Most of these parameters are obtained by reconciliation of measured data. However, for the design of the fermentation process, the solubility of the sugar, the yeast, and their mixture in water are critical. These parameters are determined through trials which are not directly related to the later process steps.

Data reconciliation

Data reconciliation is a powerful tool for estimating missing model parameters. It involves using measured data and correcting it by applying conservation equations. This is required because the mathematical models, where these parameters are used follow these fundamental laws, whereas measure data commonly is subject to errors and may not. The models that are used during the data reconciliation are described in the section on process models.

Reaction kinetics and yield coefficients

A fermentation trial is carried out in the previously described vessel reactor. The concentrations of glucose, yeast, and ethanol are monitored over time. Additionally, the CO₂ production rate is measured. A comparison of the initially added glucose with the produced ethanol and the

increased amount of yeast at the end of the experiment produces the yield coefficients. The reaction kinetic parameters in equation (2) are determined using the reaction rate regression tool implemented in CHEMCAD.

Mechanical yeast separation

Although the separation grain diameter can be calculated using equation (3), where all parameters are known, the mechanical yeast separation can not be calculated a priori. The unknown property in this case is the particle size distribution of the yeast in the mixture, which cannot be measured directly. Instead, the remaining amount of yeast in the intermediate product is analyzed.

Column start-up and total reflux profiles

Several important simulation parameters can be retrieved from the temperature profiles of the column start up. The curves from a preliminary experiment are shown in Figure 3. The next sections will refer to these profiles.

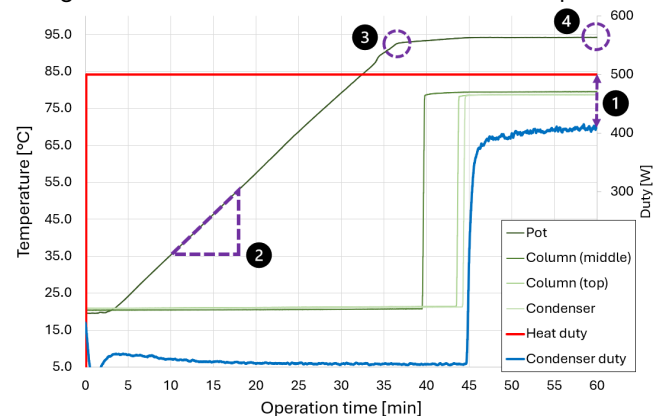


Figure 3. Temperature profiles during start-up.

Heat losses

Heat losses occur in all process steps, but they are particularly significant in the packed distillation column, where they lead to an increased reflux stream and impact the separation efficiency. These losses can be estimated by comparing the heat added to the pot with the heat removed by the cooling water in the condenser. At total reflux the difference of these values gives the overall heat loss (arrows at Point 1 in Figure 3). The heat loss from the pot can be estimated separately by analyzing the heat-up curve (Point 2 in Figure 3).

Column hold-up

The liquid hold-up in the packing and in the condenser directly influence the dynamic behavior of the batch distillation. These factors must be included in the model to make reasonable predictions of the product concentration in the distillate and receiver tanks.

Fortunately, they can be estimated from the total reflux experiment. Initially, all the column content is allocated in the pot, and its composition is known or can be derived from the temperature profiles during the heat-up

phase (Point 3 in Figure 3). Temperature and composition in the pot change over time and reach a steady state once the total reflux profile is fully established (Point 4 in Figure 3). This change in composition is a result of the transfer of mass from the pot into the column.

The correlation between the hold-up and the temperatures at Points 3 and 4 in Figure 3 is not trivial but can be determined through data reconciliation. However, no direct differentiation between the hold-up in the packing and the hold-up in the condenser is possible. Therefore, one of these parameters should be fixed to a reasonable value during the data reconciliation.

Separation efficiency

The number of equilibrium stages in the packed column, defined by the modified equation system 4-10, can be estimated using the McCabe-Thiele method, i.e. drawing steps into the x-y equilibrium diagram (Figure 4). This graphical method is not very accurate, often resulting in a non-integer value for the last stage, which is hard to read precisely from the diagram. Additionally, the energy balance is neglected, which is not a valid assumption for columns with considerable heat losses. Consequently, the separation efficiency is estimated by rigorous simulation using Murphree tray efficiencies.

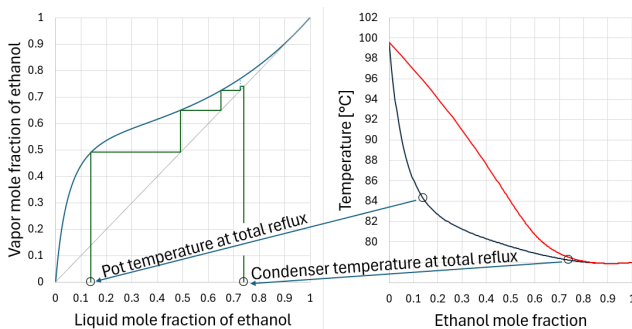


Figure 4. McCabe Thiele method for estimating the number of equilibrium stages in the packed column.

Graphically these efficiencies mean, that the step of an equilibrium tray is not drawn until the equilibrium line but ends at a certain percentage (the Murphree efficiency of the tray) of the full distance. The estimation from the McCabe Thiele method still gives a good initial guess for the data reconciliation.

Heat loss, hold-up, and separation efficiency are coupled in a highly non-linear manner, so they must be regressed together. This simultaneous regression is performed using the data reconciliation tool implemented in CHEMCAD. The measured values to be matched include the pot and condenser temperatures, as well as the heat loss over the packed column. Samples can be drawn from the pot and condenser to determine their composition, but these values correlate with the respective temperatures in the case of a binary mixture. The measurements

are still used to verify the accuracy of the method.

Adsorber capacity

The particle diameter and the adsorption isotherms for the zeolite are commonly provided by the vendor, but the packing porosity and the effective diffusivity must be estimated to apply Rosen's equation. While the packing porosity can be read from volume measurements, the effective diffusivity requires a trial run. The final missing parameter in the adsorber model can be estimated from the breakthrough curves of water.

Fermentation

The validated model for the conversion of glucose to ethanol, yeast, and carbon dioxide in the given fermenter can be used to maximize the amount of ethanol produced at minimum costs in a 150-minute run. The decision variables include the initial amounts of yeast and glucose, as well as additional glucose fed to the fermenter at any time later in the run. The feedstock content in the fermenter is limited by its solubility. While the operational costs, such as electricity consumption for stirring and cooling remain fixed, feedstock costs directly impact the profitability of the process.

Yeast removal

The two steps of yeast removal offer little room for optimization but impose constraints to the amount of fermenter broth that can be produced during the fermentation step. Additionally, the liquid volume of the batch distillation plant's pot is limited, which restricts the amount of condensate generated in the evaporation step. This step also determines the initial ethanol concentration for the distillation and, consequently the maximum product purity achievable with the existing column.

Distillation

The distillation column has only one degree of freedom during operation: the reflux ratio. In theory, the heat duty added to the pot could be adjusted, but due to the risk of flooding, it is fixed at a safe value. Nevertheless, designing the distillation step is challenging because the reflux ratio can be adjusted dynamically. Instead of optimizing a single value, the goal is to determine an optimal trajectory over the 150-minute runtime or, alternatively, a sequence of operational steps. The objective function is also complex. While the operation costs don't vary much (600 W over 150 minutes plus heat-up time), a key decision involves determining how much product should be collected and at what concentration. Product batches of varying volumes and concentrations can be collected in the receiver tanks, adding another layer of optimization.

Adsorption

Finally, the water content in the product batches

must be removed in the adsorption step, which is the bottleneck of the overall production process. While this step does not feature any decision variables, detailed planning is essential to ensure that all the product from the distillation column is processed efficiently. Due to heat-up and cool-down times, only two adsorption runs can be performed in the 180-minute timeframe.

RESULTS

All groups successfully produced bioethanol with the required purity. The utilized electrical energy was similar for all groups, but the final product mass varied significantly, ranging from 50g to 200g depending on the process design. Figure 5 presents an example of the fermentation step, comparing the planned concentration trajectories (model) with the measured values. In this specific case the students have decided for a fed-batch strategy. A similar comparison for the distillation step is shown in Figure 6. The primary cost driver in the process is the glucose feedstock, with overall operational expenditures ranging from €20 to €50 per group. The overall student feedback on the project was very positive.

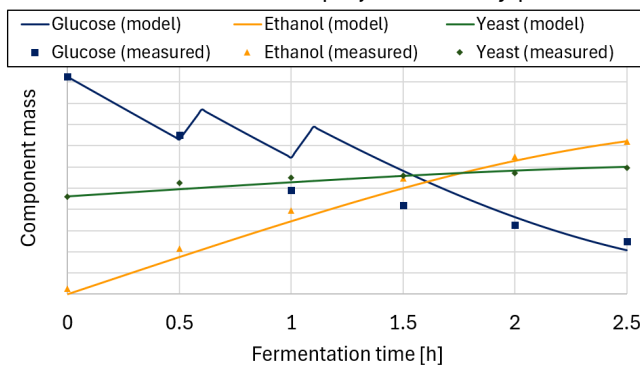


Figure 5. Exemplary results of the fermentation step.

SUMMARY

This work provides a detailed overview of the materials and methods used for a university course during which students produce bioethanol in a demanding competition. It shares key insights from the course, highlighting both challenges and successes. The study emphasizes the importance of mathematical modelling and the challenges in aligning modeled data with measured data. A key takeaway is that while the models may not perfectly capture reality, they are essential for a successful process design, particularly for inexperienced engineers transitioning from academia to industry.

Each student has an individual project, but this project is connected to those from the other group members. Providing reasonable guesses for data that is required in the other projects is very challenging, but also a great learning experience, especially if the guess was good.

This case study shows how combining modelling

tasks and experimental tasks and merging them to a project that follows a red thread leads to an extraordinary learning experience for the students. It is intended to motivate the design of similar courses.

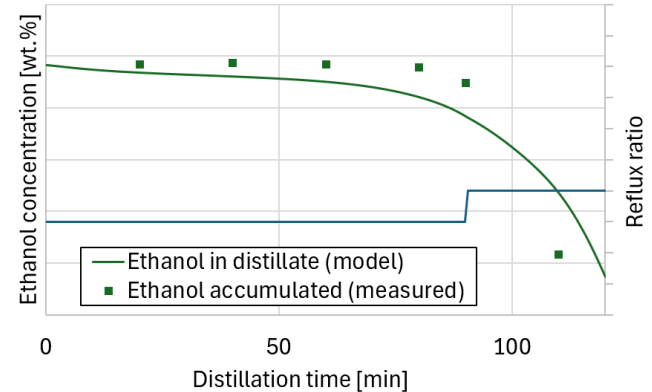


Figure 6. Exemplary results of the distillation step.

DIGITAL SUPPLEMENTARY MATERIAL

The CHEMCAD simulation files for the modelling of the fermentation step, the open distillation step and the batch distillation step are available as digital supplementary material:

<https://psecommunity.org/LAPSE:2025.0016>

<https://psecommunity.org/LAPSE:2025.0017>

<https://psecommunity.org/LAPSE:2025.0018>

Furthermore, a tutorial like detailed description of how to parametrize the batch column model in CHEMCAD can be found on the Chemstations website:

https://www.datacor.com/hubfs/Estimating_Simulation_Parameters_for_Batch_Columns.pdf

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