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Integrated modelling platforms for comprehensive assessment of biorefineries: a case study of the power-to-protein process

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ABSTRACT

Process simulation software packages are widely used to generate mass and energy balances for chemical and biochemical processes. These data are essential for techno-economic and life-cycle assessments. In this work, a method for integrating Aspen Plus and SuperPro Designer is used to simulate and study a system producing single-cell protein using methanol produced from electricity and CO_2 (e-methanol). This application was selected because of the growing importance of the protein transition and the need to replace conventional animal-based proteins with more sustainable alternatives such as microbial protein. In addition, microbial protein production from renewable carbon sources is consistent with the Sustainable Development Goals (specifically goal 2, Zero Hunger) set by the United Nations. One-factor-at-a-time sensitivity analysis, Taguchi method, and a combination of Taguchi and multi-criteria decision-making are used to highlight the capability and applicability of the applied process simulation software integration method. This method can increase the speed of modelling multiple scenarios for process optimization and can improve the accuracy of sensitivity analyses, which are critical for the design and development of microbial food production systems.

1. Introduction

Heat and mass balance data are used to conduct techno-economic analyses and life cycle assessments for evaluating the economic and environmental performances of process and energy industries. Process simulation software typically assists in generating heat and mass balance results by using predefined thermodynamic and phase equilibrium databases. Aspen Plus, Aspen HYSYS, PRO/II, and SuperPro Designer are some of the commercial software used for process simulation (Kasani et al., 2022).

Of these, Aspen Plus is primarily used for the simulation of petrochemical and refinery processes. It handles electrolytes in dissociated form, polymers, and solids by using a comprehensive database of components and thermodynamic models. However, the simulation of bioprocesses can be challenging due to its predefined unit operations and precise reaction definitions. On the other hand, SuperPro Designer is commonly used to simulate bioprocess, pharmaceutical, and food and beverage processes. It handles batch and continuous processes as well as bioreactions without requiring exact thermodynamic data. This limits its application to simulate complex unit operations such as reactive and azeotropic distillation. Aspen Plus provides phase equilibrium calculations with higher accuracy than SuperPro Designer by having a more comprehensive thermodynamic database. However, SuperPro Designer allows slight stoichiometric imbalances for reactions and provides predefined bioreactor modules such as fermenters and anaerobic digesters, which make it ideal for the simulation of bioprocesses.

Prior works have assessed methods to mitigate the limitations of process modelling using commercial simulation software packages (Table 1). Mitchell et al. (2017) proposed a method for connecting Aspen HYSYS and MATLAB via Microsoft Excel and Visual Basic for Applications (VBA) to enable the utilization of an advanced process control algorithm called Model Predictive Control (MPC). This algorithm cannot be implemented directly in Aspen HYSYS without using the proposed integration method. Taras and Woinaroschy (2011) used

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Table 1
Comparison of the present study with the previously published papers on integrating simulation software packages, VBA: visual basic for applications.

Reference	Integrated software packages	Integration interface	Purpose
Mitchell et al. (2017)	Aspen HYSYS & MATLAB	Microsoft Excel & VBA	Implementation of Model Predictive Control (MPC)
Taras and Woinaroschy (2011)	SuperPro Designer & MATLAB	VBA	Multi-objective optimization using a Genetic Algorithm
Csendes et al. (2023)	Aspen HYSYS & MATLAB	MATLAB	Estimation of kinetic constants based on experimental data and simulation results
Ponce-Ortega and Hernández-Pérez (2018)	Aspen Plus & Microsoft Excel, SuperPro Designer & Microsoft Excel, Aspen Plus & MATLAB	Microsoft Excel for Aspen Plus & MATLAB integration	Implementing metaheuristic optimization approaches
Present work	Aspen Plus & SuperPro Designer	MATLAB and VBA	Integrating two simulation software packages to study chemical/biochemical processes

MATLAB and VBA to conduct a multi-objective optimization of the penicillin production process, which was simulated in SuperPro Designer. The integration of MATLAB with SuperPro Designer enabled them to apply a Genetic Algorithm for optimization, which is not a predefined method in SuperPro Designer. Csendes et al. (2023) simulated a lab-scale reactor to produce γ-valerolactone from butyl-levulinate (BL) using predefined modules and built-in kinetic reaction models of Aspen HYSYS. Subsequently, by using experimental results for the concentrations of reactants and products, they estimated the kinetic constants using an integrated MATLAB code. Their paper also provides a comprehensive literature review on the necessity for, and methods of, integrating different simulation software packages. They concluded that software packages such as Aspen HYSYS, Aspen Plus, MATLAB, GAMS, and UniSim Design can be used in an integrated framework to conduct sensitivity analysis, operating condition optimization, and multi-objective optimization. Ponce-Ortega and Hernández-Pérez (2018), in their book, described the integration of process simulation software (such as Aspen Plus, Aspen HYSYS, and SuperPro Designer) with optimization tools (such as Microsoft Excel, MATLAB, and C++) for the implementation of metaheuristic optimization approaches. In a similar manner to these previous methods, the present work aims to integrate Aspen Plus and SuperPro Designer, which can enable reliable, rapid, and error-free data exchange for sensitivity analysis. In contrast to the work by Ponce-Ortega and Hernández-Pérez, the present work does not focus on optimization of a process modelled in Aspen Plus or SuperPro Designer using Excel or MATLAB as an intermediary; rather, in this work, data is automatically passed between several process simulation software packages (Aspen and SuperPro Designer) using MATLAB and Excel as an intermediary.

Rigorous simulation of common processes, such as anaerobic digestion cannot be achieved by solely using the predefined modules in Aspen Plus or Aspen HYSYS. Therefore, to overcome this challenge, researchers implemented the ADM1 model into the Aspen Plus simulation using Aspen Custom Modeler (Rajendran et al., 2014). More information on using Aspen Plus to simulate anaerobic digestion is available elsewhere in the literature (Inayat et al., 2021). Also, prior to the addition of the electrolyzer module in Aspen Plus V14, rigorous simulation of water electrolysis could be achieved using embedded calculations with the predefined modules in Aspen Plus or Aspen HYSYS (Jang et al., 2022; Motazedi et al., 2021). Integrating simulation software packages is also applicable to other fields of engineering, such as multi-physics simulation (Uekermann et al., 2022) or national infrastructure modeling (Usher and Russell, 2019).

Some biorefineries use both bioprocesses and chemical processes, such as producing drop-in fuels via an integrated thermochemical-biochemical pathway (Detsios et al., 2023) or biocrude production via the hydrothermal liquefaction process integrated within wastewater treatment plants (Hussain and Anastasakis, 2025). In such cases, the integration of Aspen Plus or Aspen HYSYS with SuperPro Designer would allow us to overcome the limitations of each simulation software. An example is the work done by Esmaeili-Faraj et al. (2023) where they used SuperPro Designer to simulate anaerobic digestion of palm oil mill effluent and Aspen HYSYS to simulate biogas upgrading and biomethane reforming processes. In another paper by Andrea et al. (2015) a microalgal biorefinery was simulated in SuperPro Designer, and Aspen Energy Analyzer was used for heat integration analysis, as the latter enables fast and easy design of a heat exchanger network. However, these papers do not provide details regarding the method of data exchange between the different software packages.

In this work, a method for the integration of Aspen Plus and SuperPro Designer is used . The term “integration” here means that data can be transferred automatically between software packages, which enables researchers to rapidly model multiple scenarios, conduct sensitivity analysis, and carry out process optimization while using both software packages. The manual data transfer between the simulation software packages is time-consuming and prone to errors. “Integration” makes it possible to use the strengths of both software packages and manage the limitations of each.

The integration method is applied to a single-cell protein production system using e-methanol as substrate, this is a key novelty of this work. This application is of great importance due to its potential social, economic, and environmental impacts, as it addresses challenges associated with the sustainability and transformation of current food systems through the development of alternative protein production systems. Single-cell protein refers to dried cells of algae, yeast, bacteria, or fungi, which have high protein content (Sharif et al., 2021) and can be used as an alternative to conventional proteins from livestock or poultry. Conventional protein production systems (such as those from beef) have a major impact on climate change, land use changes, water resources depletion, and ecosystem pollution (Springmann et al., 2018), and the use of single-cell proteins may reduce these environmental impacts (Fasihi et al., 2025). Examination of the economic, environmental, and social performance of single-cell protein production should be completed to compare it with conventional protein production in a sustainability assessment framework. Data required for these techno-economic and environmental assessments may be obtained from process simulation.

Prior works that have modelled single-cell protein production include: Calleja et al. (2016) who used gPROMS and MATLAB to simulate the dynamic behaviour of protein production using *Escherichia coli*; Hong et al. (2021) who provided a microscopic model for a bioreactor producing *Pichia pastoris biomass*; and Nielsen et al. (2023) who used MATLAB to develop a novel kinetic growth model for *Methylococcus capsulatus*. Vlaeminck et al. (2023) used SuperPro Designer solely for the process simulation of single-cell protein production from industrial off-gas. Modeling of the single-cell protein production process can also be done using first principle models, as exemplified by Van Peteghem et al. (2022) who assessed the feasibility of a nearly carbon-neutral process for producing single-cell protein through the use of different substrates, including formate, acetate, methanol, and ethanol. As the methanol substrate for single-cell protein production outlined in prior work by Meng et al. (2023), may be produced in chemical reactors, modelling of the methanol synthesis process is required when assessing the full single-cell protein production process.

Several studies have simulated the methanol synthesis process via CO_2 hydrogenation, such as the papers by Yousaf et al. (2022) and Do and Kim (2019) who used Aspen Plus for this purpose.

In addition to providing details of integrating Aspen Plus and SuperPro Designer in the present study, to the best of the authors' knowledge, no previous work studied the combined modelling of single-cell protein production using Aspen Plus for chemical process simulation and SuperPro Designer for bioprocess simulation. This contribution is particularly relevant in the context of developing reliable modelling tools to support the transition toward sustainable and resource-efficient food systems.

The application of the software integration method to the single-cell protein production process, as a case study, showcases the potential value of this integration method to enable a combined modelling approach to complex processes.

2. Methodology

The production process for single-cell protein using e-methanol as a substrate is analyzed using the combination of Aspen Plus and SuperPro Designer. The process starts with hydrogen generation using alkaline water electrolysis, followed by methanol synthesis and single-cell protein production using methanol as the carbon source. The model used in this study for describing the electrolyzer includes 12 nonlinear equations to calculate hydrogen and oxygen production rates as well as power consumption based on key operating and manufacturing parameters of the electrolyzer (temperature, pressure, cell current density, number of cells, and cell area). Although the electrolyzer module is added to the newer Aspen Plus versions (since version 14), the use of MATLAB for the simulation of the electrolyzer demonstrates that the proposed integration approach can enable data exchange between MATLAB, Aspen Plus, and SuperPro Designer and be applied to different software packages, regardless of which software is used for modelling each part of the process. This implies that in future studies, if a unit operation is not available as a built-in module in Aspen Plus or SuperPro Designer, it can be simulated in MATLAB, and the simulation data can then be exchanged with the other software packages, using the method provided in the present paper. The methanol synthesis process, where H_2 is reacted with CO_2, is simulated using Aspen Plus, and the single-cell protein production is simulated in SuperPro Designer (Fig. 1). Each step is described in detail in the following sections. The system boundary includes water electrolysis, methanol synthesis, and single-cell protein production, but excludes upstream processes for CO_2 capture and the conversion of single-cell protein to a final product (such as flavouring and texturizing). The focus of this paper is to present how the integration of Aspen Plus and SuperPro Designer can aid in the study of combined biological/abiotic systems such as the power-to-protein concept, rather than to provide detailed results. This focus was selected due to the wider importance of such systems in enabling the design and evaluation of sustainable food production systems with environmental, economic, and social impact. Therefore, simplifying assumptions were made and the system boundary was limited. Consequently, the results presented for the process performance are subject to further refinement.

2.1. Water electrolysis

The basis of the electrolysis simulation is an alkaline water electrolyzer with the following specifications, which are aligned with industrial-scale electrolyzers.

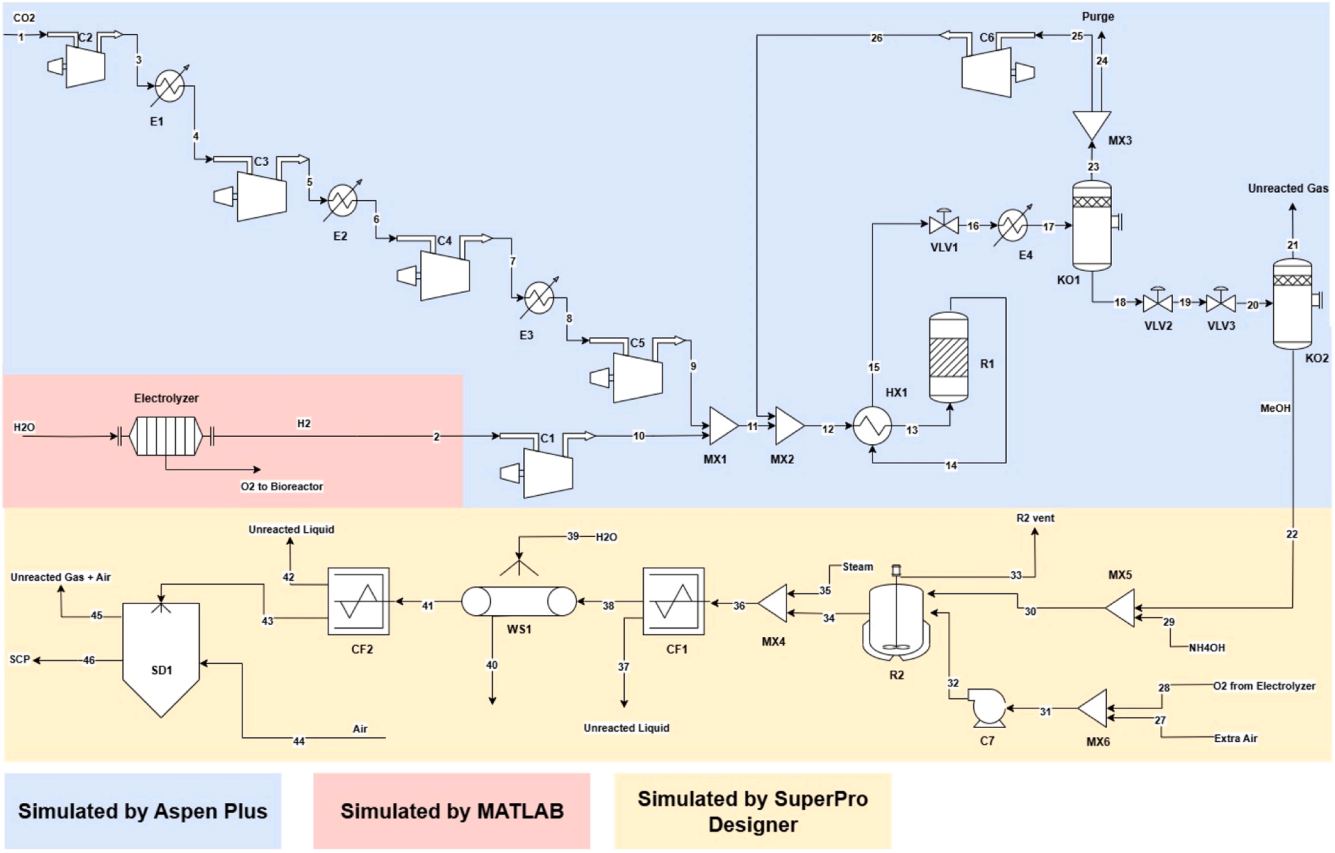


Fig. 1. Process simulation of water electrolysis, methanol synthesis from CO_2, and microbial protein production. C1-C6: compressors; MX1-MX6: mixing points; E1-E4: coolers; HX1: heat exchanger; R1: methanol synthesis reactor; R2: SCP production bioreactor; VLV1-VLV3: pressure reduction valves; KO1-KO2: 2-phase flash drums; CF1-CF2: centrifuge; WS1: washing stage; SD1: spray dryer.

- Number of cells: 326 (Sakas et al., 2022)
- Cell area: 2.66 m^2 (Sakas et al., 2022)

The alkaline water electrolyzer is based on the work by Sanchez et al. (2020) and simulated in MATLAB. Details of the constants and mathematical equations used are provided in the supplementary material (S1). According to Sanchez et al. (2020), the simulation inputs are: electrolyzer operating temperature and pressure, electrolyzer cell current density, electrolyzer cell area, and number of electrolyzer cells. Simulation results include the amount of H_2 and O_2 produced, water consumption, and the power consumption of the electrolyzer stacks. Prior literature indicates that the electrolyzer stacks are responsible for 92% of the total electrolyzer power consumption, and auxiliary equipment makes up the remaining 8% of the total power consumption (Sánchez et al., 2020). Therefore, the total power consumption of the electrolyzer is calculated using eq. 1.

$$electrolyzer\ power\ consumption = \frac{stack\ power\ consumption}{0.92} \tag{1}$$

2.2. Methanol synthesis

The simulation of methanol synthesis is completed in Aspen Plus and is based on the work by Van-Dal and Bouallou (2013) with some modifications due to the application of the produced methanol. As the methanol produced is used as a substrate for microorganisms, separation of the methanol from water is not needed, because high-purity methanol would need to be re-diluted with water prior to being used as a substrate for single-cell protein production. Therefore, the distillation tower for separating water and methanol at the end of the process is excluded. The modified Redlich-Kwong-Soave (RKSMHV2) equation of state is used for simulation sections with operating pressures higher than 10 bar, while for sections with operating pressures lower than 10 bar, the NRTL-RK thermodynamic model is used (Van-Dal and Bouallou, 2013). The CO_2 is compressed with a multi-stage compressor (C2-C5 in Fig. 1) due to the inlet-to-outlet pressure ratio (Peters and Timmerhaus, 1958) (inlet pressure: 1 bar, outlet pressure: 78 bar), and each step of the CO_2 compression is equipped with an intercooler (E1-E3 in Fig. 1). The compressed CO_2 is then mixed with H_2 (MX1in Fig. 1) and the recycled unreacted gases (MX2 in Fig. 1), and then fed to an adiabatic plug flow reactor (R1 in Fig. 1). Hydrogen is compressed in a single-stage compressor (C1 in Fig. 1). The Langmuir–Hinshelwood–Hougen–Watson (LHHW) mechanism is used due to its capability to model the catalytic synthesis of methanol from CO_2 hydrogenation (Ghosh et al., 2021). Eqs. 2 and 3 show the chemical reactions used in the methanol synthesis reactor (R1 in Fig. 1).

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O;\ \Delta H = -87\frac{kJ}{mol}\ (at\ 298\ K) \tag{2}$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O;\ \ \Delta H = +41\frac{kJ}{mol}\ (at\ 298\ K) \tag{3}$$

The reactor outlet is sent to the first flash drum (KO1in Fig. 1) after pressure reduction (VLV1in Fig. 1) and cooling (E4 in Fig. 1) to separate the gas and liquid phases. The unreacted gas phase is recycled back to the reactor inlet after compression (C6 in Fig. 1). The liquid outlet of the first flash drum (KO1 in Fig. 1) is depressurized (in VLV2 and VLV3 in Fig. 1) and sent to the second flash drum (KO2 in Fig. 1) to separate the remaining unreacted gas from the mixture of methanol and water. In this work, it was assumed that CO_2 is available at the production site at a pressure of 1 bar; therefore, the CO_2 capture process is excluded from the simulation.

2.3. Single-cell protein production

The simulation of single-cell protein production is based on work by Van Peteghem et al. (2022) with some modifications and completed using SuperPro Designer. First, ammonia was replaced with ammonium hydroxide (NH_4OH) to ensure that the entire process could be accurately simulated in the liquid phase, yielding Eqs. 4-7 in Table 2. Second, due to the organic loading rate (which will be discussed later in this section), the substrate is almost completely consumed; therefore, the bioreactor condenser, which is used to return the unreacted methanol vapor to the bioreactor, was removed. These two adjustments eliminate phase equilibrium calculations and decrease the simulation time. Storage tanks and filters were also excluded from the simulation, as they do not affect energy consumption, water usage, and CO_2 emissions.

Fresh methanol is mixed with NH_4OH (MX4 in Fig. 1), a nitrogen source for single-cell protein production, and fed to the bioreactor (R2 in Fig. 1). Oxygen produced by the electrolyzer is used to supply the required oxygen for the bioreactor (R2 in Fig. 1). If the oxygen produced by the electrolyzer is insufficient, extra air is used. The required oxygen is calculated using eq. 10. The continuous conversion fermentation module, which is a continuous stirred tank reactor (CSTR), is used for the simulation of the bioreactor (R2 in Fig. 1) at a working temperature of 37°C. The Monod kinetic model is used, as well as the maximum growth rate (μ_{max}) and substrate affinity (K_s) reported by Van Peteghem et al. (2022). Depending on the metabolic pathway, appropriate constants are used for calculations according to Table 2. The liquid outlet of the bioreactor is sent to MX6 for nucleic acid reduction by direct steam injection, and the gas phase is vented to the atmosphere. The heat treatment for nucleic acid reduction is carried out due to the potential health risks associated with their high intake (Van Peteghem et al., 2022). This step is simulated as a mixing stage (MX6 in Fig. 1) of the liquid stream from R2 (stream 34 in Fig. 1) with steam (152°C, 15 bar, stream 35 in Fig. 1). The amount of steam is manipulated so that the temperature of the effluent mixture (stream 36 in Fig. 1) will be 68°C (Risner et al., 2023) in a continuous process. The mixture after nucleic acid reduction (stream 36 in Fig. 1) is sent for two disk-stack centrifugations (CF1 and CF2) with one washing step (WS1) in between. Disc-stack centrifuges are used due to their popularity in the biotechnology industry (Green Don and Robert, 1997). The concentrated stream (stream 43 in Fig. 1) from the second centrifuge (CF2) is sent to the spray drier (SD1). Depending on the metabolic pathway in single-cell protein production, one of the reactions from Table 2 takes place in the bioreactor (R2 in Fig. 1).

In this study, it is assumed that the bioreactor feed is sterilised (no biomass present in the bioreactor feed stream), and the outlet substrate concentration (S_{out}) is calculated using eq. 8 (Ollis and Bailey, 1986).

$$S_{out} = \frac{DK_s}{\mu_{max} - D} \tag{8}$$

Where D is the dilution rate ($\frac{1}{hr}$); K_s is substrate affinity ($\frac{g}{l}$) and μ_{max} is the maximum growth rate ($\frac{1}{hr}$). Relevant constants for each metabolic pathway from Table 2 are used in eq. 8. The outlet concentration of substrate (S_{out}) is used to determine the biomass concentration in the reactor outlet (X_{out}) using Eq. 9.

$$X_{out} = \frac{S_{in} - S_{out}}{\nu_s} * \nu_x \tag{9}$$

Where ν_x and ν_s are the molar stoichiometric coefficients of biomass and substrate, respectively. In addition, the required oxygen is calculated using eq. 10.

$$O_2^{required} = \frac{S_{in} - S_{out}}{\nu_s} * \nu_{O_2} \tag{10}$$

Where S_{in} & S_{out} are the molar flow rates of substrate at the inlet and outlet of the bioreactor (R2 in Fig. 1) respectively. Also, ν_{O_2} and ν_s are the molar stoichiometric coefficients of oxygen and substrate, respectively.

Table 2
Metabolic pathways and kinetic constants during single-cell protein production.

Metabolic pathway	Maximum growth rate μ_{max} $(\frac{1}{hr})$ (Van Peteghem et al., 2022)	Substrate affinity K_s $(\frac{g}{l})$ (Van Peteghem et al., 2022)	Reaction equation (Adapted from Van Peteghem et al. (2022))	Equation number
DHA[1]	0.078	0.025	$CH_4O + 0.1\ NH_4OH + 0.99\ O_2 \rightarrow 0.48\ CH_{1.8}O_{0.5}N_{0.2} + 0.52\ CO_2 + 1.805\ H_2O$	Eq. 4
RuMP[2]	043	0.025	$CH_4O + 0.13\ NH_4OH + 0.83\ O_2 \rightarrow 0.63\ CH_{1.8}O_{0.5}N_{0.2} + 0.37\ CO_2 + 1.74\ H_2O$	Eq. 5
Serine	0.14	0.025	$CH_4O + 0.1\ NH_4OH + 0.99\ O_2 \rightarrow 0.5\ CH_{1.8}O_{0.5}N_{0.2} + 0.51\ CO_2 + 1.8\ H_2O$	Eq. 6
Calvin	0.04	0.025	$CH_4O + 0.06\ NH_4OH + 1.2\ O_2 \rightarrow 0.29\ CH_{1.8}O_{0.5}N_{0.2} + 0.709\ CO_2 + 1.9\ H_2O$	Eq. 7

1. Dihydroxyacetone, 2. Ribulose monophosphate (Zhang et al., 2022)

2.4. Integrating software packages

To conduct the process studies, Aspen Plus, and SuperPro Designer were integrated. This integration allows for automatic data exchange between these software packages when simulating different process scenarios. SuperPro Designer and Aspen Plus are controlled directly by MATLAB; therefore, operations such as running the simulation engine (for Aspen Plus or SuperPro Designer), saving the simulation files, and closing the simulation files are done directly from MATLAB. A flowchart of the described method is shown in Fig. 2.

Hydrogen produced by the electrolyzer is used as feedstock for the methanol synthesis, which is simulated using Aspen Plus. For this reason, the amount, temperature, and pressure of H_2 produced by the electrolyzer are transferred from MATLAB into Aspen Plus. MATLAB and Aspen Plus are connected directly using the "*actxserver*" command (Abril) in MATLAB. The connection enables importing and exporting data to and from Aspen Plus, as well as controlling the Aspen simulation file. Required data, which are specifications of the produced H_2 (such as temperature, pressure, mass flow rates) and the ratio of the H_2 to CO_2, are transferred between MATLAB and Aspen Plus using the "*Aspen.Tree.FindNode*" command in MATLAB. Next, the simulation engine of Aspen is run using the "*Run2*" command in MATLAB. After convergence of the simulation, the simulation results (such as cooling demand, compressor power requirement, and the amount and composition of the produced methanol) are exported from Aspen Plus to MATLAB using the "*Aspen.Tree.FindNode*" command in MATLAB.

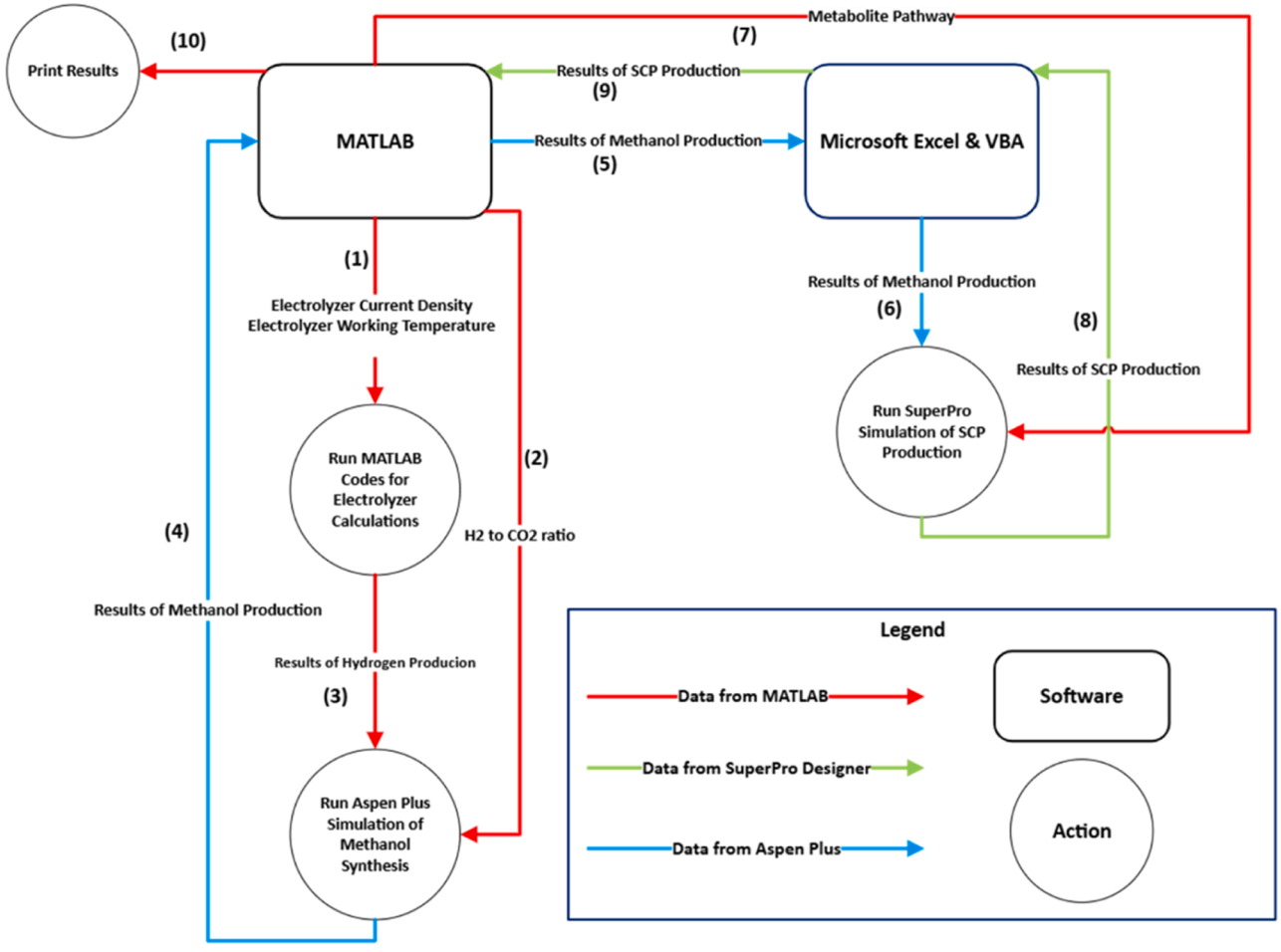


Fig. 2. Data flowchart for integrating MATLAB, Aspen Plus, and SuperPro Designer. The number beside each arrow indicates the step at which the data specified in that arrow is used; SCP: single cell protein; VBA: visual basic for applications.

The methanol produced is used as a substrate for single-cell protein production; therefore, the amount, temperature, pressure, and composition of the produced methanol must be transferred from Aspen Plus to SuperPro Designer. To the best of the authors' knowledge, there is no direct way to exchange data between Aspen Plus and SuperPro Designer. Therefore, Microsoft Excel is used as an interface. The data exchange is carried out in three steps. First, generated data in Aspen Plus are transferred to MATLAB (as explained in the previous paragraph); second, these data are transferred from MATLAB to Excel; third, these data are transferred from Excel to SuperPro Designer using the Component Object Model (COM). COM is an interface developed by Microsoft that enables software packages to exchange data (The Component Object Model, 2024). In addition, the metabolic pathway (explained in section 2.3), which is defined in MATLAB, is transferred to Excel (using the "*writematrix*" command), and then exported from Excel to SuperPro Designer.

The required code for transferring data from Excel to SuperPro Designer is written in Visual Basic for Applications (VBA). Depending on the type of data, different commands from the SuperPro Designer library in VBA are used. If the data are related to a stream (such as the amount of methanol and water in the fresh feed), the *"SetStreamVarVal"* command is used, and if the data are related to variables for a unit operation (such as bioreactor residence time), the *"SetOperVarVal"* command is used. Controlling SuperPro Designer is required because each time a parameter is changed, it requires the SuperPro Designer simulation engine to be run so that the new heat and mass balance data are generated accordingly. The *"DoMEBalances"* command in VBA is used to run the simulation engine of SuperPro Designer. After that, the generated data are first transferred to the Excel file, and then from the Excel file to MATLAB. Depending on the type of data required to be transferred, different commands are used. If the data are related to a stream (such as the amount of single-cell protein produced), the *"GetStreamVarVal"* command is used, and if the data are related to variables of a unit operation (say, centrifuge power demand), the *"GetOperVarVal"* command is used.

The software packages used in this paper are Aspen Plus V.11, SuperPro Designer V12, MATLAB R2023a, and Microsoft Excel V.2409. Simulations are run on a Dell Latitude 5420 (Processor: Intel(R) Core (TM) i5-10310U; RAM 16.0 GB)

2.5. Assessing the effect of process parameters

To study the effect of process parameters on the performance of the integrated single-cell protein plant, three performance indicators were defined as *"SCP to energy"*, *"SCP to water"*, and *"SCP to CO_2"*, which are explained in the section 2.5.1. After defining the indicators, 4 variables were selected for alteration: electrolyzer current density; electrolyzer working temperature; H_2 to CO_2 molar ratio in the methanol synthesis plant; and metabolic pathway of the single-cell protein production. These variables are explained in more detail in the section 2.5.2.

2.5.1. Performance indicators

"*SCP to energy*" is defined as the ratio of the produced single-cell protein to total energy consumed and is calculated using eq. 11:

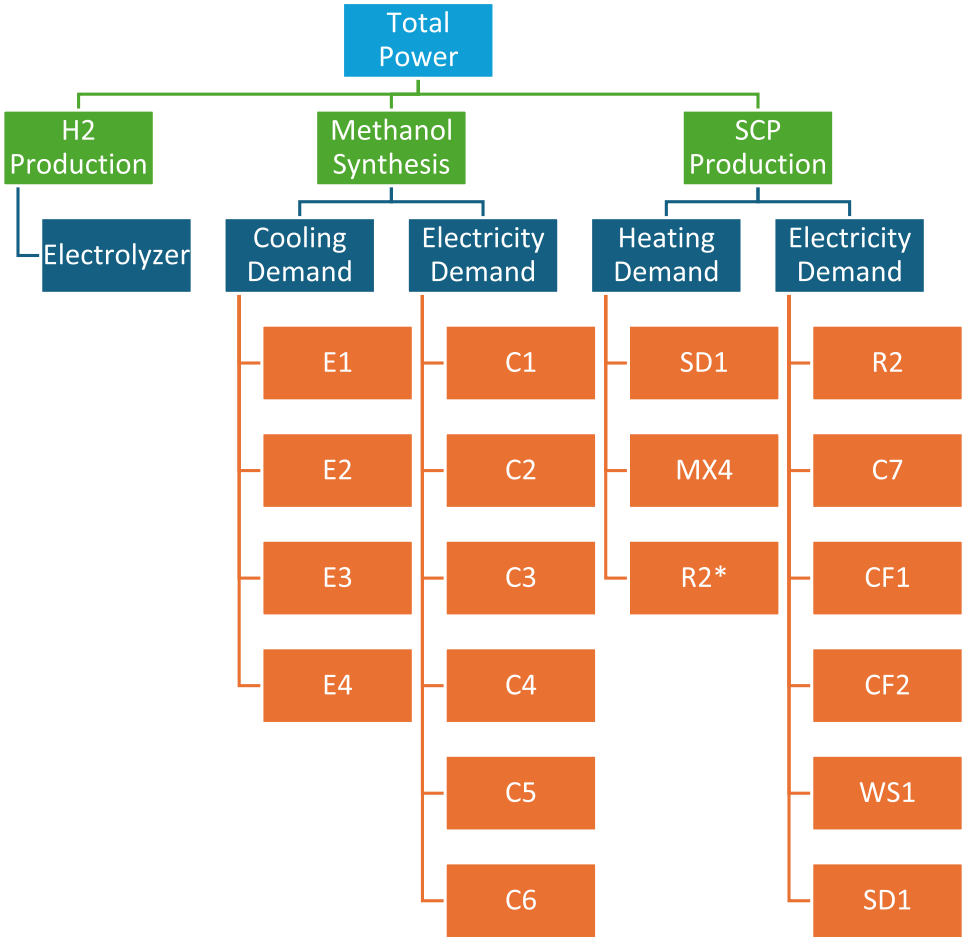


Fig. 3. Components of total energy demand- *: Only in the case of using microbes that employ the RuMP pathway, the bioreactor (R2) requires heating. The unit operation labels used in this chart correspond to the labels shown in Fig. 1; E1-E4: coolers; C1-C6: compressors; C7: bioreactor aeration fan; CF1-CF2: centrifuges; R2: bioreactor; MX4: nucleic acids reduction stage; SD1: spray dryer; SCP: single cell protein.

$$SCP \Big/ Energy = \frac{SCP\ production\ \left[\frac{kg}{hr}\right]}{total\ power\ consumption\ [kW]}\ [=]\ \frac{kg}{kW.hr} \tag{11}$$

The total power consumption in eq. 11 is made up of several components, as summarized in Fig. 3. Total power demand is divided among H_2 production, methanol synthesis, and single-cell protein production. For H_2 production, the electrolyzer is the only power-consuming unit. Eq. 1 shows the calculation of the electrolyzer power demand. Using this equation, the power required for water electrolysis is calculated, which includes the power demand by electrolyzer stacks and auxiliary equipment of the electrolyzer, such as pumps and heat exchangers.

In the methanol synthesis plant, the required power is divided between cooling demand for coolers (E1-E4) and electricity demand to run compressors (C1-C6). In the single-cell protein production plant, power consumption is divided into heating demand for the spray drier (SD1), bioreactor (R2), and steam generation for nucleic acid reduction (MX4), and electricity demand to run centrifuges (CF1, CF2), spray drier (SD1), washing stage (WS1), bioreactor aeration fan (C7), and bioreactor (R2) agitation.

To enable the combination of values for cooling, heating, and electricity demand (to run rotating equipment), the following method has been adopted to convert cooling and heating demand to electricity consumption:

- It is assumed that the cooling tower provides the cooling demand. According to Turton et al. (Turton et al., 2012) the power consumption of the cooling tower is due to the air fan and water circulation pump. For each unit of cooling duty provided by the cooling tower (with a temperature difference of 5 °C), 0.029 units of electrical power are required to operate the cooling tower (eq. 12).

$$total\,power\,demand\,of\,cooling\,(E_C) = total\,cooling\,demand * 0.029 \tag{12}$$

- It is assumed that electric heaters provide the heating demand, and power consumption is calculated using eq. 13.

$$total\ power\ demand\ of\ heating\ (E_H) = \frac{total\ heating\ demand}{electrical\ heater\ efficiency} \tag{13}$$

- The electricity demand for running rotary equipment is calculated using eq. 14.

$$\text{Electricity demand } of\ rotating\ equipment\ (E_R) = \left(\sum_{i=1}^{7} P_{C_i}\right) + P_{R2} + P_{CF1} + P_{CF2} + P_{WS1} + P_{SD1} \tag{14}$$

Where P_{C_i}, P_{R2}, P_{CF1}, P_{CF2}, P_{WS1}, P_{SD1} represent the electricity consumption of compressors and fans, bioreactor agitation, first and second centrifuges, washing stage, and spray dryer, respectively.

- The total power consumption is then calculated using eq. 15.

$$E_T = E_R + E_H + E_C \tag{15}$$

The "*SCP to water*" performance indicator is defined as the ratio of single-cell protein production to total water consumption using eq. 16.

$$SCP \Big/ Water = \frac{SCP\ production\ [kg/hr]}{total\ water\ consumption\ [kg/hr]} \tag{16}$$

Water consumption is made up of three components and described using eq. 17:

- Water consumed by electrolyzer ($Electrolyzer_{water}$)
- Water consumed by the washing stage ($WS1_{water}$)
- Water consumed for steam generation for nucleic acids reduction ($MX4_{water}$)

$$Total\,Water\,Consumption = Electrolyzer_{water} + WS1_{water} + MX4_{water} \tag{17}$$

"*SCP to* CO_2" represents the amount of single-cell protein produced per net CO_2 captured in the process. To assess the impact of using only renewable electricity sources to minimise greenhouse gas emissions, it is assumed that the electricity for running rotating equipment, as well as heating and cooling demands, is supplied by renewable sources. Therefore, there are only three sources of CO_2 emission from the integrated process:

- CO_2 in the "*Purge*" stream (stream 24 in Fig. 1) exiting "*MX3*" (in Fig. 1)
- CO_2 in the "*Unreacted Gas*" stream (stream 21 in Fig. 1) exiting "*KO2*" (in Fig. 1)
- CO_2 in the "*R2 Vent*" stream (stream 33 in Fig. 1) exiting "R2" (in Fig. 1)

In contrast to the defined sources of CO_2 emissions, the methanol synthesis plant consumes CO_2. Therefore, the net CO_2 captured is calculated using eq. 18:

$$Net\ CO_2 = CO_2^{Stream\ 1} - \left(CO_2^{Stream\ 21} + CO_2^{Stream\ 24} + CO_2^{Stream\ 33}\right) \tag{18}$$

Where $CO_2^{Stream\ 1}$ is the CO_2 consumed in methanol synthesis, $CO_2^{Stream\ 24}$ is the CO_2 emission from the purge stream (stream 24 in Fig. 1), $CO_2^{Stream\ 21}$ is the CO_2 emission from the unreacted gas stream exiting *KO2* (stream 21 in Fig. 1), and $CO_2^{Stream\ 33}$ is the CO_2 emission from the vent stream (stream 33 in Fig. 1) of the single cell protein-producing bioreactor (R2 in Fig. 1). The "*SCP to* CO_2" ratio is calculated using eq. 19:

$$\frac{SCP}{CO_2} = \frac{SCP\ production\ [kg/hr]}{net\ CO_2\ captured\ [kg/hr]} \tag{19}$$

2.5.2. Variables to be altered within the process study

For this study, 4 parameters were selected (at least one from each software package: MATLAB, Aspen Plus, SuperPro Designer) for alteration in a sensitivity analysis. This demonstrates the strength and advantages of the process simulation software integration, which enables users to alter multiple parameters across several software packages. The selected variables are summarized in Table 3. As the number of variables is limited and the methods for sensitivity analysis may not be appropriate for non-linear complex process models, in future research, other variables and sensitivity analysis methods may be applied using the integration method proposed in this work.

Table 3
Selected variables for alteration in the process study.

Variable	Base case	Range of alterations for sensitivity analysis	Step size	Number of steps
Electrolyzer current density (Current Density)	0.3 A/cm^2	0.2 – 0.4 A/cm^2 (Smolinka et al., 2010)	0.02 A/cm^2	11
Electrolyzer working temperature	70°C	60~80°C (Smolinka et al., 2010)	2°C	11
H_2 to CO_2 molar ratio for methanol synthesis	5	3-7 (Yusuf and Almomani, 2023)	0.4	11
Metabolic pathway	RuMP[1]	RuMP, DHA[2], Serine, Calvin (Van Peteghem et al., 2022)	-	4

1. Ribulose monophosphate, 2. Dihydroxyacetone

2.5.3. One-factor-at-a-time sensitivity analysis and Taguchi design of experiment

A "one-factor at a time" sensitivity analysis was completed, wherein the process parameters were changed one at a time in the range reported in Table 3, and the performance indicators (outlined in section 2.5.1) are compared with those from the base case scenario. In the base case scenario, the variables are set to the values in the "Base case" column of Table 3. A total of 37 different scenarios were assessed in the one factor at a time sensitivity analysis.

In addition, the Taguchi design of experiment (a statistical method to identify variables that influence process quality and robustness) was applied to find the influence of the variables and identify the ones that impact the results the most. These results were obtained by analyzing the main effect plots following the Taguchi design of experiment (DoE). The Taguchi design of experiment reduces the required number of experiments (which are simulation runs in the context of this paper) for the analysis by using an orthogonal array (Okolie et al., 2021). The L16 (4^4) Taguchi table is provided in supplementary material Table S3. Furthermore, it showcases the capabilities, advantages, and strengths of using the Taguchi design of experiment with process simulation software integration. For the Taguchi design of experiment, the 4 factors selected at 4 levels were the same as the variables altered in the one-factor-at-a-time sensitivity analysis, namely, electrolyzer current density, electrolyzer working temperature, H_2 to CO_2 molar ratio for methanol synthesis, and metabolic pathway for single cell protein production. The factors and levels are shown in Table 4. The responses were the performance indicators described in the section 2.5.1. The Taguchi design of experiment and related analysis are done using Minitab® 19. More information on the Taguchi method is available elsewhere in the literature (Roy, 2010). In all of the described analyses, when changing the H_2 to CO_2 molar ratio, the amount of H_2 was kept constant at the production rate of the electrolyzer, and the amount of CO_2 was manipulated accordingly.

2.6. Integrating multi-criteria decision making (MCDM) with Taguchi design of experiment

The Taguchi design of experiment can show how process parameters affect the process performance and can indicate the levels of each factor that improve process performance. If only one response is considered for the Taguchi design of experiment, the optimal value for the factors that are most favorable for the process performance can be identified. When more than one response is considered, the levels of the factors that improve each response may be different. In such situations, the multi-criteria decision-making (MCDM) method can be helpful. In this study, the design of experiment resulted in the creation of a series of distinct experiments (which are simulation runs in the context of this paper), which were then simulated and assessed. The performance values for each response were then normalized to remove units and ensure similar scales (as per the multi-criteria decision-making process). Each response was assigned a weight that indicates its importance. Then, using one of the several multi-criteria decision-making aggregation methods available, normalized performance values and weights were aggregated to obtain a single overall score for each experiment (which is a simulation run in the context of this paper). Finally, by analyzing main effect plots for the obtained overall score, the levels of the factors for which the overall MCDM score is more favorable can be identified. More information on MCDM methods is available elsewhere in the literature (Yu, 2013), (Hwang and Yoon, 1995). The combination of MCDM and the Taguchi method has been examined in the literature, such as the work by Tong et al. (Tong et al., 2007) who combined Taguchi and VIKOR MCDM approaches to improve the plasma-enhanced chemical vapor deposition process used in fabricating an integrated circuit. The combination of Taguchi design of experiment with MCDM and process simulation software integration for the assessment of single-cell protein production in the power-to-protein context constitutes the main contribution of this work.

In the present paper, the entropy method (Soleimani-damaneh and Zarepisheh, 2009) was used to calculate the response weights, and the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) (Chakraborty, 2022) was used to calculate the overall score of each simulation run. The entropy method was chosen because it is an objective weighting method and does not require human opinion to determine the response weights, which means these weights can be calculated from the results of simulations. The TOPSIS method was chosen because it is one of the most widely used MCDM methods (Pandey et al., 2023). The procedures for both methods (entropy weighting and TOPSIS) are available in the supplementary data (section S3).

Table 4
Factors, level of factors, responses, and signal-to-noise ratio method calculation used for the Taguchi design of experiment.

Factors	Levels
Electrolyzer current density (A/cm^2)	0.2, 0.26, 0.32, 0.38
Electrolyzer working temperature (°C)	60, 66, 72, 78
H_2 to CO_2 molar ratio for methanol synthesis	3, 4.3, 5.6, 6.9
Metabolic pathway	RuMP[1], DHA[2], Serine, Calvin
Responses	Signal-to-noise ratio calculation method
SCP[3]/Energy	Larger is better
SCP/ Water	Larger is better
SCP/CO_2	Smaller is better

1. Ribulose monophosphate, 2. Dihydroxyacetone, 3. single cell protein

3. Results and discussion

In this section, the results for the base case scenario are presented and discussed, followed by the results of one-factor-at-a-time sensitivity analysis, Taguchi DoE, and the combination of MCDM and Taguchi DoE.

3.1. Base case

Fig. 4 shows the power consumption of the base case scenario for each unit operation. The electrolyzer has the largest power consumption (5.5 MW, 93% of total power demand), indicating that using more energy-efficient electrolyzers could significantly improve the overall energy efficiency of single cell protein production. The second largest power consumption (217.7 kW, 3.6 %) is associated with the spray dryer (SD1 in Fig. 1), which corresponds to the heat demand for evaporation of a large volume of water included in the influent of the spray dryer. The hydrogen feed compressor (C1 in Fig. 1) is the third largest power consumer (89 kW, 1.5%), which is used to increase the pressure of hydrogen gas produced in the electrolyzer from 16 bar to 78 bar and deliver it to the methanol synthesis reactor (R2 in Fig. 1). The nucleic acid reduction stage (MX4 in Fig. 1) requires 25 kW (0.4%) of power for steam generation, highlighting that more efficient solutions for this stage can be assessed to improve the overall energy efficiency of the process. For the base case scenario, the specific energy consumption is 44.5 kilowatt hours per kilogram of single cell protein.

Fig. 5 shows the material flow of the integrated plant. The electrolyzer consumes 820 kg/hr of water (83.5% of the total water consumption), the next largest consumer is the washing stage (WS1, 137 kg/hr, 14%), then steam generation for nucleic acids reduction (25 kg/hr, 2.5 %). Using alternative methods to steam injection can decrease the water consumed during nucleic acids reduction. For the base case scenario, 7.4 kg of water is required to produce one kilogram of single-cell protein. Fig. 5 shows that 496 kg/hr (68%) of the oxygen produced by the electrolyzer is in excess of the requirement for single cell protein production and may be sold as an additional source of revenue or utilized to produce another high-value-added product in a biorefinery

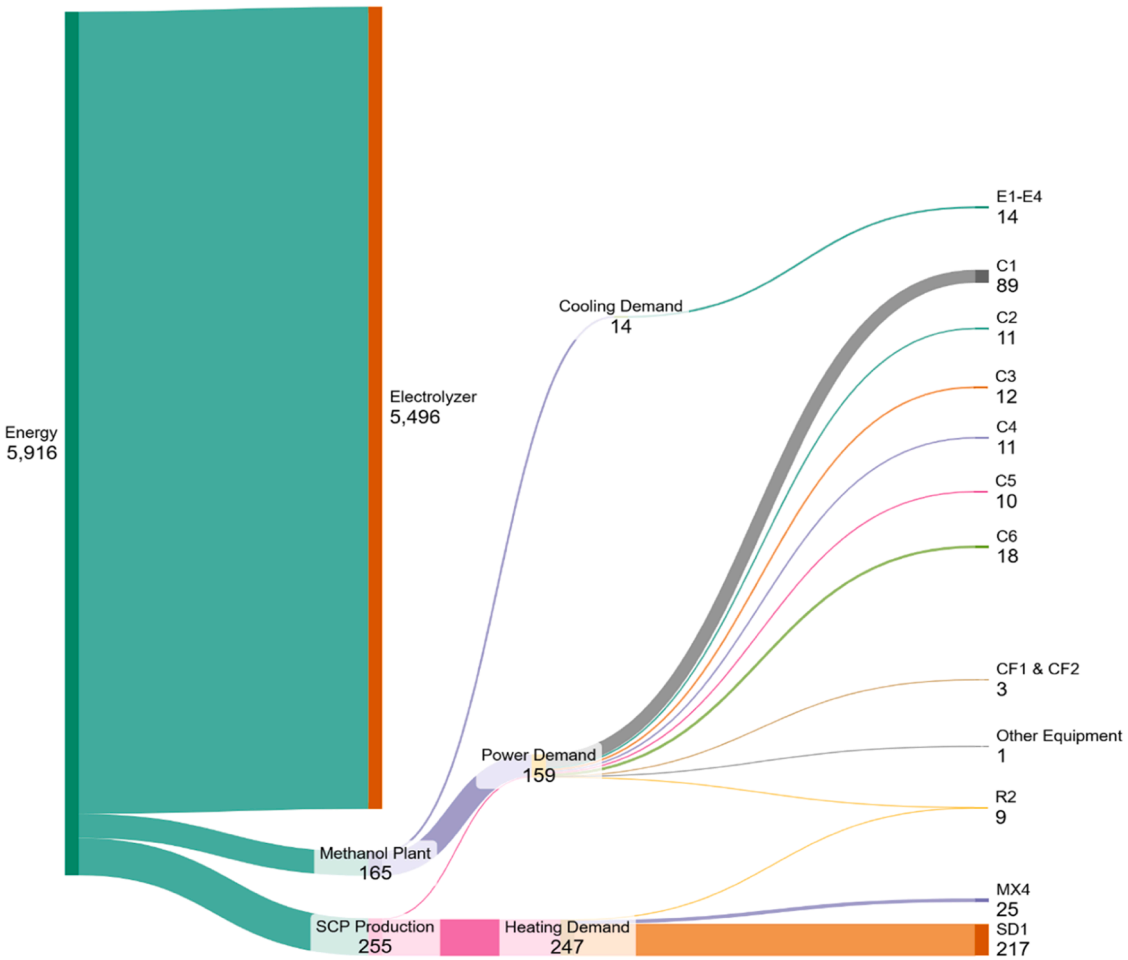


Fig. 4. Power demand of different unit operations (kW); labels of unit operations are aligned with Fig. 1, E1-E4: coolers; C1-C6: compressors; CF1-CF2: centrifuges; R2: bioreactor; MX4: nucleic acids reduction stage; SD1: spray dryer; "other equipment" label in this figure includes the power demand of WS1 and C7; SCP: single cell protein.

concept. This figure also highlights that the single cell protein production plant produces 461 kg/hr of wastewater, which contains unreacted methanol (0.03% wt) and NH_4OH (0.0044% wt). To reduce the amount of wastewater, it may be possible to recycle the effluent from the first centrifuge (CF1 in Fig. 1) and use it to dilute the fresh methanol or use it in the washing stage (WS1 in Fig. 1). Following proper treatment, the wastewater from single cell protein production may be used in the water electrolyzer or steam generation for nucleic acids reduction.

Fig. 5 also shows the emissions to the atmosphere of the integrated plant is 323 kg/hr, and single cell protein production (bioreactor (R2) and spray dryer (SD1) in Fig. 1) is responsible for 275 kg/hr (85 % of total emissions), which are mostly CO_2 and water vapor (52% CO_2 and 48% of water vapor). The methanol plant emits 49 kg/hr (15% of total emissions) of mostly unreacted CO_2 and H_2 (16% CO_2 and 73% H_2). The purge stream (from MX3 in Fig. 1) is responsible for 44.7 kg/hr (93%) of the total emissions from the methanol plant. Emission streams containing hydrogen and carbon dioxide may be reused for methanol production after appropriate purification, although economic evaluation is required before implementation of such solutions.

Fig. 5 also reveals that 400 kg/hr of CO_2 is required for the methanol synthesis. The CO_2 emission from the purge stream (stream 34 in Fig. 1) is 7 kg/hr, and this value for the emission from KO2 (flash drum; Fig. 1) is only 0.5 kg/hr. In addition, the single cell protein production plant emits 143 kg/hr of CO_2 from the bioreactor (R2). These numbers indicate that if all the energy required by the integrated plant is supplied from renewable sources, the studied system for single cell protein production can be considered as a CO_2-consuming process.

For the base case scenario, 1.88 kg of CO_2 is captured to produce one kilogram of single-cell protein. In contrast, if the energy required by the whole plant is not entirely renewable, 1242 kgCO_2eq/hr of indirect emissions due to electricity consumption (based on the Greenhouse gas emission intensity of electricity generation of the EU, 210 gCO_2eq/kWh (European environment agency, 2025)) may be emitted in addition to the plant's direct emissions, making it a CO_2 emitter.

The reduction in CO_2 emissions due to the replacement of animal proteins with microbial protein can enhance the CO_2 credit of the integrated plant. It should be noted that the results presented relate to direct emissions, and for more comprehensive conclusions, it is necessary to study the entire carbon footprint of single cell protein. Such future studies could use the results of the present work relating to the energy and material flow of the integrated plant by considering the corresponding uncertainties due to simplification assumptions and system boundary limitations.

3.2. *One factor at a time sensitivity analysis*

The results of the one factor at a time sensitivity analysis are shown in Fig. 6. Fig. 6-a indicates that the most sensitive process parameter from the ones selected in this work for the SCP/Energy ratio is the H_2 to CO_2 molar ratio, followed by current density of the electrolyzer, and finally by electrolyzer temperature. As per Fig. 6-a, an increase in the H_2 to CO_2 molar ratio results in a reduction in the SCP/Energy ratio. The

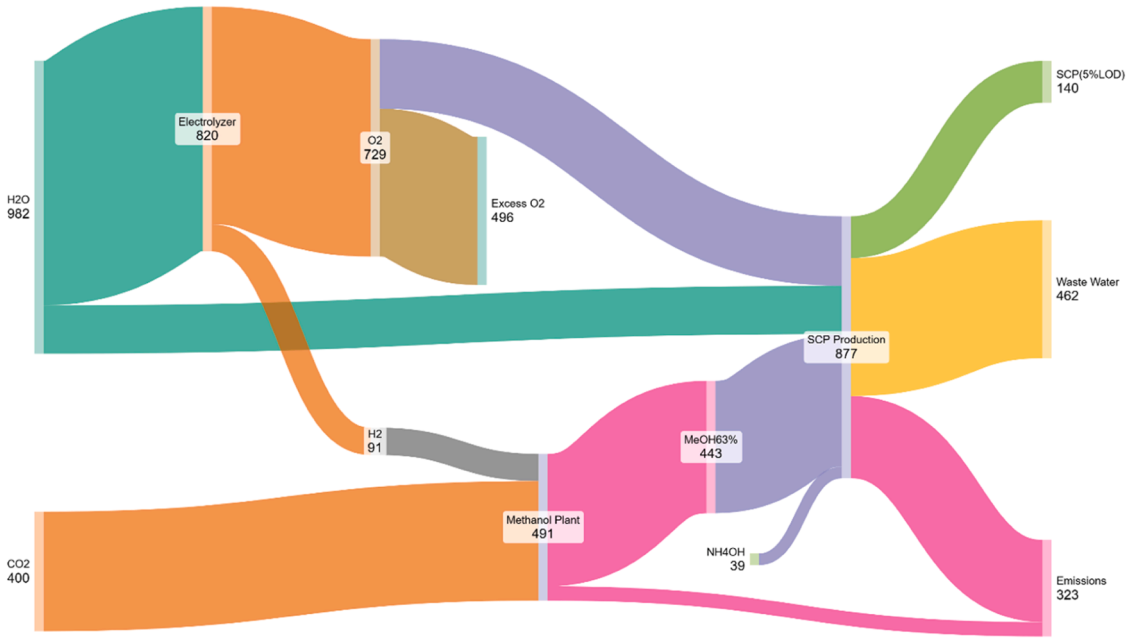


Fig. 5. Material flow (kg/hr) of the integrated plant for the base case scenario; SCP: single cell protein, LOD: loss on drying, MeOH: methanol. Emissions to the atmosphere are CO_2 produced because of microbial growth, unreacted H_2 and CO_2, and CO as well as produced H_2O in the methanol plant, and water vapor from the SCP dryer.

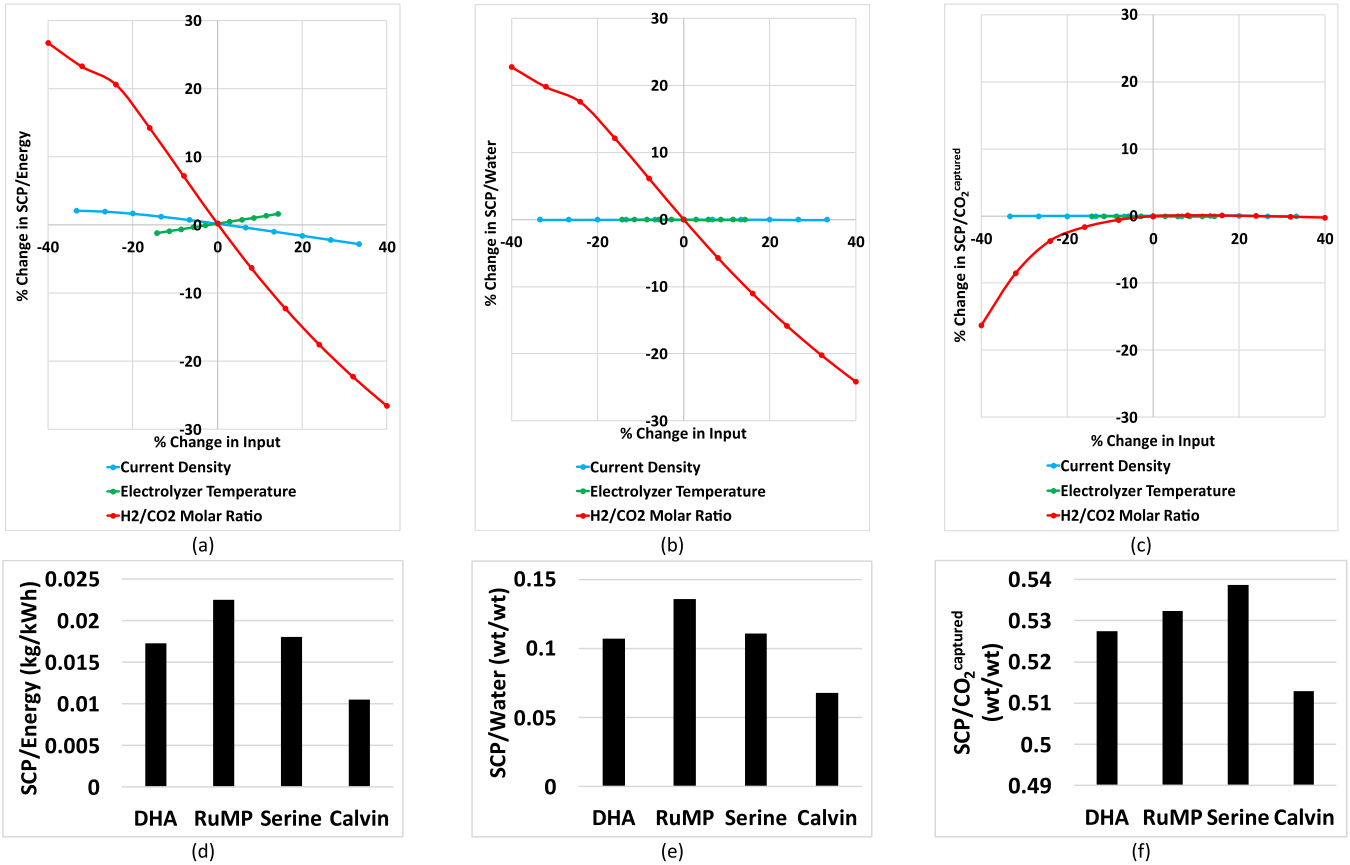


Fig. 6. Results of one-factor-at-a-time sensitivity analysis. Effect of changing variables on (a) ratio of SCP production to energy consumption (RuMP pathway), (b) ratio of SCP production to water consumption (RuMP pathway), (c) ratio of SCP production to net CO_2 captured (RuMP pathway), and changing metabolite pathway on (d) ratio of SCP production to energy consumption (CD=0.3, T=70, CH=5), (e) ratio of SCP production to water consumption, (f) ratio of SCP production to net CO_2 captured (CD=0.3, T=70, CH=5), DHA, RuMP, Serine, Calvine: metabolite pathways, CD: electrolyzer current density in A/cm^2; T: electrolyzer working temperature (°C); CH: H_2 to CO_2 molar ratio; SCP: single cell protein.

reason is that by increasing the molar ratio of H_2 to CO_2 from the smallest value (ratio of 3, 40% below the base case of 5) to the largest value (ratio of 7, 40% above the base case of 5), the amount of methanol produced decreases, and consequently, the amount of single cell protein production and energy consumption also decrease. The single cell protein production decreases by 44%, whilst the energy consumption decreases by 2.9%, which in turn reduces the SCP/Energy ratio. As a result, a lower H_2 to CO_2 ratio (not lower than 3, which is the stoichiometric ratio of H_2 to CO_2) is more favorable from the SCP/Energy ratio perspective.

Current density of the electrolyzer and its temperature have a lower impact on the SCP/Energy ratio. Results from the simulation show that as the electrolyzer temperature increases by 33% relative to the smallest value, the rate of H_2 production and consequently, methanol production decreases very slightly (both by 1.5%), which leads to a slight decrease in the amount of single cell protein produced and energy consumed. As the reduction in energy consumption (4.2%) is slightly greater than the reduction in single cell protein production (1.5%), the SCP/Energy increases; therefore, a higher temperature is more favorable.

Regarding the effect of current density, with an increase in this parameter from the smallest (33% below the base case) to the largest value (33% above the base case), the amount of H_2 production, and consequently the amount of methanol production, energy consumption, and single cell protein production increase. However, the increase in energy consumption (120%) is greater than the increase in single cell protein production (110%), resulting in a decrease in the SCP/Energy ratio; therefore, lower current density is favorable.

Regarding the SCP/Water ratio, the results in Fig. 6-b show that the H_2 to CO_2 ratio has the greatest impact on the SCP/Water ratio. By increasing the H_2 to CO_2 ratio from the lowest value (40% below the base case) to the highest value (40% above the base case), the amount of water consumption decreases (8%), but due to the higher decrease in the amount of single cell protein production (44%), the overall SCP/Water decreases. Therefore, from a water consumption perspective, a lower H_2 to CO_2 ratio is more favorable. Even though increasing the current density (100% relative to the smallest value) increases water consumption, as the magnitude of the increase in produced single cell protein (110%) and consumed water (110%) is almost equal, the SCP/Water ratio does not change by a substantial amount (less than 0.001%). This is also true for the effect of electrolyzer temperature, with the difference that increasing the electrolyzer temperature reduces both the water consumption and the single cell protein production.

Regarding the SCP/$CO_2^{captured}$ ratio (Fig. 6-c), the H_2 to CO_2 ratio has the greatest impact on the SCP/$CO_2^{captured}$ ratio. The effect of the H_2 to CO_2 ratio is nonlinear. As the H_2 to CO_2 ratio increases, the SCP/$CO_2^{captured}$ ratio increases sharply at first and then plateaus. This is because with an increase in the H_2 to CO_2 ratio, the amount of CO_2 converted into microbial biomass decreases nonlinearly. The reason for this reduction is the reduction in the amount of CO_2 consumed for methanol synthesis. From the SCP/$CO_2^{captured}$ perspective, lower H_2 to CO_2 is favorable. Similar to the previous performance indicators (SCP/Energy and SCP/Water), alterations to the electrolyzer temperature and current density had a negligible effect on the SCP/$CO_2^{captured}$ ratio. Note that, if the CO_2 used in the methanol synthesis process is from biogenic sources, its emission due to streams 21 and 24 of Fig. 1 is not considered as the system emissions. However, if this CO_2 is of fossil origin, the emissions are considered as Scope 1 emissions of the system.

The effect of the metabolic pathway on the SCP/Energy ratio, SCP/Water ratio, and SCP/$CO_2^{captured}$ ratio is shown in Fig. 6d-f, respectively. As can be seen in Fig. 6-d, the RuMP pathway has the best performance in terms of SCP/Energy ratio. This is because, although the energy consumption of the single cell protein production plant is maximum when employing this pathway, the single cell protein production rate is also maximum. This is also true for the SCP/Water ratio (Fig. 6-e). The result is different for the SCP/$CO_2^{captured}$ ratio (Fig. 6-f), in which the Calvin cycle performs best (recall that a lower SCP/$CO_2^{captured}$ ratio implies that more CO_2 is captured per kilogram of single cell protein produced). This is because the Calvin pathway has the lowest net CO_2 captured and also the lowest single cell protein production, because of the stoichiometric coefficients of the biomass production (Eq. 7).

The results show that relative performance indicators can be more helpful for decision-making purposes. For example, the absolute indicators show that increasing the H_2 to CO_2 ratio reduces energy and water consumption, which is favorable, but it also reduces the single cell protein production rate, which is not favorable. All the process performance indicators in absolute form are shown in Figures S1-S4 of the supplementary material.

The presented results demonstrate the effectiveness and applicability of the process simulation software (specifically Aspen Plus and SuperPro Designer) integration, with a focus on the study procedure itself rather than the results obtained. To perform such an analysis manually, it is necessary to transfer stream information (temperature, pressure, and mass or molar flow rates), unit operation specification (such as working temperature, pressure, and residence time), and process parameters (such as H_2 to CO_2 ratio) from one software to another. For the analysis provided in the present paper, this means the user would need to copy the aforementioned data from one software and paste it into another software 37 times to complete the one-factor-at-a-time sensitivity analysis and 16 times for the Taguchi analysis. This number of copy-paste exercises is just for completing the simulations. For the analysis of the results presented in this study, 86 different parameters (some of which are presented in the supplementary material Excel file), which were calculated by the software packages, were stored automatically. Without using the proposed integration approach, all of these 86 parameters must be retrieved manually from the three software packages (MATLAB, Aspen Plus, SuperPro Designer) and saved into a separate database for further analysis. This makes such analyses time-consuming and prone to errors.

3.3. Sensitivity assessment with Taguchi design of experiments

The results of simulations conducted using Taguchi design of experiments (DoE) are shown in Fig. 7. Current density and electrolyzer temperature have no significant effect on the SCP/Energy and the SCP/Water ratio (Fig. 7-a and Fig. 7-b, respectively). A higher H_2 to CO_2 ratio results in lower single cell protein produced per unit of energy and water consumed, making a lower H_2 to CO_2 ratio more favourable for these performance indicators. The RuMP pathway has the best performance among all metabolic pathways for both the SCP/Energy ratio and the SCP/Water ratio.

The main effect plot for SCP/$CO_2^{captured}$ is shown in Fig. 7-c. The lowest H_2 to CO_2 ratio and the Calvin pathway resulted in the lowest SCP/$CO_2^{captured}$ ratio, which is favorable in the context of the present paper.

Overall, the metabolic pathway has the greatest effect on SCP/Energy and SCP/Water, and the H_2 to CO_2 ratio has the second greatest effect. For SCP/$CO_2^{captured}$, the H_2 to CO_2 ratio has the greatest effect, followed by the metabolic pathway. The favorable level of the H_2 to CO_2 ratio aligned for SCP/Energy, SCP/Water, and SCP/$CO_2^{captured}$, meaning a lower H_2 to CO_2 ratio is better for all three performance indicators. For the metabolic pathway, the results are conflicting. This means to enhance the SCP/Energy and SCP/Water, microorganisms employing the RuMP pathway should be used, while to improve the SCP/$CO_2^{captured}$, the ones employing the Calvin pathway should be used. This conflict is where the MCDM method may be used to find a compromise solution (results are shown in the section 3.4).

Overall, the results from the Taguchi DoE are well aligned with the one-factor-at-a-time sensitivity analysis. Due to the smaller number of simulations when using the Taguchi DoE (16 simulation runs) compared to the one-factor-at-a-time sensitivity analysis (37 simulation runs), the computational cost of using a statistically informed design of experiment is much lower. The total required time for one-factor-at-a-time

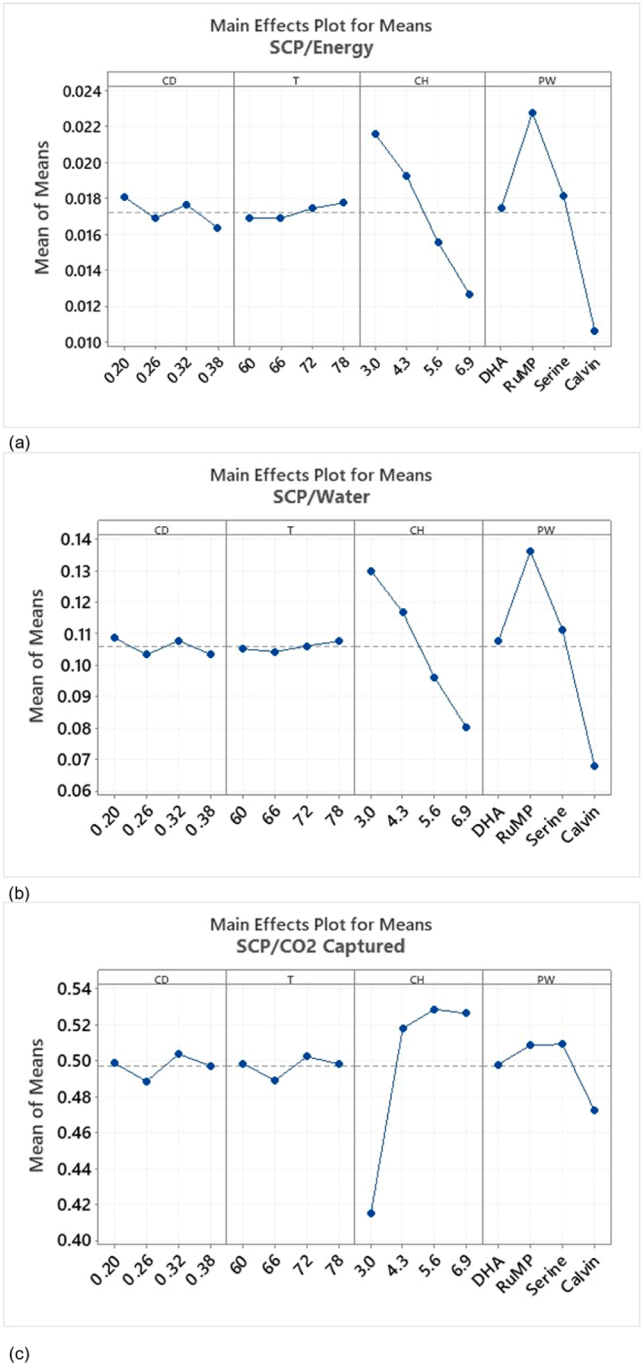


Fig. 7. Taguchi analysis, (a) Main effect plot for means of SCP/Energy, (b) Main effect plot for means of SCP/Water, (c) Main effect plot for means of SCP/$CO_2^{captured}$, CD: electrolyzer current density; T: electrolyzer working temperature; CH: H_2 to CO_2 ratio; PW: metabolic pathway.

sensitivity analysis was approximately 1726 seconds, while running the simulations designed by the Taguchi DoE required 692 seconds. Furthermore, as the type of variable for metabolic pathway (discrete) was different from the other three parameters (continuous), comparing the effect of all four factors using the spider plots (Fig. 6-a to 6-c) was not possible. This problem is not encountered when conducting the Taguchi DoE. The results of the Taguchi design of experiment are provided in the supplementary materials (section S4). The aforementioned points highlight the ability of the process simulation software integration (specifically with Aspen Plus and SuperPro Designer) to facilitate analyses such as the Taguchi method to enable more nuanced sensitivity analyses. The results of the analyses completed in this work are indicative owing to modelling limitations and simplifying assumptions, rather the ability to obtain such results from the OFAT and Taguchi method, using software integration, is of wider applicability and potential impact.

3.4. Integrating MCDM and Taguchi

As stated in the previous section, a lower H_2 to CO_2 ratio is favorable for SCP/Energy, SCP/Water, and SCP/$CO_2^{captured}$. In contrast to this unanimity, the RuMP pathway should be selected to enhance SCP/Energy and SCP/Water, while the Calvin pathway should be selected to enhance the SCP/$CO_2^{captured}$. This leads to a trade-off process that can be addressed using the MCDM method.

The results of the entropy weight calculation are shown in Fig. 8-a. Due to the greater variation in the SCP/Energy results, this performance indicator received the highest weight. The SCP/Water and SCP/$CO_2^{captured}$ received lower weights. Fig. 8-b shows the TOPSIS score and ranking of each simulation run; a higher score indicates a better ranking; therefore, run 11 (metabolite pathway: RuMP; H_2 to CO_2 ratio: 3; electrolyzer temperature: 72°C; electrolyzer current density: 0.32 A/cm^2) obtains the best score and ranking out of the 16 simulations completed for the Taguchi analysis.

The Taguchi analysis of the TOPSIS scores is shown in Fig. 8-c. Once again, the current density of the electrolyzer and the electrolyzer temperature have no significant effect on the TOPSIS scores (main effects plot, Fig. 8-c), whilst a lower H_2 to CO_2 ratio results in a better TOPSIS score (better overall performance). The RuMP pathway yields the best overall performance of the 4 pathways assessed in this work (Fig. 8-c).

3.5. Key advantages of the integrated process modelling approach

The necessity and application of integrating software packages have been highlighted in the literature (Csendes et al., 2023). In the present study, an application for the integration of process simulation software packages (Aspen Plus and SuperPro Designer using MATLAB and Microsoft Excel) is presented. This approach enables the automatic data exchange between the software packages, and it eliminates the need for manual data transfer by the user. While manual data exchange may not be challenging for a single simulation run, it becomes highly inefficient in studies where multiple simulation runs are needed, such as sensitivity analysis, identifying optimal ranges for parameters, or conducting multi-objective optimization. In addition to being time-consuming, manual data transfer is prone to error. In the current study, a one-factor-at-a-time sensitivity analysis and a design of experiment-based sensitivity assessment using the Taguchi method with 37 and 16 simulation runs, respectively, were completed in approximately 40 minutes. This is significantly easier compared to performing the same number of simulation runs by manual data exchange.

In addition to automatic data exchange, the applied integration method allows for automatic retrieval and storage of simulation results for subsequent analysis. Eighty-six different parameters were retrieved from the software packages (MATLAB, Aspen Plus, and SuperPro Designer), and all were stored automatically. Without the applied integration approach, extracting and managing this volume of results would be highly time-consuming and also prone to human error. This study also demonstrates that the applied integration method is compatible with various types of analyses, including sensitivity analysis, design of experiments, and multi-criteria decision-making.

In the study of biorefinery processes, it may be necessary to optimize multiple objectives simultaneously, as optimizing a single objective may lead to deterioration in the performance of others. Under such conditions, the application of multi-objective optimization becomes essential. Prior work by Ponce-Ortega and Hernández-Pérez (Ponce-Ortega and Hernández-Pérez, 2018) may be used as a starting point for such optimization approaches. Two main approaches are available for conducting

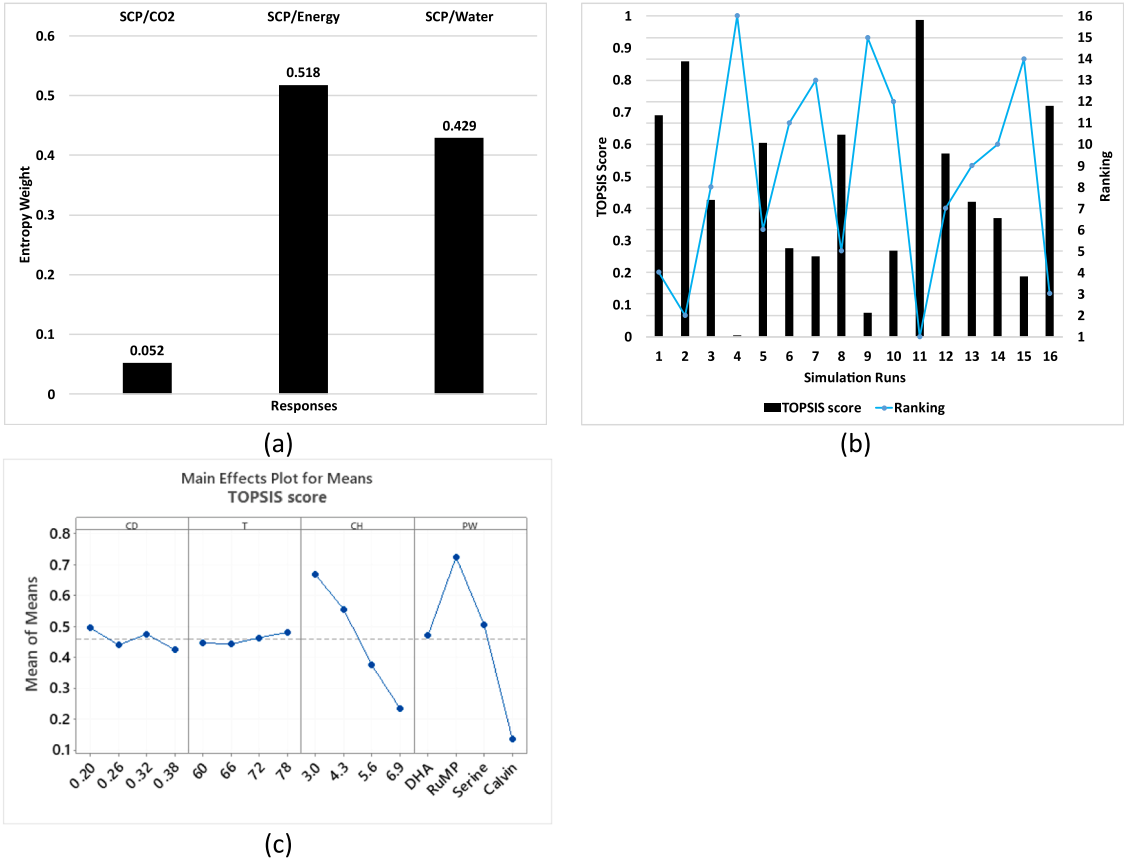


Fig. 8. Results of integrating MCDM and Taguchi method, (a) Entropy weights of indicators, (b) TOPSIS scores and rankings of simulation runs, (c) main effect plot for means of TOPSIS score; SCP: single cell protein, CD: electrolyzer current density, T: electrolyzer working temperature, CH: H2 to CO2 ratio, PW: metabolic pathway.

multi-objective optimization. In the first approach, functions that correlate the objective parameters with the process variables are derived. Subsequently, mathematical methods are used to determine the variable values at which these functions reach their extrema. Such functions can be developed using Response Surface Methodology (RSM), followed by Analysis of Variance (ANOVA). If developing such functions is not feasible, Genetic Algorithms may be employed in the optimization approach. Regardless of the optimization approach, the applied integration method in this study can facilitate and accelerate the execution of simulation cases and the extraction of results.

4. Limitations and future studies

4.1. Limitations of the proposed method

As stated in the section 2.5.2, of all the available variables in the integrated plant, only 4 are studied in this paper. Therefore, future research can examine the impact of variables that are not addressed here, such as electrolyzer working pressure, operating pressure of compressors and the reactor of the methanol synthesis plant, the Monod kinetic constants for single cell protein production, and other parameters linked to the biological conversion of methanol to single cell protein (such as temperature, pH, retention time).

The calculation of biomass concentration at the outlet of the bioreactor, which is simulated in SuperPro Designer, was performed considering ideal conditions for the substrate to biomass conversion. However, in many cases, the actual performance is far from ideal. If sufficient information is available, the substrate and biomass concentrations can be calculated under conditions closer to reality.

4.2. Limitations of software packages

The simulated process for the methanol synthesis plant contains a recycle stream (stream 26 in Fig. 1). The process simulations containing recycle streams are solved by built-in trial-and-error methods in both Aspen Plus and SuperPro Designer, as outlined in the supplementary material (section S6). Since the initial guess affects the convergence of the process simulation in both software packages, when conducting a sensitivity analysis, the parameters must be changed within a range that still allows the simulations to converge. Furthermore, a wide range of variations for the parameters studied in the sensitivity analysis means a larger number of simulations, and the longer the time required to perform it. Note that process models without recycle streams have lower computational costs and are less susceptible to divergence because the equations are solved with one iteration, and there is no need for an initial guess (affecting divergence possibility) and trial and error (affecting computational cost).

Some parameters from the SuperPro Designer software package are not accessible through the Excel library, such as substrate affinity in a kinetic fermentation reaction. This makes it impossible to study the impact of these parameters on system performance using the applied integration method.

Ideal reactor models are used to simulate the methanol synthesis (plug flow reactor) and single cell protein production (continuous stirred tank reactor); however, industrial reactors do not follow ideal reactor behavior (Levenspiel, 1998). This can lead to a difference between the simulation results and what can happen on an industrial scale in terms of flow rates and compositions of products and byproducts. Therefore, using non-ideal reactor models can lead to more accurate and realistic results. Neither Aspen Plus nor SuperPro Designer has a built-in

module for the simulation of non-ideal reactors; therefore, using Aspen Custom Modeler or MATLAB may be required for this purpose. Using the applied integration method, it is possible to use MATLAB to simulate the non-ideal reactors and integrate it with Aspen Plus and SuperPro Designer.

4.3. Limitations of the studied processes

The CO_2 capture process was not simulated in the present study (see Fig. 1 for the system boundary), and future research could include adding this process to the entire plant and assessing its effects on the overall plant performance. Furthermore, this study did not include texturing or flavouring processes, which are important for single-cell protein applications in food or feed. In the context of single cell protein, protein extraction from different microbial biomass types could also be incorporated into the simulation. Future studies could explore other types of high-value microbial products, such as nutritional oils, pigments, or specific proteins produced via precision fermentation.

There are several different substrates, microorganisms, and metabolic pathways available for single cell protein production, and each of them can affect the economic and environmental performance of the whole process (Sakarika et al., 2022). In future work, other substrates with different metabolic pathways and kinetic constants can be studied. Similarly, there are multiple different types of water electrolyzers (such as proton exchange membrane and solid oxide electrolyzer) and methanol synthesis processes (such as biomethane to methanol and biomass gasification to methanol), which can be the subject of future studies.

The limitations discussed in this section, as well as the simplification assumptions, reduce the potential level of accuracy of the results presented regarding the performance of the power-to-protein process. It should be noted that the primary focus of this study is presenting a method for integrating Aspen Plus and SuperPro Designer. Future research can address some of the limitations of the process modelling completed for the power to protein process, thereby enhancing the certainty and robustness of process studies on power-to-protein systems.

5. Conclusion

In this paper, a method for integrating Aspen Plus, and SuperPro Designer using MATLAB and Microsoft Excel is applied to study single-cell protein production using methanol as substrate, within the power-to-protein concept. By using the aforementioned method, 53 simulation cases were run in approximately 40 minutes. All the data are automatically exchanged between software packages, and the results of simulation runs are retrieved automatically. Manual data exchange and recording for such many simulations would be a difficult, time-consuming task, and prone to error.

The simulation results show that the electrolyzer has the largest share of energy and water consumption (90% and 83.5%, respectively). Also, the energy and water consumption for the reduction of nucleic acids is significant (0.4% and 2.5%). The amount of oxygen produced by the electrolyzer (729 kg/hr) is much higher than the amount required by the bioreactor (233 kg/hr); therefore, the excess oxygen may be used in other bioreactions or be sold for additional revenue. The CO_2 emissions from the system show that the single-cell protein production using methanol (produced via CO_2 hydrogenation) as substrate may be considered as a carbon-consuming process with a high-value product, if the energy required is provided by renewable sources. By examining the process parameters, it was determined that the ratio of H_2 to CO_2 and the metabolic pathway have the greatest impact on energy consumption, water consumption, and consumed CO_2. In addition, reducing the H_2 to CO_2 ratio and using microorganisms employing the RuMP pathway improves the system's performance across all three performance indicators (water, energy, and CO_2 consumption). It should be noted that due to the simplifying assumptions and system boundary limitations applied within this work, future work is required to refine the results obtained. The results can be a guide to investigate the feasibility of using the circular economy approaches for single-cell protein production and highlight the capabilities of the process simulation software integration.

CRediT authorship contribution statement

Mohammadali Babanejadi Sorkhab: Writing – original draft, Methodology, Formal analysis, Conceptualization. **Myrsini Sakarika:** Writing – review & editing. **Archishman Bose:** Writing – review & editing, Supervision. **Jerry D. Murphy:** Writing – review & editing, Supervision. **Richard O'Shea:** Writing – review & editing, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2026.109725.

Data availability

Data will be made available on request.

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