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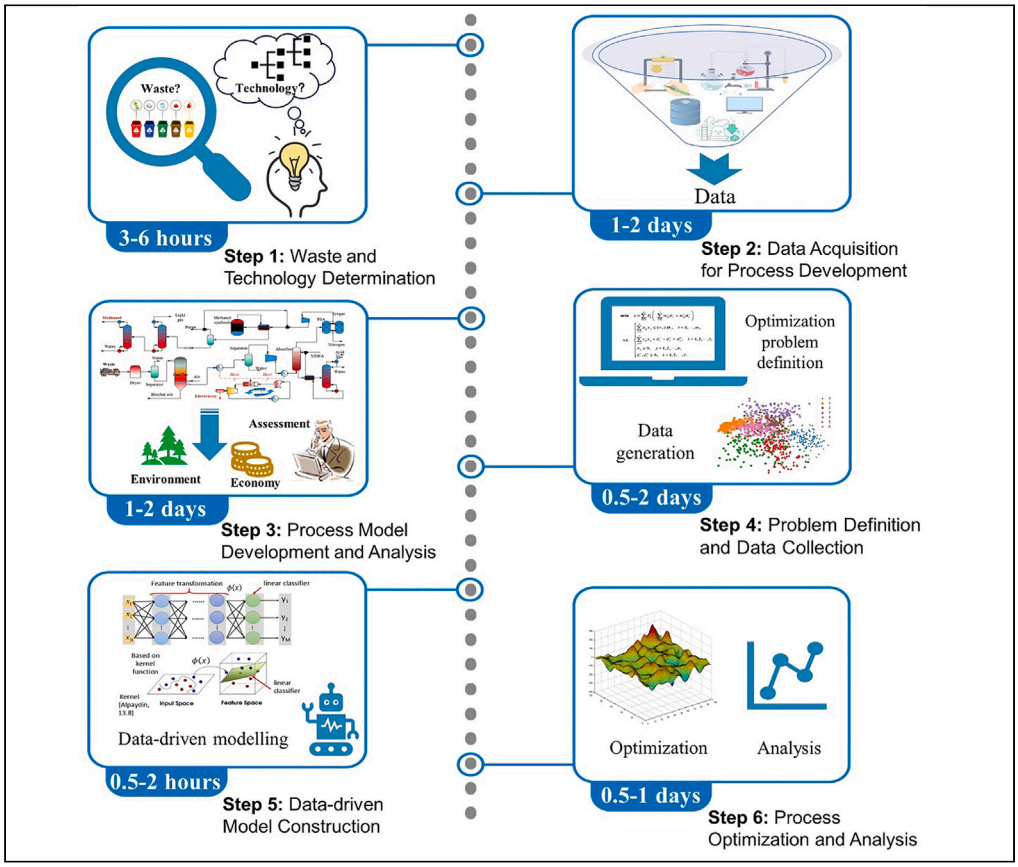
Protocol for the design and accelerated optimization of a waste-to-energy system using AI tools



Amid a surge in waste volume, the need to achieve sustainable waste treatment has become increasingly important. Here, we present a protocol for the design and accelerated optimization of a waste-to-energy system using artificial intelligence tools. We describe steps for waste treatment process advancement as demonstrated by the medical waste-to-methanol conversion and implementing data-driven process optimization. We then detail procedures for streamlining tasks by establishing connectivity between systems such as Aspen Plus and MATLAB.

Publisher's note: Undertaking any experimental protocol requires adherence to local institutional guidelines for laboratory safety and ethics.

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Highlights

Guidelines for designing a sustainable waste treatment process

A novel process of medical waste-to-methanol conversion is demonstrated

Detailed steps for implementing AI-based optimization

Operations are efficiently optimized for minimum greenhouse gas emissions

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Protocol for the design and accelerated optimization of a waste-to-energy system using AI tools

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SUMMARY

Amid a surge in waste volume, the need to achieve sustainable waste treatment has become increasingly important. Here, we present a protocol for the design and accelerated optimization of a waste-to-energy system using artificial intelligence tools. We describe steps for waste treatment process advancement as demonstrated by the medical waste-to-methanol conversion and implementing data-driven process optimization. We then detail procedures for streamlining tasks by establishing connectivity between systems such as Aspen Plus and MATLAB.

For complete details on the use and execution of this protocol, please refer to Shi et al. (2022)[1] and Fang et al. (2022).[2]

BEFORE YOU BEGIN

Scope

This protocol describes a framework that integrates the design of sustainable process for converting waste into energy and the optimization of operating parameters with high efficiency. The case illustrated here is to design and optimize a valorization process of converting medical waste (MW) into methanol (MeOH) while this framework is also adaptive to other types of waste such as sewage sludge, plastic waste, food waste. A systemic classification of these wastes is presented in Table 1. Through the implementation of this framework, new insights into the waste valorization with economic viability and carbon neutrality can be obtained. Besides, optimization of operating parameters provides the maximum potential of the process for application. The framework represents a significant step toward more sustainable waste management practices and mitigating the impacts of climate change. It aligns with global efforts to transition to a low-carbon economy and reduce greenhouse gas emissions while still harnessing the energy potential of waste materials.

Structure of AI-based operation optimization

Though a detailed first-principle model exhibits accuracy in capturing the complex relationships between process parameters and process performance, it becomes computationally challenging due to the incorporation of numerous nonlinearities. Thus, data-driven optimization has emerged as a promising approach, particularly in the era of artificial intelligence (AI) and machine learning. Figure 1 provides an overview of data-driven operational optimization grounded in machine learning. Shaded boxes represent the procedural steps, while dashed boxes signify the necessary information or techniques employed to accomplish these steps. When dealing with novel processes for which there is no existing production data, a detailed process model is developed to facilitate data generation through process simulation. This is achieved by employing a suitable sampling strategy.

Table 1. Systematic groups of different wastes

Waste categories	Descriptions	Examples
Municipal solid waste	• Wet organic materials that are derived from living animals and anthropical activities.	• Sewage sludge, food waste, livestock, manure.
	• Anthropical waste derived from the consumption of industrial products with relatively lower moisture	• Plastics, paper, cardboard, medical waste, waste tires.
Biomass waste	• Biodegradable waste and residues from agriculture and forestry sections.	• Crop residue, woody biomass, rice husk, sugarcane bagasse.

Subsequently, this generated data becomes the foundation for constructing a data-driven model through machine learning and AI techniques. The resulting model holds the potential to accurately represent process behaviors while maintaining a relatively lower level of complexity. Consequently, the utilization of AI-based model is expected to accelerate the optimization process. In cases where the identified optimal solution is unattainable, such as when the validated error exceeds the maximum acceptable threshold, this solution can serve as a new data point within training set to retrain the model. This allows for updating model iteratively and ensuring the achievement of a feasible solution.

Hardware and software requirements

An increasing number of process simulators have facilitated the ease of conducting process design simulations. Table 2 provides an overview of common software packages suitable for chemical process simulations. It's noteworthy that, with the exception of DWSIM, the listed software is not open-source. Given the rapid advancements in AI, numerous software platforms are now available, compatible with Windows, Linux, and macOS, making AI-based process optimization accessible. Table 3 presents some of the commonly used platforms and outlines their respective features. These options include Python-based tools such as PyCharm and Spyder, as well as RStudio and MATLAB, among others. The hardware prerequisites for the target waste treatment process rely significantly on the size and complexity of process. To ensure optimal performance, we highly recommend utilizing a modern quad-core processor accompanied by a minimum of 16 GB of RAM. In this protocol, Aspen Plus and MATLAB are used to develop and optimize a novel MW-to-MeOH process.

Note: Aspen Plus V11 and MATLAB 2021a are used in our case study.

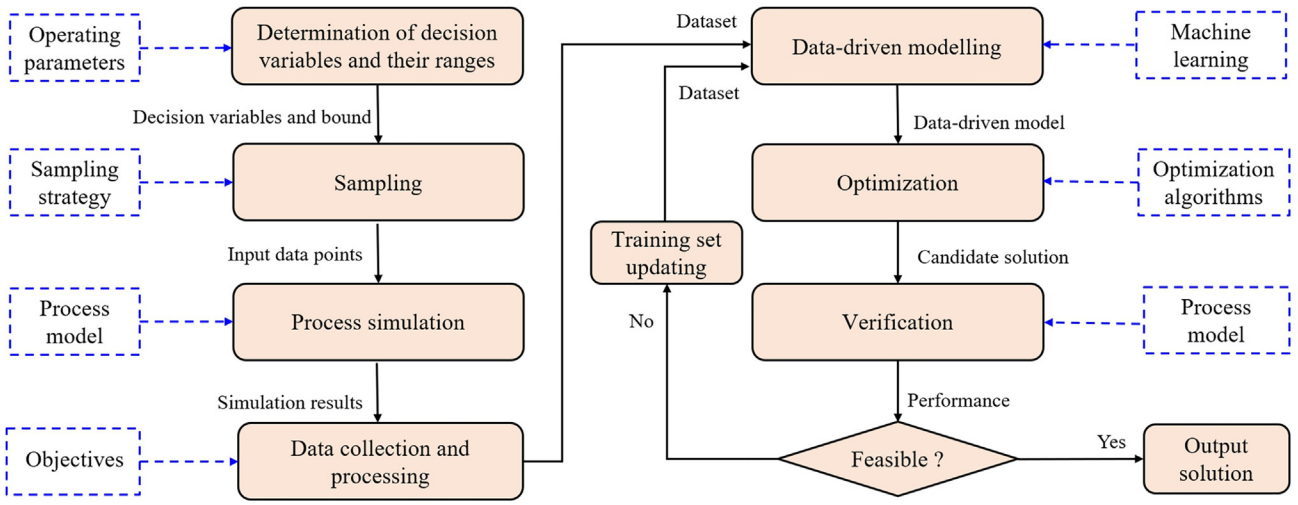

Figure 1. Overview of data-driven operation optimization based on machine learning (AI)

Table 2. Software packages for chemical process simulation

Software	Key features	Limitations and drawbacks	Supported OS
Aspen Plus	• Extensive library of components and models • Comprehensive modules for simulation • Widely used in the industry	• Expensive licensing • Steeper learning curve	• Windows
Aspen HYSYS	• Extensive modeling capabilities • Integration with AspenTech suite	• Expensive licensing • Specialized for certain industries	• Windows
DWSIM	• Open-source and free • User-friendly interface • Suitable for education and smaller-scale simulations	• Limited application support • Smaller user community	• Windows, macOS, Linux
gPROMS	• Advanced process modeling and optimization • Used in chemical and pharmaceutical industries	• High licensing costs • Complex for beginners	• Windows, Linux
ProSimPlus	• Rich process engineering software • Extensive modeling and optimization capabilities	• Expensive • Need a steeper learning curve	• Windows
ChemCAD	• User-friendly interface • Versatile for unit operations and reactions • Good for educational purposes	• Limited component library • May lack advanced features	• Windows

Note: Aspen Plus is a large-size commercial software which requires a suitable operating system version, processor type, memory size and most important, the valid license. The installation procedure should be carried out following the instructions provided in the official documentation.

Note: For convenience of using optimization tools integrated in MATLAB, we recommend installation of optimization toolbox available in MATLAB applications.

KEY RESOURCES TABLE

REAGENT or RESOURCE	SOURCE	IDENTIFIER
Deposited data		
Dataset for data-driven modeling	This paper	https://doi.org/10.17632/vmh244j5s9.2
Software and algorithms		
Aspen Plus file containing MW-to-MeOH process model	This paper	https://doi.org/10.17632/vmh244j5s9.2
MATLAB file containing data-driven operation optimization program	This paper	https://doi.org/10.17632/vmh244j5s9.2

STEP-BY-STEP METHOD DETAILS

The following section describes in detail the steps to design and optimize a waste-to energy process by synergistically using Aspen Plus, MATLAB. The delineation of these steps divides into two aspects: Steps 1–3 encompass process design and development while Steps 4–6 are related to process optimization based on machine learning technique. We have developed a MATLAB code to streamline this optimization process automatically (see key resources table). To illustrate these principles, we present a practical case study involving the conversion of MW into MeOH.

Step 1: Waste determination and feasible technology selection

Timing: 3–6 h

In this step, the focus is on defining waste and selecting feasible technologies, including reaction synthesis and separation synthesis.

Table 3. Platforms for AI-based process optimization

Platforms	Advantages	Disadvantages	Supported OS
PyCharm	• User-friendly interface • Rich ecosystem of plugins • Excellent support for Python	• Commercial license required • Heavier on system resources • May have a learning curve for beginners	• Windows, Linux, macOS
Spyder	• Open-source and free • Built-in support for data analysis • Integration with scientific libraries	• May not be as feature-rich as commercial tools • User interface may be less polished	• Windows, Linux, macOS
Jupyter	• Open-source and highly customizable • Supports interactive data exploration • Great for sharing code and results	• Requires some Python programming proficiency • Lacks mature IDE for development • May require additional setup for some languages	• Windows, Linux, macOS
RStudio	• Specialized for R language • Comprehensive tools for data analysis • Excellent for statistical modeling	• Limited support for languages other than R • Not as versatile for general-purpose programming • May have a steeper learning curve for beginners	• Windows, Linux, macOS
MATLAB	• Strong support for parallel and GPU computing	• Commercial license required • Expensive for individual users • Not open source, limiting customization	• Windows, Linux, macOS
GAMS	• Tailored for mathematical optimization problems • Excellent solver support • Suitable for large-scale optimization	• Requires licensing and may not be cost-effective • Steeper learning curve for beginners • Less suitable for general-purpose programming	Windows, Linux, macOS
Julia	• High-performance, dynamic language • Exceptional numerical and scientific computing • Seamless integration with C, Fortran, and Python	• Smaller user base compared to Python and R • Fewer mature libraries compared to Python and R • Learning curve for those new to the language	Windows, Linux, macOS

1. Waste determination:
   a. Determine the type of waste.
      i. In the exemplary deployment of the protocol, our target waste is MW, characterized by its hazardous and infectious nature.

⚠ CRITICAL: Different types of waste has different characteristic, which play an important role in the selection of treatment technologies.

2. Feasible reaction pathway selection:
   a. Select the primary treatment technology.
      i. Plasma Gasification.

⚠ CRITICAL: The selection of reaction pathways should be conducted according to the experimental studies which has proved the feasibility and safety.

Note: We select plasma gasification for primary treatment of MW because it yields syngas mainly composed of H_2, CO, and CO_2, with the added advantage of no toxic by-products.[3]

   b. Select the Downstream upgrade technology for energy vector production.
      i. MeOH synthesis.

⚠ CRITICAL: Designing the downstream conversion process is of paramount significance, as it aims to enhance economic profitability while concurrently mitigating the environmental footprint.

Note: we determine syngas-to-MeOH synthesis by the following rationales: 1) MeOH holds a notable market value, serving both as a versatile fuel and a kind of valuable chemicals; 2) The MeOH derived from MW via syngas intermediates presents a promising avenue for the development of carbon-neutral fuels.[4]

3. Feasible separation technology selection:
   a. Analyze the potential components to be separated.
      i. H_2S in the syngas.
      ii. CO_2 in the syngas.
      iii. N_2 in the syngas.
      iv. Light gas in the initial product (MeOH).
      v. Water in the initial product (MeOH).

Note: Analyze the mixture in the potential stream first. In the demonstrated example, we determine the potential components to be separated based on the following analysis: 1) Given the presence of acid gases such as H_2S in the syngas, which have the potential to deactivate catalysts during MeOH synthesis[1]; 2) Effective capture of CO_2 within the syngas is vital to achieving carbon reduction objectives; 3) The significant presence of nitrogen gas (N_2), sourced from air as the gasification agent, has the potential to substantially increase equipment capacity requirements; 4) Following MeOH synthesis, the resultant product stream comprises MeOH, water, and various light gases, necessitating further purification.

   b. Select a separation technology for each stream to be purified.
      i. Methyldiethanolamine (MDEA)-based method for separating H_2S in the syngas.
      ii. Monoethanolamine (MEA)-based method for CO2 capture after removing acid gases.
      iii. Pressure swing adsorption (PSA) technology for N_2 removal.
      iv. Distillation for MeOH purification.

Note: We opt for a methyldiethanolamine (MDEA)-based method due to its remarkable selectivity in absorbing H_2S and its lower heat requirement for regeneration compared to other amines.[5] Since MDEA-based systems have limited CO_2 adsorption capacity when there are some acid gas impurities,[5] we employ a monoethanolamine (MEA)-based system additionally for CO_2 capture after removing acid gas. In the purification of MeOH, a traditional distillation approach has been employed, as it remains one of the most widely accepted and utilized methods for separating liquid mixtures effectively.

Note: For simple gas-liquid separation involved in the process, flash is usually employed.

Step 2: Acquire data to support process model development

Timing: 1–2 days

This step aims at acquiring data related to characteristic of feedstock and the modeling of main units from experiments, plants, literature, waste treatment departments, or open databases.

4. Waste analysis data acquirement:
   a. Collect data that can be used to characterize the waste.
      i. In this protocol, proximate and ultimate analysis results of MW are derived from previous experimental studies,[6] as illustrated in Table 4.
5. Data acquirement process modeling:
   a. Collect data related to technologies including the involved reactions, reaction conversion rates, kinetic parameters, etc.

Note: Detailed insights into the modeling of MW gasification and MeOH synthesis can be referenced in our previous studies.[1,7]

   b. Determine base design features and assumptions for the key units.

Table 4. Proximate and ultimate analysis of MW

	Proximate analysis (wt %)				Ultimate analysis (wt %)					
Waste	Moisture	Ash	Volatiles	FC	C	H	O	N	S	LHV (kJ/kg)
MW[6]	7.04	1.89	82.37	8.70	48.99	7.20	43.52	0.22	0.08	15,570

FC: fixed carbon. LHV: lower heating value.

i. In the context of MW-to-energy technologies, we derive the values of key operating parameters based on previous work and domain knowledge, which are elaborated in Table 5.

Note: Due to the complexity of gasification reactions, there presently exists no comprehensive mechanism for modeling the process. Therefore, we consider a simplified modeling approach.

Note: We determine some values of operating parameters like number of trays, reflux ratio and distillate flowrate involved in the distillation column through iterative trials in the subsequent process simulation.

Step 3: Process model development and analysis

Timing: 1–2 days

This step is to develop and analyze a detailed process based on the determined waste type, reaction and synthesis technologies. Figure 2 presents the main procedures.

6. Model development for key units:
   a. Construct models for the key units.
      i. The operational units are represented by various blocks in Aspen Plus, as outlined in Table 6.

Note: Notably, the plasma gasification unit holds paramount significance within the entire process, yet there is no predefined block to model it. Therefore, we decompose it into drying, pyrolysis, and gasification stages, informed by prior observations,[12] and subsequently

Table 5. Summary of the process design features and simulation assumptions

Operation units	Parameter/characteristic	Values	Units
Plasma gasification	Temperature	1560.5[8]	°C
	ER	0.1[8]	–
	SMR	0.99[8]	–
MDEA system	CO_2 removal efficiency	10[1]	%
	Acid gas removal efficiency	100[1]	%
	Duty	6.668[1]	kwh/kg CO_2
MEA system	CO_2 removal efficiency	85[9]	%
	Duty	4[9]	MJ/kg
PSA	N_2 removal efficiency	100[10]	%
	Duty	0.069[10]	kwh/kg feed
MeOH synthesis	Temperature	240[11]	°C
Distillation (removal of light gas)	number of trays	10	–
	Reflux ratio (RR)	0.5	–
	Distillate flowrate (DF)	0.39	Kmol/h
Distillation (removal of water)	number of trays	12	–
	Reflux ratio (RR)	1	–
	Distillate flowrate (DF)	11	Kmol/h

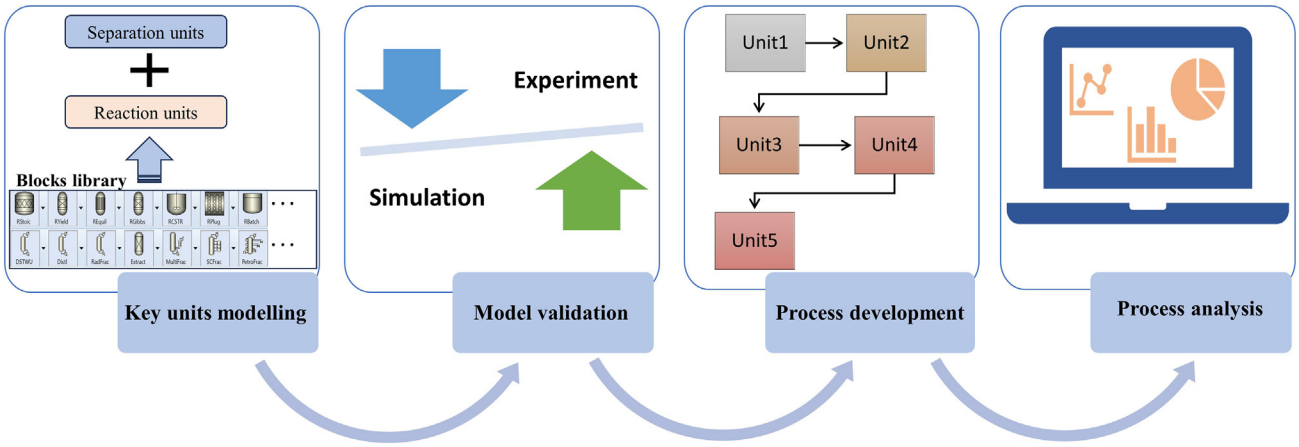

Figure 2. Workflow of process model development and analysis

employed suitable blocks to model these stages. For the MeOH synthesis reactor, we employ the RPlug block.

Note: Using simplified models for units that may not hold a critical role in the overall process can effectively reduce the laborites.

7. Model verification:
   a. Validate the model for units lacking established blocks in the simulator.
      i. To validate our developed plasma gasification model, we compare the simulated results with experiments conducted under identical feed and operating conditions.

Note: In this study, we utilize the Gibbs reactor module within Aspen Plus to simulate the gasification zone. This reactor module is adaptable, allowing us to fine-tune its settings to achieve results that align with experimental data. Initially, we recommend employing chemical and phase equilibrium settings in the Gibbs reactor. If this approach does not yield satisfactory results, we can use a restricted chemical equilibrium approach. This involves specifying predefined reactions within the Gibbs reactor and subsequently adjusting the temperature parameters for these reactions to ensure a more consistent match between our simulation results and the experimental data. For a more comprehensive understanding of these procedures, please refer to our previous work.[1]

8. Comprehensive process development:
   a. Intensify process.
      i. To recover and harness energy contained in the high-temperature syngas from plasma gasification, we incorporate a steam cycle (SC) into the process, enhancing energy efficiency while simultaneously reducing carbon emissions.

Note: In pursuit of process intensification, identify critical spot that can be further improved.

   b. Assemble the entire process.
      i. Construct the complete by integrating the requisite equipment for pressurization, decompression, and the heating and cooling of various streams.
   c. Test the process by simulation.
      i. In Aspen Plus, we execute the simulation to check the convergence of the process.

Table 6. Blocks used for modeling in Aspen Plus

Operation units	Blocks in aspen plus
Plasma gasification	RStoic (drying)
	RYield (decomposition)
	RGibbs (gasification)
MDEA system	Sep
MEA system	Sep
PSA	Sep
MeOH synthesis	RPlug
Distillation	RadFrac

⚠ CRITICAL: When errors or warnings arise, we must identify the problematic modules and appropriately adjust the block parameters.

Note: Trial-and-error parameter adjustments may be necessary to achieve process model convergence.

9. Process analysis:
   a. Assess the process.
      i. To evaluate process performance, we calculate key metrics such as product conversion rates, equipment capital costs, annual utility expenses, and total greenhouse gas (GHG) emissions of the MW-to-MeOH process as an illustrative example.

Step 4: Optimization problem definition and data collection

Timing: 0.5–2 days

10. Optimization problem definition:
    a. Define the objective.
       i. In this context, our objective is to minimize the total GHG emissions.

Note: Selecting a comprehensive metric as optimization objective is important. In our example, we use GHG emissions as the objective based on the following two reasons: It significantly impacts environmental performance while is negatively related to economic performance. The process's primary product, MeOH, derives from CO_2 and H_2, and fewer CO_2 emission signify higher product yield. Reduced emissions derived from utility usage also translate to lower annual costs.

    b. Select appropriate operating parameters as decision variables.
       i. Gasification temperature (GT).
       ii. Equivalent ratio in gasification (ER).
       iii. MeOH synthesis temperature (MT).
       iv. Distillate flow rate of the distillation column for light gas removal (DF).
       v. Reflux ratio of the distillation column for light gas removal (RR).

Note: To represent the chosen objective, we should carefully select pertinent operating parameters based on knowledge, literature, experience, or thorough analysis. We select the demonstrated operating parameters within MW-to-MeOH process because extensive analysis has identified them as the principal factors influencing the process.[13]

    c. Determine the ranges of decision variables.
       i. Table 7 provides details regarding the selected decision variables and their respective ranges.

Table 7. Operating parameters and their ranges defined in the studied case

Operating parameters	Lower bound	Upper bound
GT (°C)	1500	1700
ER	0.1	0.42
MT (°C)	250	280
DF (kmol/h)	0.2	0.5
RR	0.3	0.7

Note: The selection of operating parameters and the definition of their acceptable ranges hinge significantly on the distinctive attributes of the specific problem under consideration. In our particular case, the primary aim is to demonstrate the viability of AI-driven optimization. Consequently, we did not dedicate extensive efforts to meticulously refining the variables and specifying their associated ranges.

Note: For easily calling, we program the GHG emissions (see quantification and statistical analysis) using calculator built in Aspen Plus.

11. Data collection:
    a. Establish the Sampling Strategy.
        i. In our case study, we utilize Latin hypercube sampling (LHS), which is elaborated upon in the quantification and statistical analysis.
    b. Collect data by running simulation.
        i. We efficiently collect data by establishing a connection between Aspen Plus and MATLAB.

Note: The quantity of data essential for machine learning relies on the dimensionality of input variables and the complexity of process model. Typically, high-dimensional and complex problems require more data.

Note: It's advisable to augment the target data collection volume suitably. This is necessary since certain inputs may be unfeasible during simulation, failing to adhere to the constraints inherent in the process model, and potentially leading to unreliable simulation results.

Step 5: Data-driven model construction using AI techniques

Timing: 0.5–2 days

12. Data processing:
    a. Data cleaning.
        i. Remove data points with errors or warnings simulation running state.
        ii. Normalize and transform the data to ensure its quality and suitability for machine learning algorithms.

Note: In Aspen Plus, the feasible running state is identified as "8", which serves as a data screening criterion.

    b. Data splitting.
        i. To prevent overfitting and ensure robust model evaluation, we divide the dataset into 80% and 20% as training set and test set. Besides, we use 5-fold cross validation to optimize the structure of model.
13. Data-driven model construction:
    a. Determine the machine learning technique.

i. We select typical 3-layer artificial neural network (ANN) with rectified linear unit (ReLU) activation, which has simple structure while allows for accurate representation of the nonlinear systems involved in chemical processes. For an in-depth performance comparison of ANNs with various activation functions, please refer to our previous studies.[14]

Note: An appropriate machine learning technique is important for constructing data-driven models to describe the relationship between the decision variables and the objective.

b. Train a data-driven model.
   i. Train the selected model using the training dataset.
   ii. Use 5-fold cross validation to optimize the number of neurons in the hidden layer of ANN for better performance.
c. Test the data-driven model.
   i. Calculate the mean absolute error (MAE), mean relative error (MRE), mean square error (MSE) and coefficient of determination (R^2) base on test data for assessing generalization ability.

Note: The utilization of established functions integrated within the MATLAB platform accelerates the construction of most machine learning models.

Step 6: Process optimization and analysis

Timing: 0.5–1 day

14. Process optimization:
    a. Select an appropriate optimization algorithm.
       i. Employ particle swarm optimization (PSO) to optimize the decision variables to achieve minimum GHG emissions based on the constructed data-driven model.

Note: We have demonstrated the effectiveness and efficiency of PSO in our previous studies.[15]

    b. Conduct optimization.
       i. Run the optimization algorithm until the termination criteria is achieved.

Note: We recommend installing optimization toolbox in MATLAB for successfully executing the code of optimization.

Note: We determine the population size of PSO as 30[15] while the other parameters are mainly according to the default value of toolbox.

15. Solution validation:
    a. Run simulation model based on the optimal solution.
       i. Input the candidate solutions obtained through optimization into the process model and simulate their performance.
    b. Assess the optimization results.
       i. Calculate the error between simulated objective value and predicted value using data-driven model.

Note: If the error is over the maximum allowed value, see "troubleshooting: Feasibility of data-driven optimization result".

16. Validate the efficiency of optimization based on data-driven model:
    a. Employ the selected optimization algorithm to optimize the process based on the detailed model.
        i. Employ PSO to optimize the MW-to-MeOH process based on the Aspen Plus model.
    b. Compare the optimization time and objective value derived from different optimization schemes. This step provides valuable insights into the trade-offs between detailed modeling and data-driven optimization approaches.

Note: Considering the computational load involved in optimization based on process model, we relax the optimization termination criteria appropriately.

EXPECTED OUTCOMES

Analysis of waste-to-energy process

Steps 1–3 encompass the design and development phases of waste treatment processes. In a case study, we focus on the MW-to-MeOH process and successfully develop the process model within Aspen Plus, as depicted in Figure 3. (For the detailed file containing the process model, please see key resources table). The process begins with MW (stream FEED) entering the plasma gasifier to produce syngas. Plasma gasification's feasibility is verified through comparison with experimental results, as shown in Table 8, where the mole fractions of key syngas components align between model predictions and experiments with quite low absolute errors. To harness the heat energy within the high-temperature syngas (stream MSG), we employ a SC for power generation. Subsequently, the cooling syngas (stream CGS) undergoes gas cleaning, with separation units modeled using Sep blocks in Aspen Plus. The cleaned syngas (stream H2CO) is pressurized and enters the MeOH synthesis reactor. To enhance the conversion rate, unreacted gases are recycled to the reactor, with a small portion (stream PURGE) being purged. Primary MeOH production (stream L-MEOH) then undergoes further purification through two distillation columns in series for light gas and water removal.

The developed process model facilitates comprehensive assessments of its potential. Figure 4 illustrates exemplary economic analysis results for MW-to-MeOH process, with a MeOH conversion rate of 0.69 kg MeOH/kg waste, resulting in a total capital investment of 10.20 MM$ for equipment procurement. Additionally, annual utility costs for electricity, steam, coal, and cooling water are estimated at 0.188 MM$/year, 0.067 MM$/year, 0.132 MM$/year, and 0.023 MM$/year, respectively. It's important to note that the economic analysis includes additional factors such as operator salaries

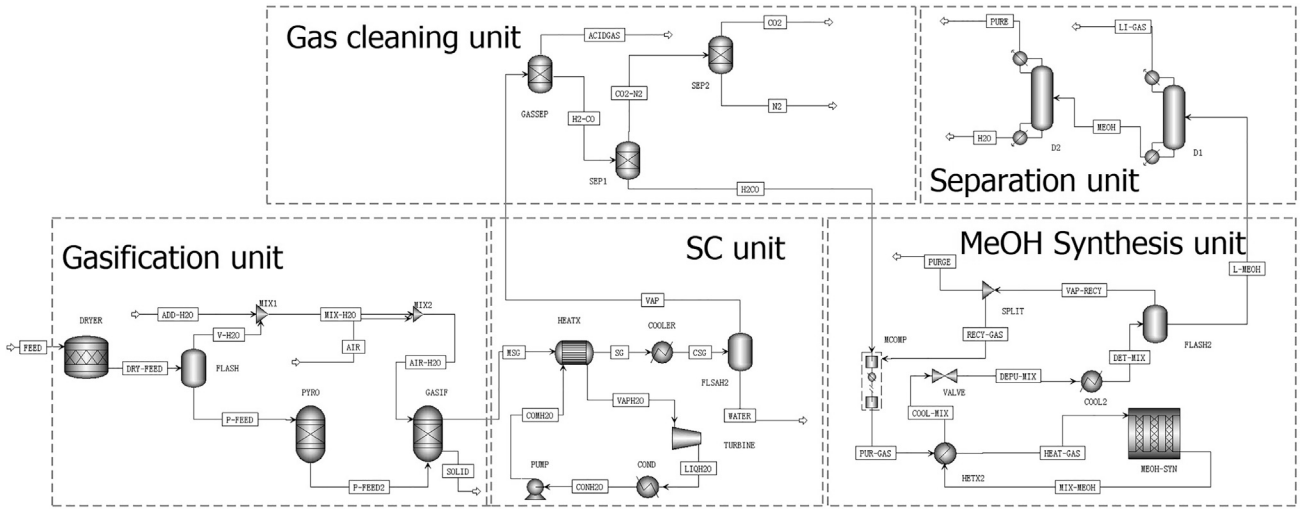

Figure 3. Flowsheet of MW-to-MeOH process

Table 8. Validation results of plasma gasification model

Syngas composition	H_2	CO	CO_2	H_2O	N_2
Simulation results (mol %)	42.73	33.89	0.016	16.26	5.39
Experimental results (mol %)[16]	43.5	34.5	0.03	16.22	5.63
Absolute error (mol %)	0.77	0.61	0.014	0.04	0.24

and land costs. These factors are typically proportional to the main contributors to total capital and costs. In this demonstration, we primarily focus on calculating two key elements that significantly contribute to the overall capital and cost figures. Assessing the environmental impact of the developed process is a crucial aspect of evaluating its sustainability. In this study, we conducted an estimation of the GHG emissions associated with the process to reflect its environmental performance. A comprehensive breakdown of emission sources and categories can be found in Figure 5. Notably, emissions from utilities dominate the overall emissions profile. Despite the offsetting effect of power generation in SC, there remains an annual emission of nearly 30,000 tons of equivalent CO_2, which is approximately ten times higher than the direct emissions from the process itself. To put this into perspective, the treatment of each kilogram of MW results in 2.71 kg of equivalent CO_2 emissions, with a daily total of 32.52 tons of equivalent CO_2 emissions. Notably, in 2021, the emission from Hong Kong industry process and product use sector is 4684.93 t eqCO_2/day.[17] Detailed equations for calculating economic and environmental indicators can be found in the quantification and statistical analysis.

Analysis of AI-based process optimization

After determining the optimization objective and the related decision variables, data is collected by running simulation (For detailed dataset, please see key resources table). Sensitivity analysis of hyperparameters on the model accuracy is required to avoid over fitting. 5-fold cross validation is employed in analyzing influence of neuron number within hidden layer on the ANN performance. The results shown in Figure 6 indicate that with ten neurons in the hidden layer, the ANN model yields satisfactory performance. The ANN model's performance in test set is illustrated in Figure 7, with low MSE, MAE, MRE and high R^2 (These metrics are calculated by equations presented in quantification and statistical analysis). The results demonstrate a high-performance data-driven model with computational advantages has been constructed.

The machine learning model facilitates accelerated process optimization by simplifying the relationship between objectives and selected operations. In our case study, the ANN model is used with

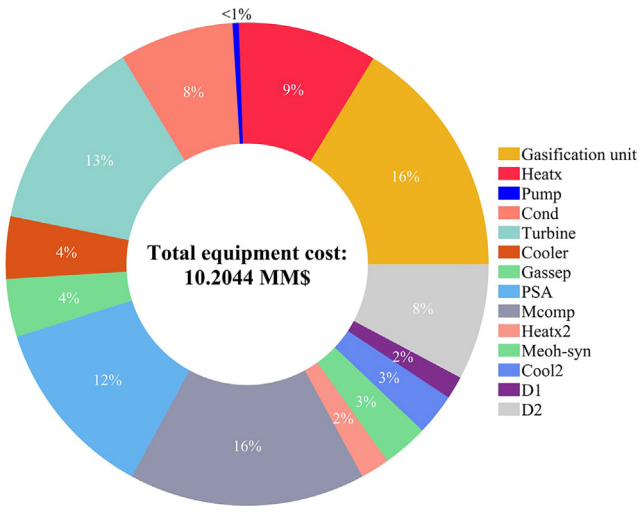

Figure 4. Capital cost of equipment procurement

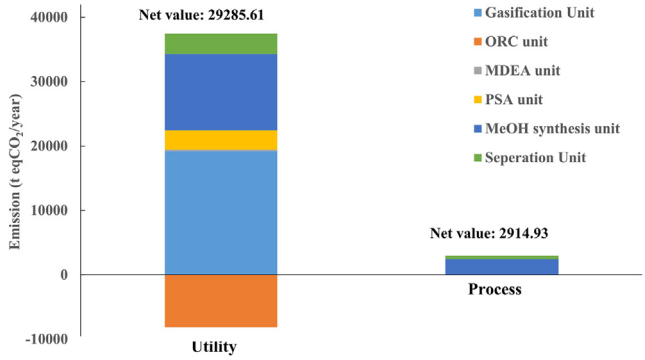

Figure 5. Carbon emission analysis

PSO for minimizing total GHG emissions. Figure 8 illustrates the PSO-based optimization process, with the total GHG emissions stabilizing around the 5th iteration. The optimal solution requires validation using a rigorous model. Table 9 compares process model and data-driven model results when the process operates optimally, confirming the effectiveness of data-driven optimization (22.64 t eqCO_2/day vs. 22.46 t eqCO_2/day). Furthermore, the efficiency of this novel optimization strategy is demonstrated by comparing it with process model-based optimization. The findings indicate that, despite achieving similar GHG emissions (22.64 t eqCO_2/d vs. 21.25 t eqCO_2/d), the execution time for process model-based optimization is significantly longer, taking approximately 2083.02 s. In contrast, AI-based optimization is notably more efficient, requiring only around 8.53 s, making it 243.2 times faster. Importantly, while the latter approach does necessitate a substantial amount of time for data collection, the advantage lies in the ability to repeatedly employ the developed model in various optimization scenarios. For instance, it allows for the fixation of certain operating parameters at constant values while the trained data-driven model can be used again.

QUANTIFICATION AND STATISTICAL ANALYSIS

1. Process analysis
   a. Economic analysis

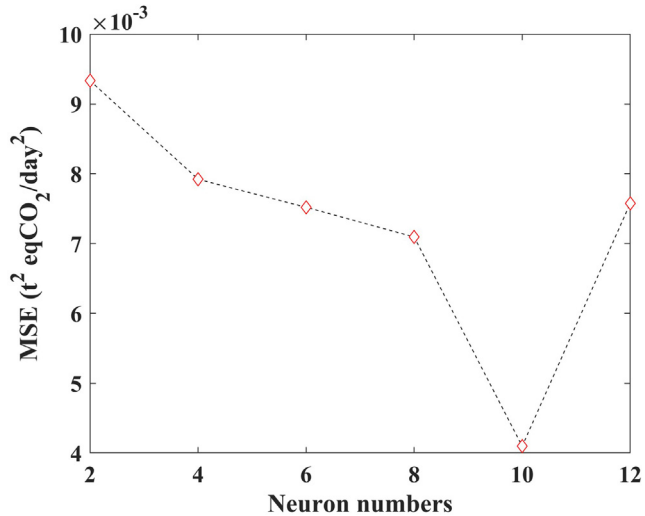

Figure 6. Neuron number effect on ANN accuracy

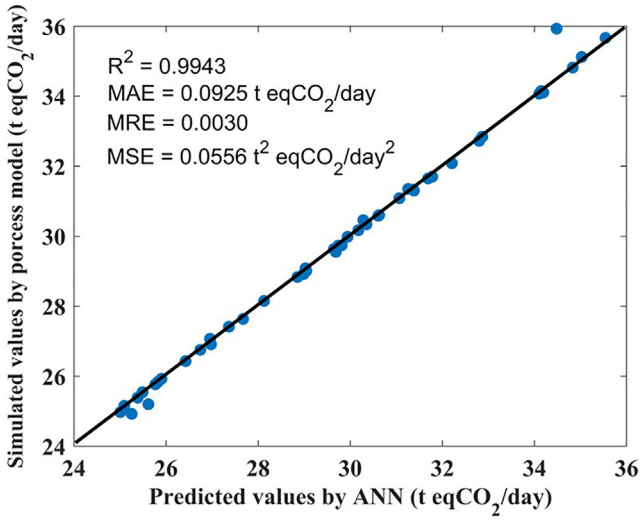

Figure 7. Performance of ANN model in test set

The economic assessment includes the equipment cost and energy consumption in this protocol, which is a simplified calculation considering the initial evaluation stage. Specifically, the total equipment procurement cost (*TEPC*) can be seen as the sum of the cost of all involved equipment or operation units while the energy consumption cost (*ECC*) is estimated based on the energy amount and prices. The estimation equations are given as follows:[1]

$$TEPC = \sum_{i}^{N}\left(EPC_p^i \times \left(\frac{cap_n^i}{cap_p^i}\right)^{\varphi} \times \frac{CEPCI}{CEPCI_p}\right) \quad \text{(Equation 1)}$$

$$ECC = \sum_{i}^{N}(U_i \times P_i) \quad \text{(Equation 2)}$$

where EPC_p^i is the cost of *i-th* unit operation in the past year according to the literature or research reports. cap_p^i and cap_n^i are the disposal capacities of ith unit operation or equipment in the past year and in this study, respectively. *CEPCI* represents the chemical engineering plant cost index which

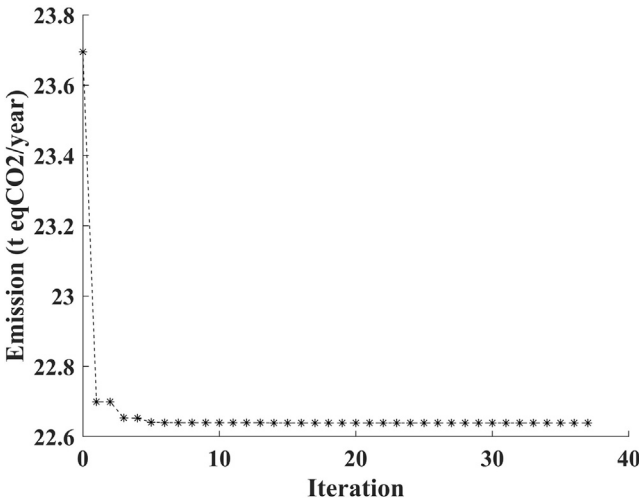

Figure 8. Optimization process based on ANN and PSO

Table 9. Validation the optimum solution by process model

Operating parameters					Calculated emissions by models (t eqCO_2 /day)	
GT (°C)	ER	MT (°C)	DF (kmol/h)	RR	ANN	Process model
1700	0.42	250	0.38	0.51	22.64	22.46

can be determined according to the monthly report in Chemical Engineering magazine.[18] In 2022, the *CEPCI* value is 831.7. Additionally, φ is the scale factor associated with each unit operation and equipment. U_i and P_i stand for utility consumption and the associated price, respectively. The involved parameters for the economic analysis regard to this work are summarized in the Table 10 and Table 11. It should be mentioned the coal is assumed to be the energy source for heating the gasification reactor.

b. Environmental analysis

The environmental analysis is conducted by estimating the greenhouse gas emissions from the perspective of direct carbon emissions and indirect emissions caused by the energy consumptions of various types like steam, coal, electricity and cooling water. A major assumption throughout the calculation is that only CO_2, CH_4 and N_2O gases are applied to evaluate the greenhouse gas emissions according to Equations 3, 4, 5, and 6[1] because other type of emissions accounts very little.

$$CO_2^E = \sum_i PE_i \left(D_{CO2}^i + I_{CO2}^i\right) \quad \text{(Equation 3)}$$

$$CH_4^E = \sum_i PE_i \left(D_{CH4}^i + I_{CH4}^i\right) \quad \text{(Equation 4)}$$

$$N_2O^E = \sum_i PE_i \left(D_{N2O}^i + I_{N2O}^i\right) \quad \text{(Equation 5)}$$

$$GHG = CO_2^P + CO_2^E + 23\left(CH_4^P + CH_4^E\right) + 296\left(N_2O^P + N_2O^E\right) \quad \text{(Equation 6)}$$

where D_{gas}^i and I_{gas}^i are the direct and indirect emission factors of greenhouse gases regarding to different energy sources *i*. PE_i stands for the process energy consumption of *i-th* energy type. Meanwhile, CO_2^P CH_4^P, N_2O^P are the gas emissions from the waste treatment process which can be calculated through the process simulation. The direct and indirect emission factors of the selected process energy along with their price are given in Table 11.

2. Data-driven modeling

a. Latin hypercube sampling

Latin hypercube sampling (LHS) is employed in this case. LHS is a statistical technique employed to generate a quasi-random set of parameter values sampled from a multidimensional distribution. LHS accomplishes this by partitioning the subspace of each vector component S_i

Table 10. The detailed information of equipment costs, capacities, and scale factors

Unit operation	Capacity unit	Base capacity	Base cost ($)	φ	Base year	$CEPCI_p$
Gasification unit[20]	tons/day	1000.00	14700000	0.60	2010	550.8
Heat exchanger[21]	MW	138.10	8100000	0.60	2002	395.6
Pump[22]	kg/s	0.025	1654	0.70	2003	402
Turbine[21]	MW	13.20	15176470	0.85	2002	395.6
Gas separation[1]	kmol/h	192.00	14400000	0.60	2022	831.7
PSA unit[9]	tons/year	1000000.00	48675000	0.60	2013	567.3
Compressor[21]	MW	13.20	15176470	0.85	2002	395.6
MeOH synthesis reactor[23]	kg/s	117.98	17050000	0.82	2007	525.4
Distillation column[24]	m^3	4.700	100599	0.60	2018	603.1

Table 11. Environmental analysis factors along with the price of different energy types

Process energy	DCO_2[25] (g/MJ)	ICO_2[25] (g/MJ)	DCH_4[25] (g/MJ)	ICH_4[25] (g/MJ)	DN_2O[25] (g/MJ)	IN_2O[25] (g/MJ)	Price[9,26] ($/Kwh)
Electricity	0	248.02	0	2.16	0	0.62	0.052
Steam	113.87	0.29	1.79	0	0	0	0.028
Coal	81.642	5.73	0.001	0.43	0.001	0.17	0.0072
Cooling water	–	–	–	–	–	–	0.0013

($i = 1,2,\ldots,N$) into $M = n$ distinct subsets or strata, each having an equal probability denoted as $\Omega_{i,k}$ ($i = 1,2,\ldots,N$; $k = 1,2,\ldots,M$). Samples for each vector component are then selected from their corresponding strata in accordance with:[19]

$$x_{i,k} = D_{X_i}^{-1}(U_{ik}) \quad \text{(Equation 7)}$$

where U_{ik} represents independently and identically distributed (iid) samples within the interval $[\xi_k^l, \xi_k^\mu]$ with:

$$\xi_k^l = (k-1)/M \quad \text{(Equation 8)}$$

$$\xi_k^\mu = k/M \quad \text{(Equation 9)}$$

The resulting samples X are formed by assembling the terms of the generated vector components through a random grouping process. That is, a term $x_{i,k}$ is randomly selected from each vector component (without replacement) and these terms are grouped together to create one sample. This entire procedure is repeated $M = n$ times.

b. Artificial neural network

Three-layer ANN is employed in this work for data-driven modeling of waste-to energy process. An Artificial Neural Network (ANN) is a computational model inspired by the structure and functioning of the human brain. It is a fundamental component of machine learning and artificial intelligence (AI). Its schematic diagram is demonstrated in Figure 9. The values of neurons in hidden layer (H_l) are calculated by values of neurons in input layer (x_i) as shown in Equation 10[14] and further used to calculate the output values (y_o) through Equation 11.[14] The model parameters ω, b are determined by model training.

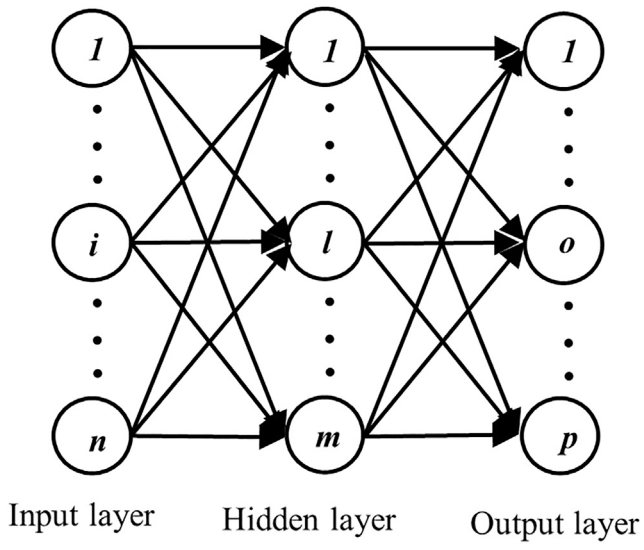

Figure 9. Three-layer ANN topology diagram

$$H_l = max\left(\sum_{i=1}^{n} \omega_{i,l} x_i + b_l, 0\right) \quad \text{(Equation 10)}$$

$$y_o = \sum_{i=1}^{m} \omega_{l,o} H_l + b_o \quad \text{(Equation 11)}$$

$\omega_{i,l}$ is the connecting weight of *i-th* node in the input layer and *l-th* node in the hidden layer, b_l is the bias of *l*-th node in the hidden layer, and *n* is the number of nodes in the input layer. Similarly, $\omega_{l,o}$ is the connecting weight of *l-th* node in the hidden layer and *o-th* node in the output layer, b_o is the bias of *o*-th node in the output layer, and *m* is the number of nodes in the hidden layer.

c. Metrics of data-driven model evaluation

In model performance assessment, mean square error (MSE), mean absolute error (MAE), mean relative error (MRE) and determination coefficient (R^2) are used and their calculations are based on Equations 12, 13, 14, and 15.

$$MSE = \frac{\sum_{i=1}^{n} \left(y_i^{pre} - y_i\right)^2}{n} \quad \text{(Equation 12)}$$

$$MAE = \frac{\sum_{i=1}^{n} \left(y_i^{pre} - y_i\right)}{n} \quad \text{(Equation 13)}$$

$$MRE = \frac{\sum_{i=1}^{n} \left(y_i^{pre} - y_i\right)}{y_i \times n} \quad \text{(Equation 14)}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n} \left(y_i^{pre} - y_i\right)^2}{\sum_{i=1}^{n} \left(y_i - \overline{y}\right)^2} \quad \text{(Equation 15)}$$

where n is the number of data points, y_i^{pre} is the predicted output value of the *i-th* data point, y_i is the actual output value of the *i-th* data point, $\overline{y}$ is the average value of output in the dataset.

3. Optimization

a. Particle swarm optimization

Particle swarm optimization (PSO), as a heuristic optimization algorithm, is known for its simplicity in both structure and programming.[27] In this algorithm, each potential solution is represented as a particle, denoted as *i*, with distinct velocity vectors (v_i) and position vectors (x_i) in an N-dimensional space. These particles iteratively explore different positions to seek optimal values for the objective function and a global optimum across all possible solutions. The PSO algorithm operates through a series of iterations. Initially, the particle's velocity and position vectors are randomly selected within specified limits. Subsequent iterations update the position vector and velocity vector based on inertia, individual best values (p_i), and global best value (p_g), as defined by the following equations:[28]

$$v_i^{k+1} = \omega v_i^k + c_1 r_1 \left(p_i - x_i^k\right) + c_2 r_2 \left(p_g - x_i^k\right) \quad \text{(Equation 16)}$$

$$x_i^{k+1} = x_i^k + v_i^{k+1} \quad \text{(Equation 17)}$$

where x_i^k and v_i^k denote the position and the instantaneous velocity of the particle, *i*, in iteration, k, ω is the inertia coefficient, c_1 and c_2 are the acceleration factors, and r_1 and r_2 are the random numbers ranging from 0 to 1.

Consequently, the objective value (obj_i^k) for a particle *i* during iteration *k* is determined based on its updated position vector (x_i^k). If obj_i^k exceeds the previous optimal value (obj_i^{k-1}), x_i^k is set as p_i; otherwise, p_i is retained. This process is used to compare obj_i^k values among all particles, and the optimal

obj_i^k value is selected as the global optimum. If this global optimum surpasses the previous iteration's global best value (p_g), p_g is replaced with x_i^k; otherwise, p_g remains unchanged. This iterative procedure continues until the maximum number of iterations is reached.

LIMITATIONS

In presenting our framework for integrating process design and optimization in waste valorization, certain limitations should be acknowledged. Firstly, it is important to highlight the absence of actual operational data during the prospect analysis phase. As the designed process has not yet been implemented, the data used for various aspects of the analysis, such as equipment cost in economic evaluations, is derived from studies and reports based on similar processes. While efforts are made to select relevant data sources, this reliance on analogous systems introduces a degree of inherent uncertainty and potential error into our findings. Additionally, for the successful implementation of data-driven optimization, access to a comprehensive dataset is imperative. Therefore, AI-based optimization can only be realized when designed process becomes amenable to simulation and data collection, emphasizing the importance of its practical applicability and data availability in future studies.

TROUBLESHOOTING

Problem 1

Efficiency of technologies selection (step 1)

The initial challenge in the context of waste valorization process design is the huge magnitude of potentially viable technologies, both in terms of reaction synthesis and separation methodologies. This issue is further exacerbated by the evolving landscape of waste valorization technologies, wherein novel approaches continually emerge, thus expanding the search space.

Potential solution

One viable strategy is the adoption of more suitable metrics that facilitate a rapid yet comprehensive evaluation of technology performance. These metrics should encompass key criteria, including environmental impact, economic viability, scalability, and safety, among others. By strategically focusing on these metrics, the assessment process can be refined, enabling the identification of technologies by ranking that align most closely with project objectives.

Furthermore, to navigate the complex landscape of technology selection, the implementation of optimization techniques, such as mixed-integer nonlinear programming (MINLP), holds substantial promise. Through mathematical optimization, it becomes possible to identify optimal technologies combination. This quantitative approach enhances the rigor and objectivity of technology selection, thereby mitigating the challenge posed by the multitude of feasible options.

Problem 2

Economic viability in waste treatment (step 3)

To achieve waste valorization with carbon reduction, a critical issue revolves around economic sustainability. The necessity to capture and utilize carbon from waste streams can strain financial feasibility.

Potential solution

To tackle this, a two-pronged approach is needed. First, optimize carbon-derived product pathways, exemplified by waste-to-MeOH processes, where intermediate syngas is further converted, enhancing overall economic viability. Simultaneously, consider subsidies for technologies contributing to carbon reduction, bridging the economic gap between novel and conventional waste treatment. This fosters sustainable waste management while mitigating financial obstacles tied to carbon capture and utilization.

Problem 3

Simulation errors and warnings (step 3)

In the realm of process simulation, errors and warnings are unavoidable, potentially stemming from input inaccuracies, convergence difficulties, or model limitations. These issues obstruct smooth simulation runs, hampering data accuracy and result meaningfulness.

Potential solution

Efficient resolution involves systematic diagnosis to locate the source of the problem, often within specific process blocks or model settings. Adjustments to simulation parameters, like convergence tolerances or specifying conditions, may be necessary and might require iterative fine-tuning. In software such as Aspen Plus, accessing the control panel aids in problem localization, and detailed reports guide corrective actions, expediting resolution.

Problem 4

Feasibility of data-driven optimization result (step 6)

In data-driven optimization, a challenge arises when solutions obtained may not be practically feasible within the simulation model.

Potential solution

To address this, adopt an iterative approach. When infeasible solutions emerge, treat them as new data points for training the data-driven model. This iterative process enhances model adaptability, improving accuracy and practicality.

Problem 5

Simulation interruptions due to high computational load (step 4)

During data collection via process simulation, a persistent challenge arises when the simulation process unexpectedly terminates or breaks down. This disruption is primarily attributed to the substantial computational demands associated with first-principle simulations, resulting in unanticipated interruption during data collection.

Potential solution

To effectively address this challenge, it is recommended to implement a proactive memory management approach during the data collection process. This approach involves periodically closing the simulation program and subsequently reopening it to alleviate memory constraints. Furthermore, it is advisable to save simulation results incrementally through generating running logs to ensure data preservation.

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources and reagents should be directed to and will be fulfilled by the lead contact, Dr. J. Ren (jzhren@polyu.edu.hk).

Materials availability

This study did not generate new unique reagents.

Data and code availability

Original data have been deposited to Mendeley Data: https://doi.org/10.17632/vmh244j5s9.2.

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AUTHOR CONTRIBUTIONS

J.Z.: conceptualization, data curation, visualization, methodology, models development, formal analysis, writing – original draft, and writing – review and editing; T.S.: data curation, visualization, methodology, models development, formal analysis, and writing – review and editing; Q.Q.: investigation and writing – review and editing; C.H.: methodology and writing – review and editing; J.R.: supervision, methodology, project administration, writing – review and editing, and funding acquisition.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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