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Reinforcement Learning-driven Process Intensification Synthesis – Design and Optimization of Reaction/Separation Systems

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ABSTRACT

This work aims to systematically generate intensified process designs by integrating reinforcement learning (RL)-driven process synthesis and phenomena-based modeling via Generalized Modular Framework (GMF). Rather than considering flowsheet synthesis with conventional unit-operations, GMF utilizes fundamental building blocks, also known as mass and heat exchange modules, to describe the physiochemical phenomena and to enhance novel process discovery. At its core are driving forces which characterize the mass transfer feasibility based on the total change in Gibbs free energy of the system. RL is integrated with this phenomena-based modeling strategy to drive flowsheet generation by exploring much of the total action space and minimizing pre-postulation of stream connections. All possible inlets, outlets, and interconnections between modules are contained in a stream matrix. Deep Q-Network is used as the RL agent, which contains a multi-layer convolution neural network followed by a multi-layer feedforward neural network. This network computes q values for each possible stream connection contained in the stream matrix and determines an optimal action from the maximum q-value (e.g., varying the stream interconnections). New designs can thus be generated and iteratively improved. This approach is demonstrated using two case studies: (1) binary separation of benzene and toluene, and (2) membrane-assisted reaction for methanol production.

Keywords: Process Intensification, Machine Learning, Optimization, Process Synthesis, Process Design

1. INTRODUCTION

With the demand for sustainable chemical production rising, novel processes are more pertinent now than ever before. These technologies should simultaneously improve cost efficiency, energy consumption, and environmental outlook. An emerging process design technique known as process intensification is a promising innovation in the chemical sector [1-2]. It is capable of significant improvements versus conventional designs by intensifying physiochemical fundamentals to overcome equilibrium limitations, often leading to equipment featuring multifunctional tasks. Representative process intensification examples are reactive distillation, membrane reactors, dividing wall columns, etc. Despite these advantages, there are limited examples of intensified systems deployed in industry. This is due to the high complexity for the conceptual process design of these units and their integration with existing processes/plants [3].

Recent research has been investigating reinforcement learning (RL) as a tool to drive process synthesis to address computational complexity associated with traditional approaches using mixed-integer nonlinear programming (MINLP) [4-7]. The RL-based methods typically start with a pool of unit operations in which connections between each can be defined using an inlet-outlet stream matrix, graphical representation, etc. without explicit postulation of a superstructure. The RL agent will

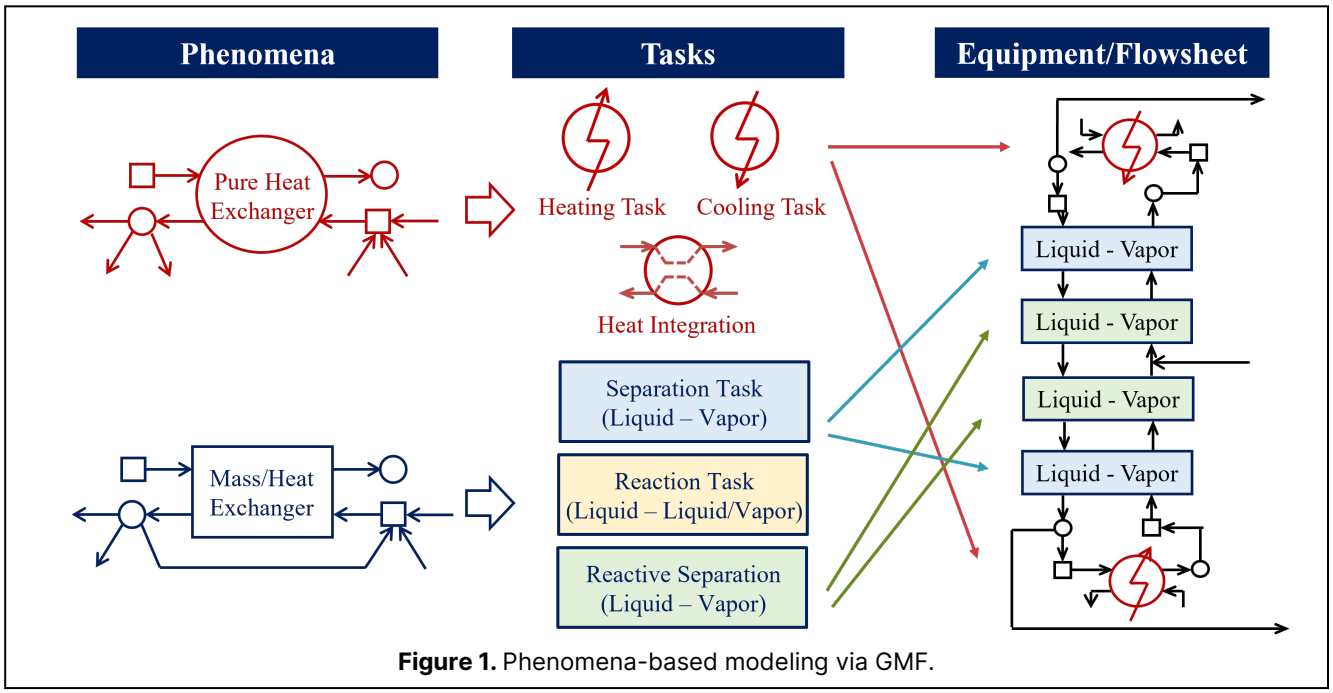

Figure 1. Phenomena-based modeling via GMF.

explore the design space and make decisions on e.g., changing unit operation selections or stream connections, thus generating new process designs.

This work aims to extend RL-driven process synthesis towards systematic process intensification. An integrated framework is presented which augments phenomena-based process modelling though the Generalized Modular Framework (GMF) and automated flowsheet generation through RL's exploration capabilities. The remainder of this paper is organized as follows: Section 2 introduces the RL-GMF methodology for process intensification synthesis. Section 3 showcases the proposed approach on two representative case studies including benzene/toluene binary separation and CO_2 to methanol production via membrane-assisted reaction. Section 4 concludes this paper with key findings and ongoing work.

2. RL-DRIVEN PROCESS INTENSIFICATION SYNTHESIS

2.1. Overview of Generalized Modular Framework

The Generalized Modular Framework is a phenomena-based modeling strategy which, rather than considering conventional chemical processing equipment, considers two fundamental building blocks describing general physiochemical phenomena [8]. As shown in Fig. 1, these phenomena building blocks include: (1) a pure heat exchange module (HE) and (2) a mass/heat exchange module (MH). The pure heat exchange module acts as a heat exchanger where the process stream can be heated, cooled, or utilized in heat integration. The mass/heat exchange module can represent any of the following tasks: separation, reaction, or reactive separation. These tasks can then be synergistically combined to model conventional/intensified units or flowsheets.

The core of GMF is its Gibbs-based driving forces which enforce the total Gibbs free energy of the system to always be decreasing or at zero for feasible mass/heat transfer to occur. While equilibrium is considered, it is not strictly enforced. Eqs. 1-3 present the driving force constraints for reaction/separation systems driven by vapor-liquid equilibrium (VLE), such as distillation-based systems [9]. For these systems, $G1$ defines the net mass transfer direction and $G2$ defines the mass transfer feasibility which is the distance from physical and chemical equilibrium. The product of $G1$ and $G2$ approximates the total change in Gibbs free energy of the system.

$$d(nG)^{tot}_{T,P} \approx G1_i \times G2_i \leq 0 \tag{1}$$

$$G1_i = dn^L_{ei} \approx f^{LO}_e x^{LO}_{ei} - f^{LI}_e x^{LI}_{ei} \tag{2}$$

$$G2_i = \left[\frac{\partial (nG)^{tot}}{d(n^L_{ei})}\right]_{T,P} \approx \ln\left[\frac{\gamma^L_{ei} x^L_{ei} P^{sat,L}_{ei}}{\phi^V_{ei} x^V_{ei} P_{tot}}\right] + \sum_i \sum_k \left[\frac{\upsilon_{ik} \Delta G^f_i}{RT^L_e} + \upsilon_{ik} \ln\left(\phi^V_{ei} x^V_{ei} P_e\right)\right] \frac{\partial \epsilon_k}{\partial n^L_{ei}} \tag{3}$$

Eqs. 4-5 give the driving force constraints for membrane-assisted reaction/separation systems [10]. μ^V_i in Eq. 4 is the chemical potential in the reaction zone and is determined from the mass transfer across the membrane calculated by Eq. 5. The product of the chemical potential and the change in material approximates the total change in Gibbs free energy for the reaction zone.

$$d(nG)^{tot}_{T,P} = \sum_i \mu^V_i dn^V_i \leq 0 \tag{4}$$

$$J_i = \lambda_i A(\mu_i^M - \mu_i^V) \quad (5)$$

The GMF process synthesis model is built with a physical model, structural model, and objective function. The physical model specifies a set of physical and/or chemical constraints of the system. These are broken down into: (1) mass balances, (2) energy balances, (3) thermodynamic properties, (4) phase defining, (5) driving forces, etc. Thermodynamic properties can be defined through any given thermodynamic model and phase defining to ensure that liquid and vapor streams are accurately represented. The structural model represents the existence (or not) of modules and streams along with the interconnectivity of the system, defined through binary variables. Mixers are placed before the module inlet stream, and splitters are placed after the module outlet stream. These allow for interconnecting streams between modules. The objective function can be defined to maximize or minimize any desired performance metric.

2.2. RL-GMF Methodology

The RL-driven process synthesis algorithm applied in this work is built on that developed by Wang et al. [5] for unit operation-based process design. Tian et al. [11] presented a follow-up work to accelerate the RL design search. This work introduces the RL-GMF process intensification synthesis strategy, as shown stepwise in Fig. 2.

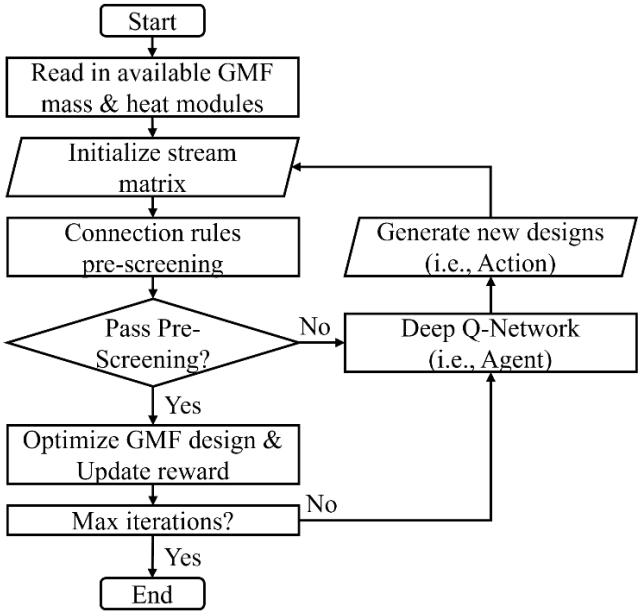

Figure 2. RL-GMF algorithm for process intensification synthesis.

2.2.1 Stream Matrix Initialization

The methodology starts off by reading in the available GMF MH and HE modules where the maximum number of available modules are user defined. Compared to our prior work for GMF process intensification synthesis using mixed-integer nonlinear optimization (MINLP) [8-9], the binary variables are redefined as parameters in RL and used to construct an inlet-outlet stream matrix. For example, the matrix for a two MH module system is shown below in Table 1. The rows correlate to inlets and the columns correlate to outlets. 18 binary parameters are present, generating a 6×3 matrix.

Table 1. Stream matrix representation: An example of 2 MH modules.

	Liquid Outlets		
Liquid Inlets	$y^{IP,L}$	y_1^{LP}	y_2^{LP}
	y_1^{IL}	$y_{1,1}^{LL}$	$y_{2,1}^{LL}$
	y_2^{IL}	$y_{1,2}^{LL}$	$y_{2,2}^{LL}$
	Vapor Outlets		
Vapor Inlets	$y^{IP,V}$	y_1^{VP}	y_2^{VP}
	y_1^{IV}	$y_{1,1}^{VV}$	$y_{2,1}^{VV}$
	y_2^{IV}	$y_{1,2}^{VV}$	$y_{2,2}^{VV}$

2.2.2 Connection Rules Pre-Screening

As per Fig. 2, after the stream matrix gets initialized, it is sent to a series of pre-screening checks to ensure that the constructed flowsheet satisfies the most basic requirements on connectivity. This helps to reduce computational time by completely skipping the GMF modelling of any nonsensical solution generated by RL. Examples of these checks include:

- There exists at least one feed stream connection to the system.
- There exists at least one product stream connection from the system.
- There is at least one liquid inlet and one vapor outlet for heater modules to exist.
- There is at least one vapor inlet and one liquid outlet for cooler modules to exist.
- Inlet and outlet streams from both sides of each module must exist to enforce module existence.

The last connection rule requires that there should be vapor and liquid inlets/outlets or permeate and retentate inlets/outlets on both sides for VLE-driven systems or membrane assisted reaction-driven systems respectively. Failure of any of these checks will assign either the minimum pre-score or incur a penalty to the pre-score, resulting in a failed pre-screening and negative reward.

2.2.3. GMF Optimization & Reward Update

Upon successfully passing pre-screening, the associated stream matrix will be translated to a GMF phenomena-based flowsheet for optimization. If there is no inlet or no outlet streams to/from a module, the module is treated as non-existing. A reward is generated based on the status of the optimizer and the value of the objective function. If the optimizer fails to converge (e.g., infeasible

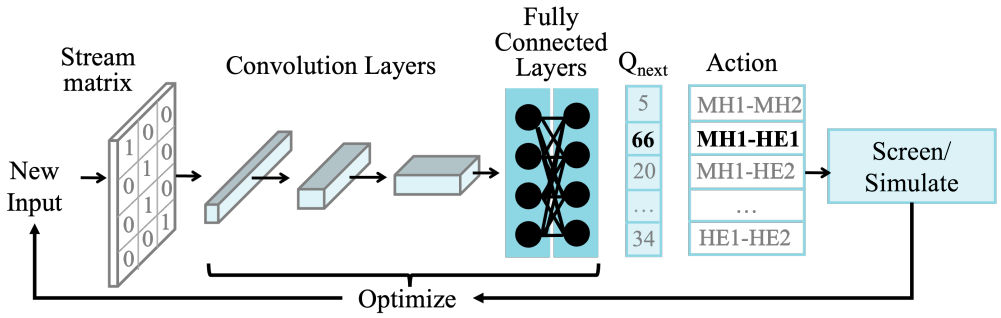

Figure 3. RL agent with Deep Q-Network.

solution), the minimum reward is assigned. If it successfully converges to a solution, a reward value is calculated based on e.g. objective value and process variables.

2.2.4. Deep Q-Network and Generation of New Design

Upon failing pre-screening or passing through GMF optimization, the current state and reward is sent to the DQN [5]. This step uses the agent in RL to learn from given conditions and intelligently make changes to the stream matrix to drive the algorithm towards improved designs. As illustrated in Fig. 3, the DQN is comprised of a three-layer one-dimensional convolution neural (CNN) network followed by a two-layer feed forward neural network (FNN). The state is a two-dimensional matrix of the batch number and flattened stream matrix (e.g., Table 1). This is used as the input to the CNN where key features are extracted, reshaped, and subsequently processed through the fully connected layers which determine the q-values for each row. An optimal decision is made where the index of the maximum q-value in each row takes a value of one. To open the possibility for every index in a single row to take a value of zero, an additional column is generated in this step to act as a placeholder for the optimal choice. These decisions translate to the switching of module inter-connections, elimination of modules, and adjustment of inlet/product streams. In this way, a new design can be generated with a unique inlet-outlet stream matrix and is then sent back to the workflow as shown in Fig. 2.

This integration of RL and GMF allows for automated flowsheet synthesis, scanning much of the total action space. Through the reduction of flowsheet pre-postulation, enhanced discovery of innovative process designs and non-intuitive flowsheets can be observed. Additionally, GMF is inherently a MINLP problem where solution convergence is time consuming and may be infeasible without good initial guesses. In this proposed approach, RL takes care of parameterizing the GMF binary variables, and the problem can then be solved as a nonlinear problem (NLP) with enhanced solution convergence. This framework is built in Python version 3.8.20 using TensorFlow for RL development, IPOPT as the NLP solver for Case Study 1 (VLE-driven GMF), and BARON as the NLP solver for Case Study 2 (membrane reaction-driven GMF).

3. CASE STUDIES

This section discusses two case studies performed to test the RL-GMF framework. These are representative of the two modelling trajectories of GMF with VLE-driven systems tested through the binary separation of benzene and toluene and membrane assisted reaction-driven systems tested with modular methanol production.

3.1. Binary Separation of Benzene/Toluene

3.1.1. Problem Statement

As a first motivating example, this case study describes a conventional separation scheme where a high purity product is to be obtained for at least 99% benzene from a liquid benzene/toluene mixture feed. Ideal vapor-liquid equilibrium conditions are used in the phenomena-based modelling with purely separation considered, neglecting the need for a reactive term in the driving force (Eq. 3). Table 2 shows the feed conditions of this scheme adopted from Proios and Pistikopoulos [12]. The GMF objective function is formulated to maximize the mole fraction of benzene from the column distillate (Eq. 6). The reward for RL is defined as the difference between the distillate rate and scaled reflux ratio (Eq. 7), which was the objective function used in [12].

$$\max \left(x_2^{VO,benzene}\right) \tag{6}$$

$$\text{reward} = f_{2,p_{liq}}^{CP} - 50\frac{f_{2,2}^{CL}}{f_{2,p_{liq}}^{CP}} \tag{7}$$

Table 2. Feed Stream Conditions for VLE-driven System

Liquid Feed	
Flowrate (kmol/hr)	360.00
Temperature (K)	359.89
Pressure (bar)	1.01
Benzene	0.70
Toluene	0.30

Proios and Pistikopoulos [12] solved this GMF process synthesis problem via MINLP. The resulting optimal design used two MH modules and two HE modules shown in Fig. 4. It featured a compact representation of a trayed distillation column. In what follows, we number the MH modules in ascending order. Namely, the MH module at the bottom is numbered as MH 1, the existence or not defined by binary parameter y_1. The MH module at the top is numbered as MH 2, the existence or not defined by binary parameter y_2. Each MH module has two associated HE modules. For the optimal MINLP solution shown in Fig. 4, the HE module for MH 1 acts as the reboiler. The HE module for MH 2 acts as the condenser. MH 1 defines the stripping section capturing separation below the feed stage. MH 2 defines the rectifying section capturing separation above the feed stage.

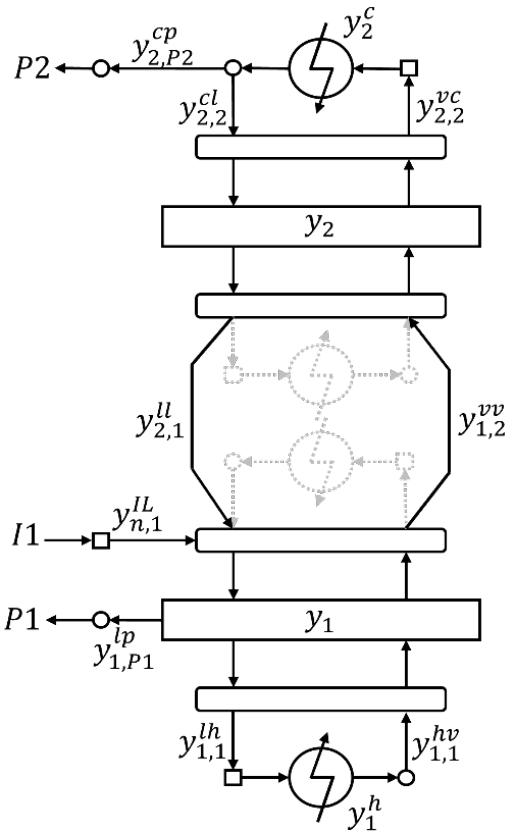

Figure 4. GMF representation of trayed distillation column (reproduced from [12]).

3.1.2. RL-GMF Implementation

The goal of this case study is to test if the RL-GMF methodology can successfully generate good design configuration(s) for this binary separation problem. A maximum of two mass heat exchange modules and four pure heat exchange modules are provided to the RL-GMF process synthesis. There are forty-two total binary variables associated with the design. All inlets, outlets, and interconnections are available for RL to explore resulting in a stream matrix of size 16×3. Note that for the stream matrix shown in Table 1, the current RL algorithm only allows one index in each row of the stream matrix to take a value of one. If it is possible that multiple indices in a single row would take the value of one, the stream matrix can be restructured.

Over 100, 000 episodes, eight unique feasible solutions were found as shown in Fig. 5. The total run time for 100, 000 episodes is 146 minutes. Out of this total run time, 139 minutes are spent on GMF optimization to evaluate the more than 2, 700 configurations which have passed the pre-screening step.

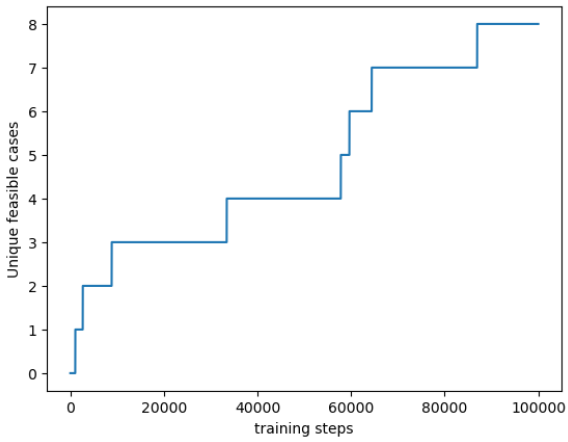

Figure 5. Benzene/toluene binary separation: Unique feasible solutions during RL-GMF training.

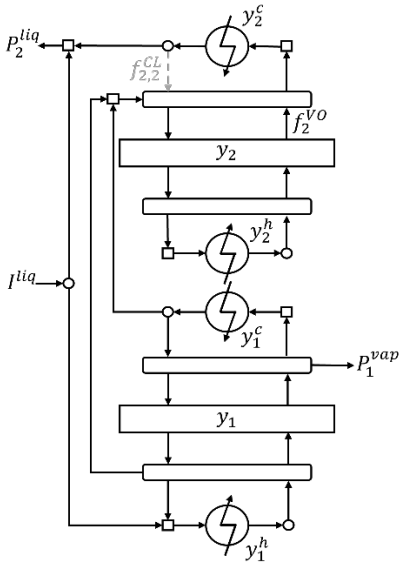

Figure 6. Benzene/toluene binary separation: RL-GMF design with the highest reward value.

The highest reward value achieved is 3120, the design of which is shown in Fig. 6. Using the trayed distillation column structure as base case (Fig. 4), its reward value corresponds to 2094. From optimization point of view, the RL algorithm successfully identifies a better

solution with non-intuitive design structure. However, from physical point of view, we notice that part of the initial feed stream (I^{liq}) is directly mixed with the product stream (P_2^{liq}). This happens as the problem statement only poses constraint for the purity of benzene vapor outlet from module 2 (f_2^{VO}). Additionally, the choice of the reward function (Eq. 3) strives to maximize the flowrate of the distillate product (P_2^{liq}) and minimize that of the reflux ($f_{2,2}^{CL}$), enforcing nonexistence of the reflux stream. This altogether drives the RL algorithm to identify Fig. 6 as the best solution.

The 2, 700 GMF configurations generated by RL do not include the base case configuration presented in Fig. 4. We hypothesize that this may be due to the large combinatorial design space with the forty-two total binary variables. To test this, a simplified case study is run with the HE module connections predefined and the MH connections open for RL to explore. This leads to a total of eighteen binary parameters. This simplified scenario is able to identify twelve unique feasible design structures over only 10, 000 episodes, and the base case configuration is generated on the 2, 308th episode. The increase from eighteen to forty-two parameters significantly adds to the design space (especially the infeasible design space), requiring longer run times to identify good design solutions.

3.2. Membrane-Assisted Methanol Production

3.2.1. Problem Statement

This case study investigates the design of a water selective membrane-assisted reaction scheme to produce methanol from CO_2 direct hydrogenation [13]. Kinetic models are adopted from Van den Bussche and Froment [14] using commercial catalyst $Cu/ZnO/Al_2O_3$. This kinetic model considers stoichiometric methanol production (Eq. 8) with reverse water gas shift (rWGS) as a side reaction (Eq. 9). The reactions take place in gas phase. An adiabatic reactor is considered with pressure drop negligible per the low flowrate. Feed conditions are listed in Table 3 at pilot scale. A total of ten membrane tubes are used with water permeance as 10^{-4} mol/s/m^2/Pa. Note that this permeance value is adopted higher than the reported values to more clearly showcase the impact of the membrane. A parametric study has been performed to quantify the impact of water permeance from 10^{-6} – 10^{-4} mol/s/m2/Pa but is not included here due to the page limit. The objective function for GMF optimization is to maximize CO_2 conversion. The reward function for RL is adopted as 10^4 times of the CO_2 conversion, to drive the design toward higher conversion.

$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \quad (8)$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \quad (9)$$

Table 3. Feed conditions for methanol production.

	Feed	Sweep Gas
Flowrate (kmol/hr)	44.5	2.5
Temperature (K)	483.15	483.15
Pressure (bar)	77.9	1.00
CO_2	0.1850	0
H_2	0.7561	0
CH_3OH	0.0017	0
CO	0.0567	0
H_2O	0.0004	0
N_2	0	1

3.2.2. RL-GMF Implementation

A maximum of three MH modules are allowed for this study, which generates a stream matrix with thirty-two parameters of shape 8×4. The length of each MH module is set to 0.5 m. This model is run through the RL algorithm over 30, 000 episodes finding three unique feasible designs as shown in Fig. 7. The total computational time is 20 minutes.

Fig. 8(1-3) depict RL-GMF design solutions. Fig. 8(1) features the use of a single MH module with a CO_2 conversion of 9.55%. Fig. 8(2-3) use all three MH modules with CO_2 conversions as 26.51% and 26.34% respectively. The sweep gas recycle streams formed in Fig. 8(3) are not physically correct, but often created by the RL algorithm to obtain higher rewards numerically. This is consistent with the observation in our prior work for RL-driven unit operation-based process synthesis [11]. As such, Fig. 8(2) presents the best design solution identified by RL-GMF.

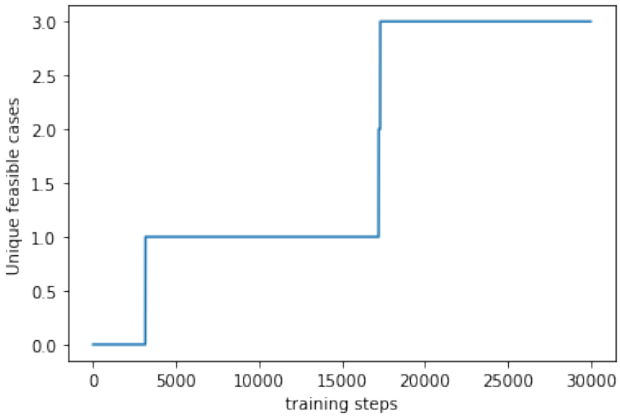

Figure 7. Unique feasible solutions during RL-GMF training – membrane assisted reaction-driven model.

The base case design is adopted as a counter-current membrane reactor as that shown in Fig. 8(4). The corresponding CO_2 conversion is 17.39%, which is lower than the 26.51% conversion provided by the design in Fig. 8(2). Table 4 compares the reaction rates and membrane permeance flux for the two designs. In the counter-flow

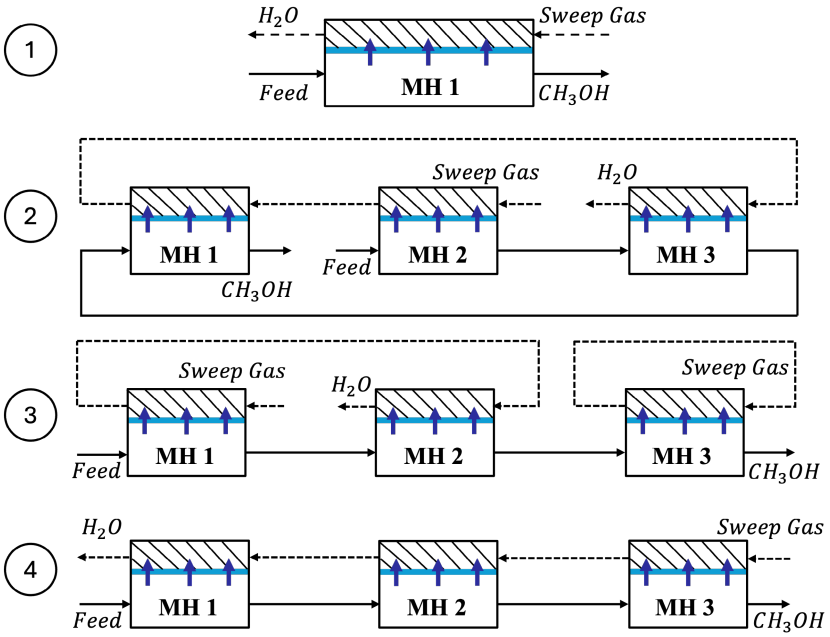

Figure 8. Membrane-assisted methanol production: (1-3) Feasible designs from RL-GMF, (4) base case design.

Table 4. Comparison of reaction rates and membrane permeance flux.

	Reaction Rate (Eq. 8) Unit: kmol/h/kg catalyst		**Membrane Permeance Flux (Water)** Unit: kmol/h/m^2	
	RL-GMF best design (Fig. 8(2))	Base case counter-current (Fig. 8(4))	RL-GMF best design (Fig. 8(2))	Base case counter-current (Fig. 8(4))
MH 1	0.80	1.89	0.55	0.84
MH 2	1.89	0.52	1.00	0.35
MH 3	2.43	0.94	1.09	0.63

structure in Fig. 8(4), MH 2 presents a bottleneck with small driving forces for both reaction and membrane separation. However, the more non-intuitive design structure in Fig. 8(2) successfully debottlenecks this by altering the sequences of feed and sweep gas flowing through the three MH modules.

4. CONCLUDING REMARKS

This paper introduced the use of reinforcement learning and phenomena-based modeling to enhance the discovery of novel process designs. Problem complexity was reduced from MINLP to NLP with the parameterization of GMF binary variables through the RL stream matrices. Two case studies were presented to demonstrate the RL-GMF algorithm, including benzene/toluene binary separation and membrane-assisted methanol production. For both case studies, the RL-GMF algorithm was able to identify non-intuitive process design solutions which provided higher rewards than the base case designs. The large infeasible design space still presented challenges for large-scale process synthesis. Future work should address this to reduce the run time and drive more efficient solution generation. Ongoing efforts are incorporating masking methods to RL and investigating classification neural networks to rule out the infeasible designs.

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REFERENCES

1. Tian Y, Demirel SE, Hasan MMF, Pistikopoulos EN. An overview of process systems engineering approaches for process intensification: state of the art. Chemical Engineering and Processing - Process Intensification 133:160-210 (2018). https://doi.org/10.1016/j.cep.2018.07.014
2. Ramírez-Márquez C, Al-Thubaiti MM, Martín M, El-

Halwagi MM, Ponce-Ortega JM. Processes intensification for sustainability: prospects and opportunities. Ind. Eng. Chem. Res. 62:2428-2443 (2023). https://doi.org/10.1021/acs.iecr.2c04305
3. Patel BA, Pereira CS. Process intensification at scale: an industrial perspective. Chemical Engineering and Processing - Process Intensification 181:109098 (2022). https://doi.org/10.1016/j.cep.2022.109098
4. Khan AA, Lapkin AA. Designing the process designer: hierarchical reinforcement learning for optimisation-based process design. Chemical Engineering and Processing - Process Intensification 180:108885 (2022). https://doi.org/10.1016/j.cep.2022.108885
5. Wang D, Bao J, Zamarripa-Perez MA, Paul B, Chen Y, Gao P, Ma T, Noring AA, Iyengar AKS, Schwartz DT, Eggleton EE, He Q, Liu A, Marina OA, Koeppel B, Xu Z. A coupled reinforcement learning and IDAES process modeling framework for automated conceptual design of energy and chemical systems. Energy Adv. 2:1735-1751 (2023). https://doi.org/10.1039/d3ya00310h
6. Gao Q, Schweidtmann AM. Deep reinforcement learning for process design: review and perspective. Current Opinion in Chemical Engineering 44:101012 (2024). https://doi.org/10.1016/j.coche.2024.101012
7. Reynoso?Donzelli S, Ricardez?Sandoval LA. A reinforcement learning approach with masked agents for chemical process flowsheet design. AIChE Journal 71: (2024). https://doi.org/10.1002/aic.18584
8. Pistikopoulos EN, Tian Y. Computer-aided modular process intensification: design, synthesis, and operability. Synthesis and Operability Strategies for Computer-Aided Modular Process Intensification :19-41 (2022). https://doi.org/10.1016/b978-0-32-385587-7.00011-7
9. Tian Y, Pistikopoulos EN. Synthesis of operable process intensification systems—steady-state design with safety and operability considerations. Ind. Eng. Chem. Res. 58:6049-6068 (2018). https://doi.org/10.1021/acs.iecr.8b04389
10. Tian, Y., Akintola, A., & Akoh, B. (2023). A Process Design, Intensification, and Modularization Approach for Membrane-Assisted Reaction Systems. *In Comput. Aided Chem. Eng.* (Vol. 52, pp. 3159-3164). Elsevier.
11. Tian Y, Akintola A, Jiang Y, Wang D, Bao J, Zamarripa MA, Paul B, Chen Y, Gao P, Noring A, Iyengar A, Liu A, Marina O, Koeppel B, Xu Z. Reinforcement learning-driven process design: a hydrodealkylation example. Systems and Control Transactions 3:387-393 (2024). https://doi.org/10.69997/sct.119603
12. Proios P, Pistikopoulos EN. Generalized modular framework for the representation and synthesis of complex distillation column sequences. Ind. Eng. Chem. Res. 44:4656-4675 (2005). https://doi.org/10.1021/ie040163m
13. Hamedi H, Brinkmann T, Shishatskiy S. Membrane-assisted methanol synthesis processes and the required permselectivity. Membranes 11:596 (2021). https://doi.org/10.3390/membranes11080596
14. Bussche KMV, Froment GF. A steady-state kinetic model for methanol synthesis and the water gas shift reaction on a commercial cu/zno/al2o3catalyst. Journal of Catalysis 161:1-10 (1996). https://doi.org/10.1006/jcat.1996.0156