Automated Generative Process Synthesis via Generative AI-based Dual-Loop Simulation and Optimization

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1. Introduction

The design of chemical processes is a foundational challenge requiring the simultaneous optimization of discrete topologies and continuous operating variables. Traditional mathematical programming, such as MINLP based on superstructures, often struggles with combinatorial complexity and remains limited to pre-postulated design alternatives [1].

While recent generative AI models propose flowsheet structures, they often lack integration with rigorous simulators to evaluate thermodynamic feasibility [2]. This study proposes a novel dual-loop framework that synergistically integrates generative Transformers with rigorous simulation to address the multi-level complexity of simultaneously optimizing discrete process topologies and continuous operating variables.

2. Methodology

Our framework utilizes the Simplified Flowsheet Input-Line Entry System (SFILES) [3] to encode process structures into textual sequences. These sequences are mapped onto a continuous latent manifold using a hybrid architecture of a Transformer-based encoder-decoder and a deep hierarchical VAE [4, 5].

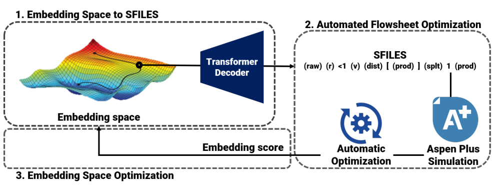

Fig. 1: Schematic of the integrated dual-loop framework: (1) topology decoding, (2) PFD-level optimization, and (3) PSO-based embedding space search.

2.1 Dual-Loop Optimization Strategy

The optimization is formulated as a bi-level problem where topology exploration is decoupled from variable optimization:

$$\max_{x \in X} \left(\max_{v \in O(x)} f_x(v) \right) \tag{1}$$

where x denotes the process topology and v represents the operating variables.

- **Outer Loop:** Leverages Particle Swarm Optimization (PSO) to explore the continuous embedding space for candidate topologies [6].
- **Inner Loop:** Acts as an automated evaluation agent that converts SFILES into simulation-able Aspen Plus flowsheets and performs rigorous Equation-Oriented (EO) optimization.

2.2 Feasibility and Post-processing

To ensure the generated designs are thermodynamically and syntactically valid, we incorporate strict grammar-based validation and process-specific engineering filters. This allows the AI to avoid physically impossible configurations [4].

3. Case Study: Ethylene Glycol Production

The framework was validated using the hydrolysis of ethylene oxide for monoethylene glycol (MEG) production [7].

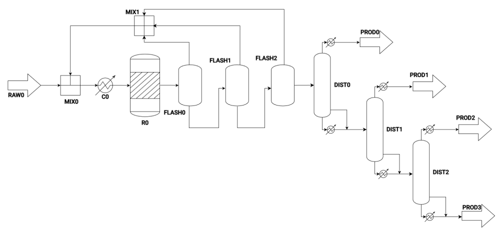

Fig. 2: PFD for the base case ethylene glycol plant.

3.1 Scenario 1: Penalty-Agnostic (Excluding Capital Cost)

In this scenario, only product revenue and utility costs were considered. As shown in Figure 3, the PSO algorithm identified a global recycle loop from the final distillation column ('DIST2') back to the reactor inlet ('MIX0'). As shown in Table 1, this deep integration strategy resulted in a total profit of 35,598.16 USD/hr, a significant improvement over the base case. Figure 4 confirms the PSO's robust search capability, demonstrating its extensive migration across the embedding manifold to escape multiple local optima and reach the high-performance design frontier.

3.2 Scenario 2: Cost-Constrained (Including Capital Cost)

Operational cost penalties (1,000 USD/hr for flash drums, 2,000 USD/hr for distillation columns) were introduced. As shown in Figure 5, the framework strategically replaced an expensive distillation column with a lower-cost flash unit ('FLASH1'). The total profit reached 29,270.37 USD/hr (Table 2), successfully navigating the discrete trade-off between separation

Table 1: Comparison of optimization results across different cases (Scenario 1)

	Base Case	**Best Case (Random)**	**Best Case (PSO)**
	[USD/hr]	*[USD/hr]*	*[USD/hr]*
Utility	-4,486.22	-4,530.96	-4,319.00
Product	39,099.96	39,502.08	39,908.16
Total	**34,613.74**	**34,971.12**	**35,598.16**

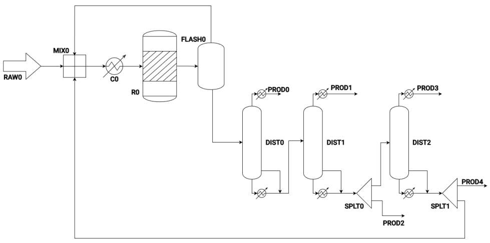

Fig. 3: The optimal flowsheet discovered using particle swarm optimization (PSO) while excluding unit cost.

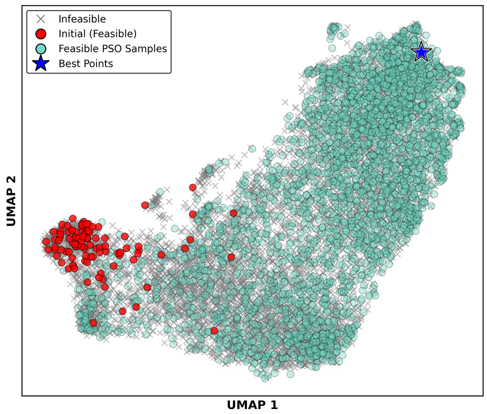

Fig. 4: UMAP visualization of the PSO search trajectory for Scenario 1. The plot illustrates the migration from the initial swarm (red) to the global optimum (blue star) through extensive exploration of the embedding manifold [8].

performance and capital expenditure. As visualized in Figure 6, the PSO swarm effectively traversed the rugged design space, successfully migrating away from the capital-intensive initialization region toward a distinct, low-capital basin of attraction.

4. Conclusion

The proposed dual-loop framework successfully decouples topology discovery from operating variable optimization. It not only rediscovers established industrial configurations but also identifies novel, capital-efficient alternatives. Future work will incorporate comprehensive life cycle assessment (LCA) to optimize for environmental sustainability alongside profitability.

Table 2: Comparison of optimization results considering unit block cost penalties (Scenario 2)

	Base Case	**Best Case (Random)**	**Best Case (PSO)**
	[USD/hr]	*[USD/hr]*	*[USD/hr]*
Utility	-4,486.22	-4,321.07	-4,414.95
Product	39,099.96	38,884.68	39,685.32
Unit Cost	-9,000	-6,000	-6,000
Total	**25,613.74**	**28,563.61**	**29,270.37**

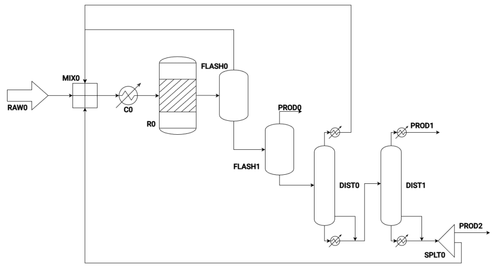

Fig. 5: The optimal flowsheet discovered using particle swarm optimization (PSO) while considering unit cost.

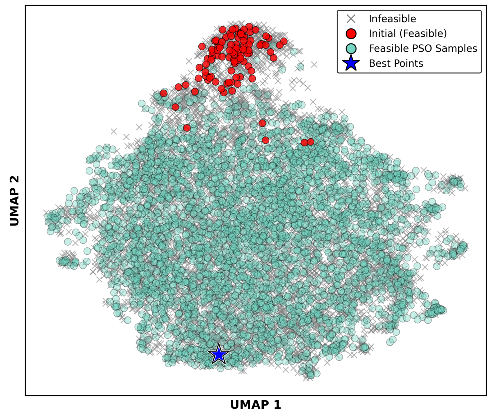

Fig. 6: UMAP visualization of the PSO search trajectory for Scenario 2. The plot illustrates the migration from the initial swarm (red) to the global optimum (blue star) through extensive exploration of the embedding manifold [8].

Acknowledgments

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Appendix A. Details of the Optimization Problem Setup

The economic performance for the Ethylene Glycol (EG) process is evaluated based on the following objective function formulations and cost parameters.

1.1 Objective Function Formulation

Two scenarios were considered to evaluate the trade-off between operational efficiency and capital expenditure:

- **Scenario 1 (Penalty-Agnostic):** Focused solely on maximizing operational profit.

$$J_1 = C_{prod} \cdot F_{prod} - \sum_{j \in Utilities} C_j \cdot E_j \qquad \text{(A1)}$$

- **Scenario 2 (Cost-Constrained):** Incorporated unit capital penalties to discourage excessive topological complexity.

$$J_2 = J_1 - \sum_{i \in Units} C_i \cdot N_i \qquad \text{(A2)}$$

Both scenarios are subject to a product purity constraint of $x_{MEG} \geq 0.99$.

1.2 Cost Parameters and Constants

The pricing and utility costs used in the optimization are summarized below [9]:

- **Product Price (C_{prod}):** 36 USD/kmol for MEG.
- **Utility Costs (C_j):**
  - Cooling water (30°C): 0.000378 USD/MJ.
  - High-pressure steam (254°C): 0.00566 USD/MJ.
- **Capital Cost Penalties (C_i):**
  - Distillation Column: 2,000 USD/Unit·hr.
  - Flash Drum: 1,000 USD/Unit·hr.

Appendix B. SFILES Post-processing and Feasibility Rules

To ensure the generated topologies are simulator-ready and physically consistent, a series of post-processing steps are applied to the raw SFILES strings.

2.1 Generic Rules

Generic simplifications applied to all topologies include merging consecutive mixer units into a single block to reduce simulation complexity.

2.2 Process-Specific Rules for EG

Custom rules tailored for the ethylene glycol hydrolysis process include:

- **Unit Removal:** Valves ('v'), pumps ('pp'), and heat exchangers ('hex') are removed as their functions are integrated into primary unit specifications.
- **Standardization:** All general separators ('sep') are specified as flash drums to standardize the search space.
- **Simulation Compatibility:** A mixer block is automatically inserted upstream of the reactor if multiple inlets exist.
- **Thermal Conditioning:** A cooler is mandated upstream of the reactor if not present to ensure explicit temperature control.

Appendix C. Particle Swarm Optimization (PSO) Hyperparameters

The outer-loop optimization utilizes PSO to navigate the continuous 32-dimensional embedding space. The specific hyperparameters used to balance exploration and exploitation are detailed in Table A1.

Table A1: Hyperparameters for the PSO algorithm.

Hyperparameter	**Value**
Number of particles, N	200
Maximum iterations, t_{max}	100
Early stopping patience	50
Acceleration coefficients (c_1, c_2)	2.0
Inertia weight (w)	$0.9 \times (1 - \alpha) + 0.4 \times \alpha$
α (Iteration ratio)	t/t_{max}