Process design through deep reinforcement learning and graph neural networks

Qinghe Gao, Artur M. Schweidtmann

Graph seminar

Process Intelligence Research
Dept. Chemical Engineering
Delft University of Technology

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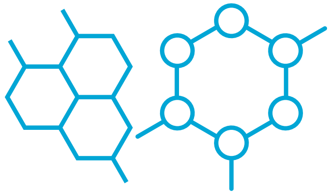
TU Delft Process Intelligence RESEARCH

What is chemical process?

Raw material



Chemical process

Product

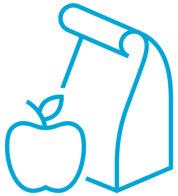
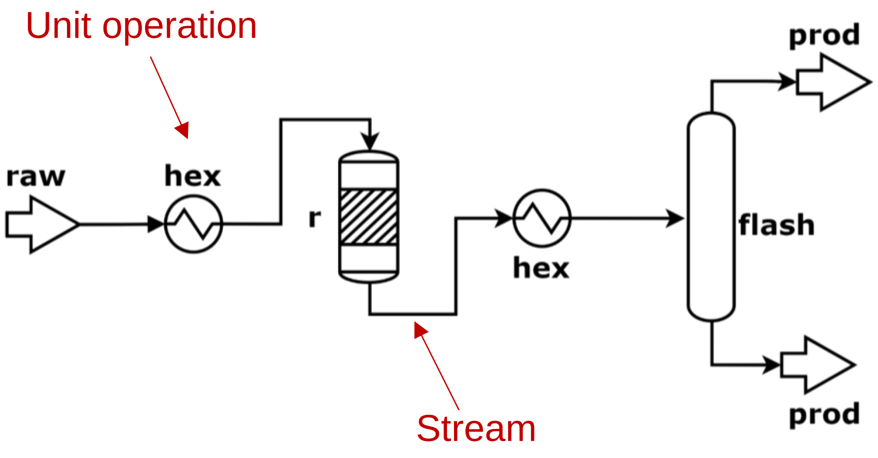


Figure: https://cen.acs.org/business/finance/CENs-top-50-US-chemical-producers-for-2020/99/i17

What is chemical process design

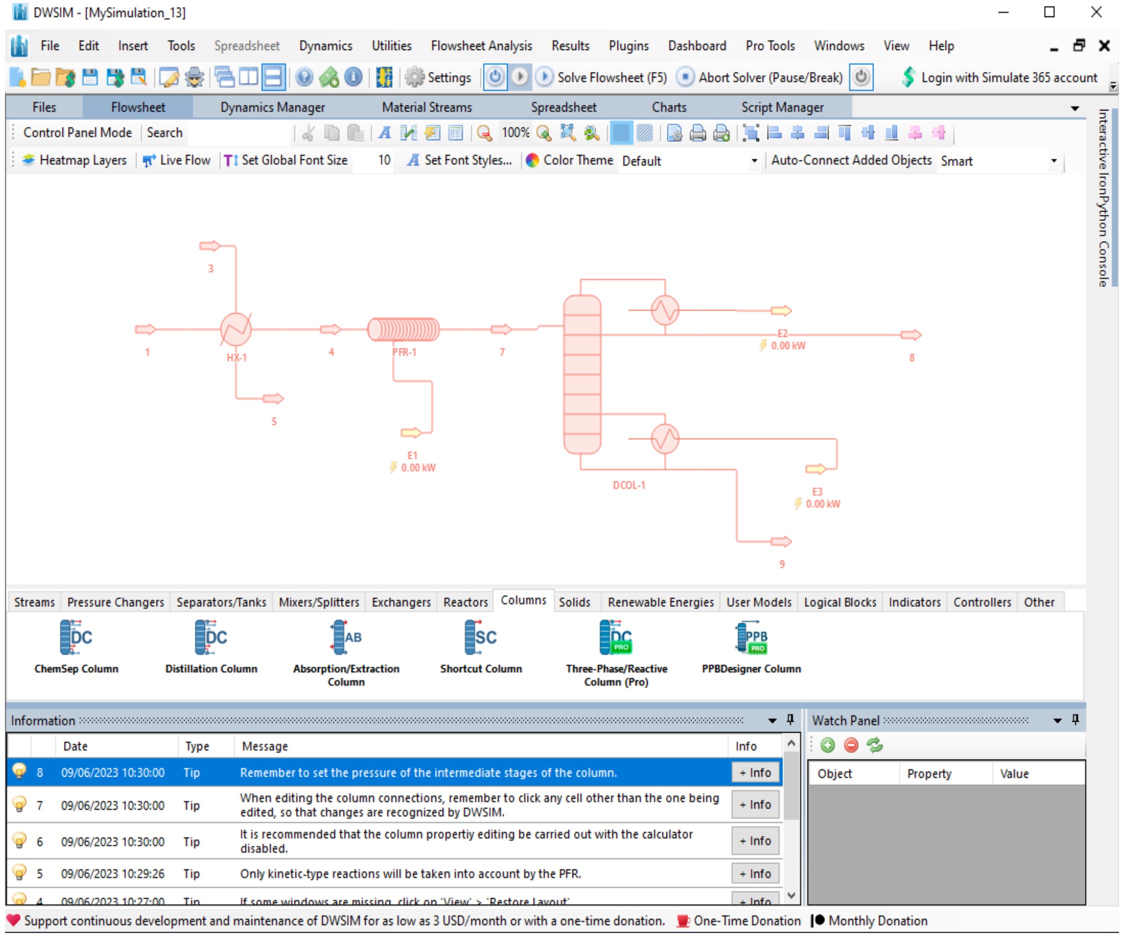
Stream

Flowsheet



Current process design methods

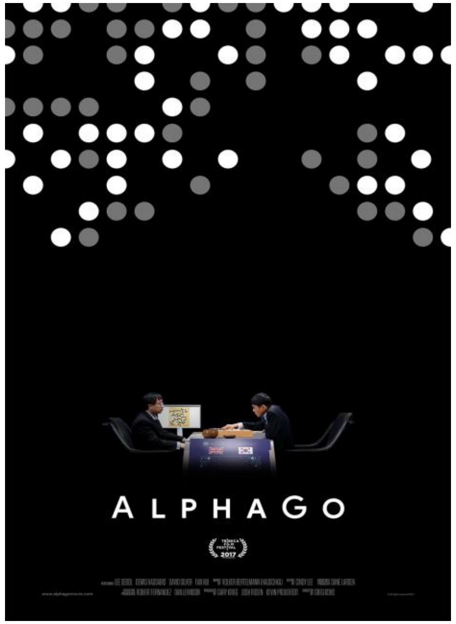
- Current process design methods are mostly trail-and-error based on experience
- Engineers utilize the commercial process simulator to manually add unit operation one by one and simulate the flowsheet
- This requires a long simulation time



→ Can we leverage ML in process design?

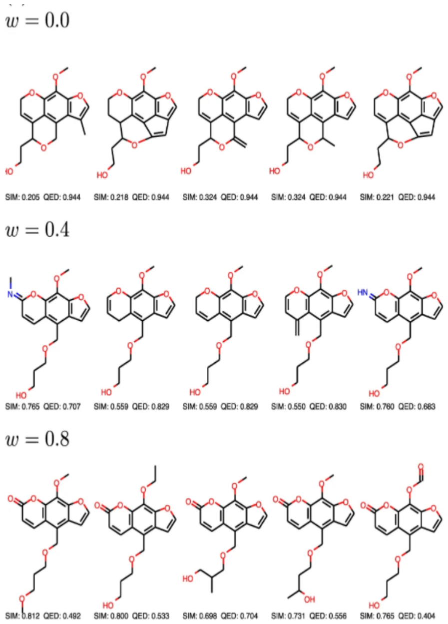
Reinforcement learning shows super-human performance

Board game: GO[1]

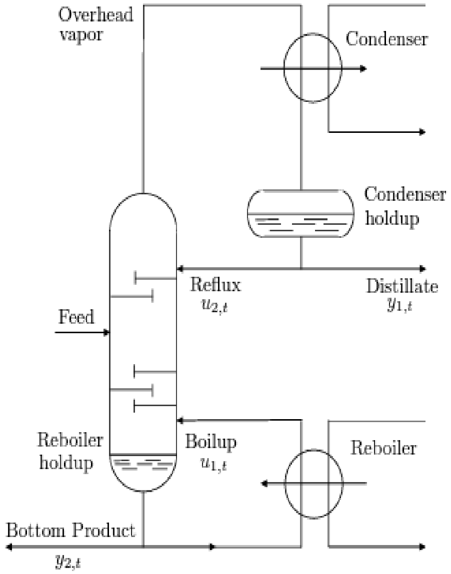


Computer game [2]

Molecular design [3]



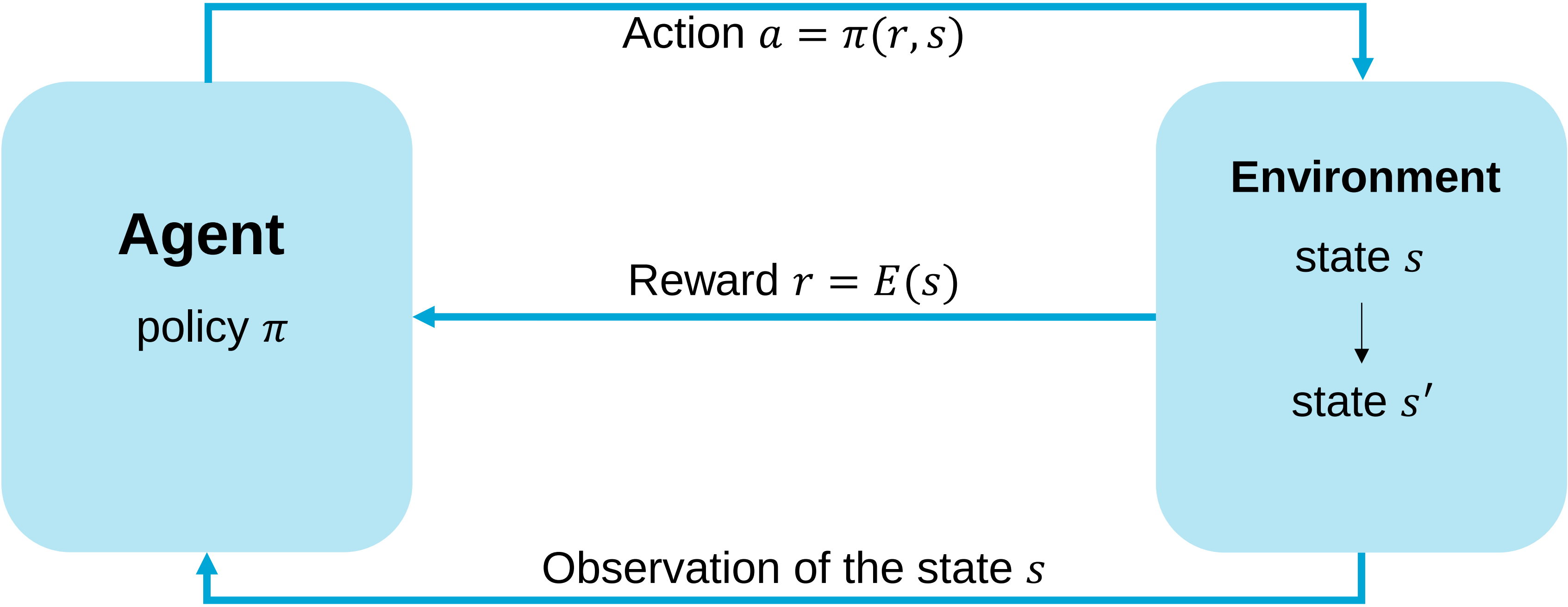
Process control [4]



→ **Can we use reinforcement learning in process design?**

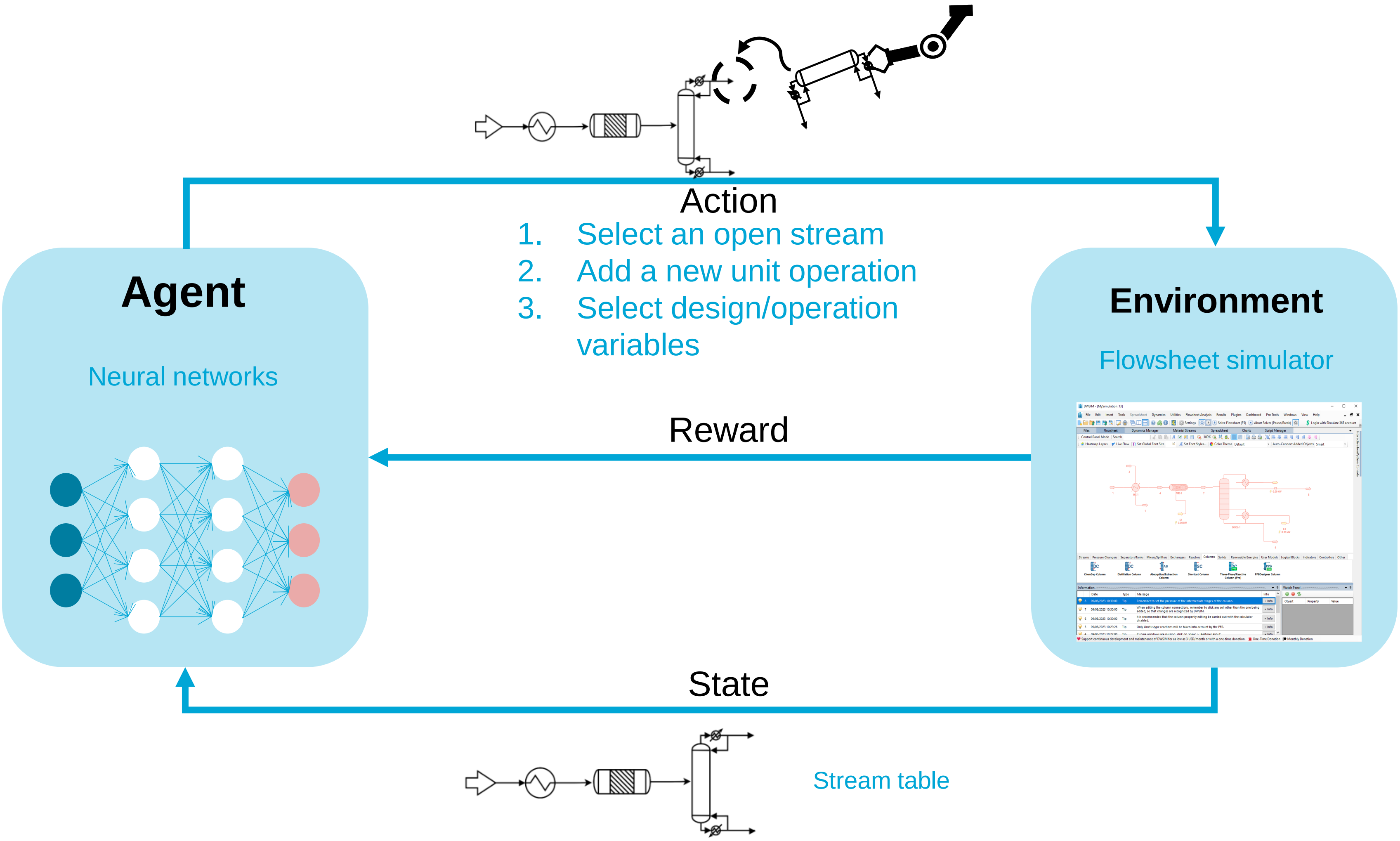
[1] Figure 1: Silver, D., Huang, A., Maddison, C. et al. Mastering the game of Go with deep neural networks and tree search. Nature 529, 484–489 (2016). https://doi.org/10.1038/nature16961
[2] Figure 2: https://analyticsindiamag.com/this-ai-agent-uses-reinforcement-learning-to-self-drive-in-a-video-game/
[3] Figure 3: Zhou, Z., Kearnes, S., Li, L. et al. Optimization of Molecules via Deep Reinforcement Learning. Sci Rep 9, 10752 (2019). https://doi.org/10.1038/s41598-019-47148-x
[4] Figure 4: Spielberg, S., Tulsyan, A., Lawrence, N. P., Loewen, P. D., & Gopaluni, R. B. (2020). Deep reinforcement learning for process control: A primer for beginners. arXiv preprint arXiv:2004.05490.

What is reinforcement learning?



[1] R. S. Sutton and A. G. Barto. Reinforcement Learning: An Introduction. The MIT Press, second edition, 2018

Reinforcement learning for process design



[1] R. S. Sutton and A. G. Barto. Reinforcement Learning: An Introduction. The MIT Press, second edition, 2018
[2] Gao, Q., & Schweidtmann, A. M. (2024). Deep reinforcement learning for process design: Review and perspective. Current Opinion in Chemical Engineering, 44, 101012.

Three components in RL framework

Information representation

Agent architecture

Action space

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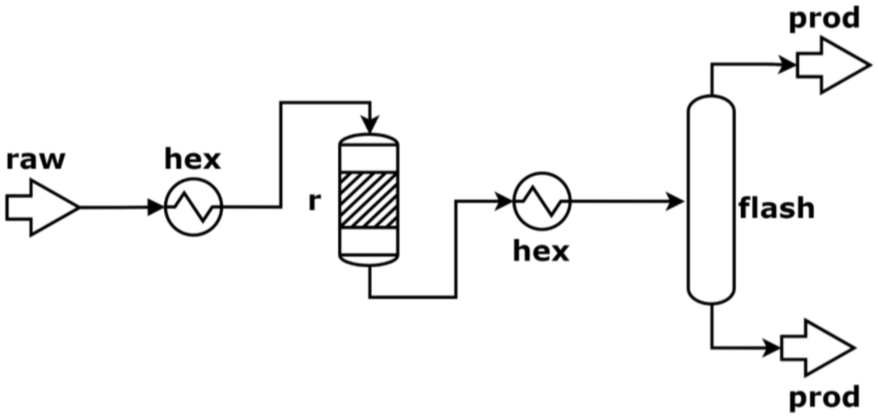
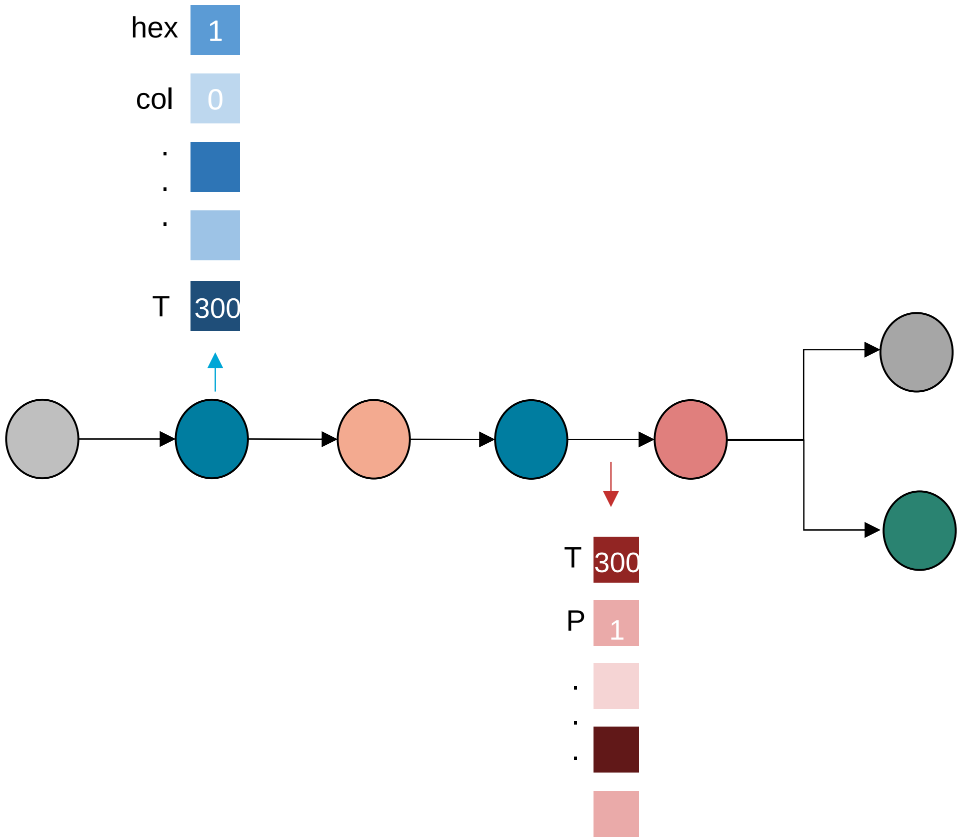
Agent architecture

Action space

Information representation: Flowsheet graph





[1] Göttl, Q., Grimm, D., & Burger, J. (2021). Automated Process Synthesis Using Reinforcement Learning. In Computer Aided Chemical Engineering (Vol. 50, pp. 209-214). Elsevier
[2] Stops, L., Leenhouts, R., Gao, Q., & Schweidtmann, A. M. (2023). Flowsheet generation through hierarchical reinforcement learning and graph neural networks. AIChE Journal, 69(1), e17938.

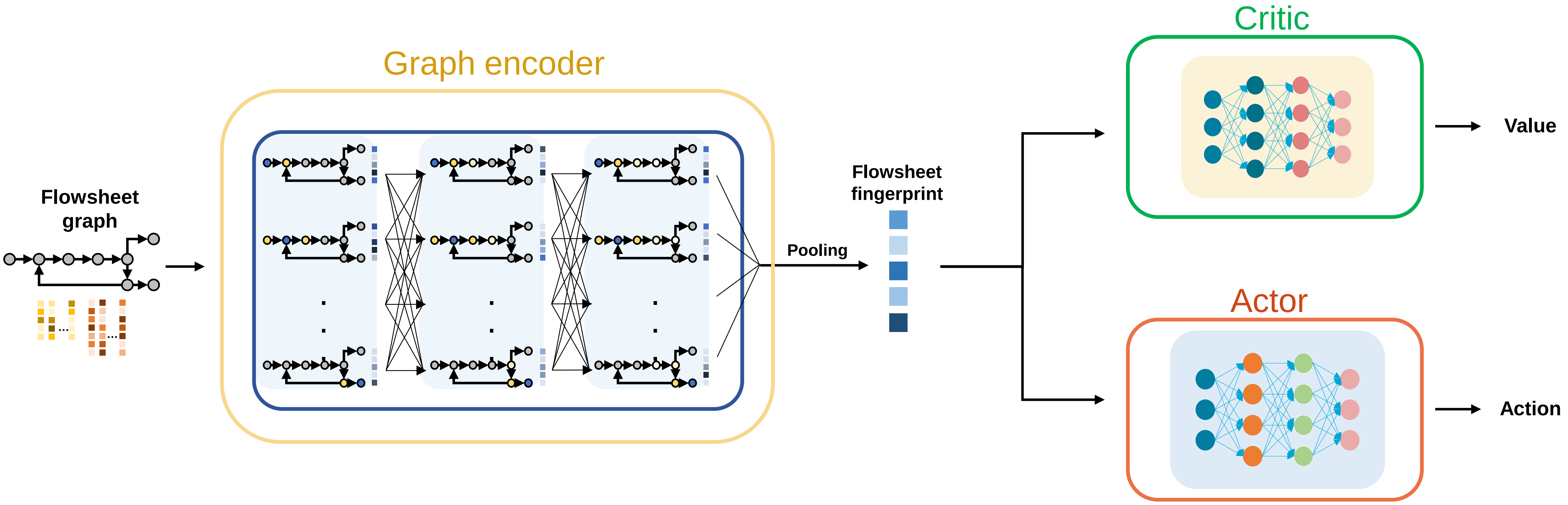
Three components in RL framework

Information representation

Agent architecture

Action space

Actor-critic agent structure



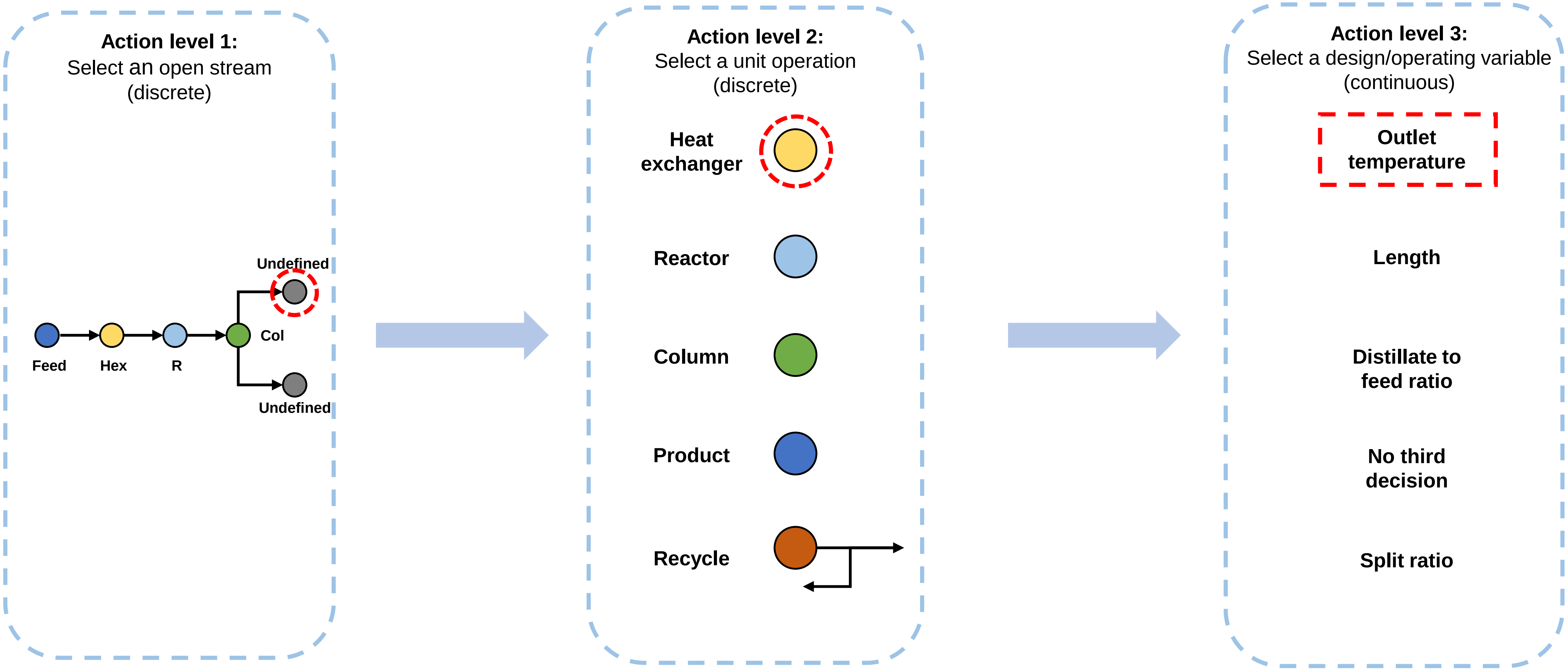
Three components in RL framework

Information representation

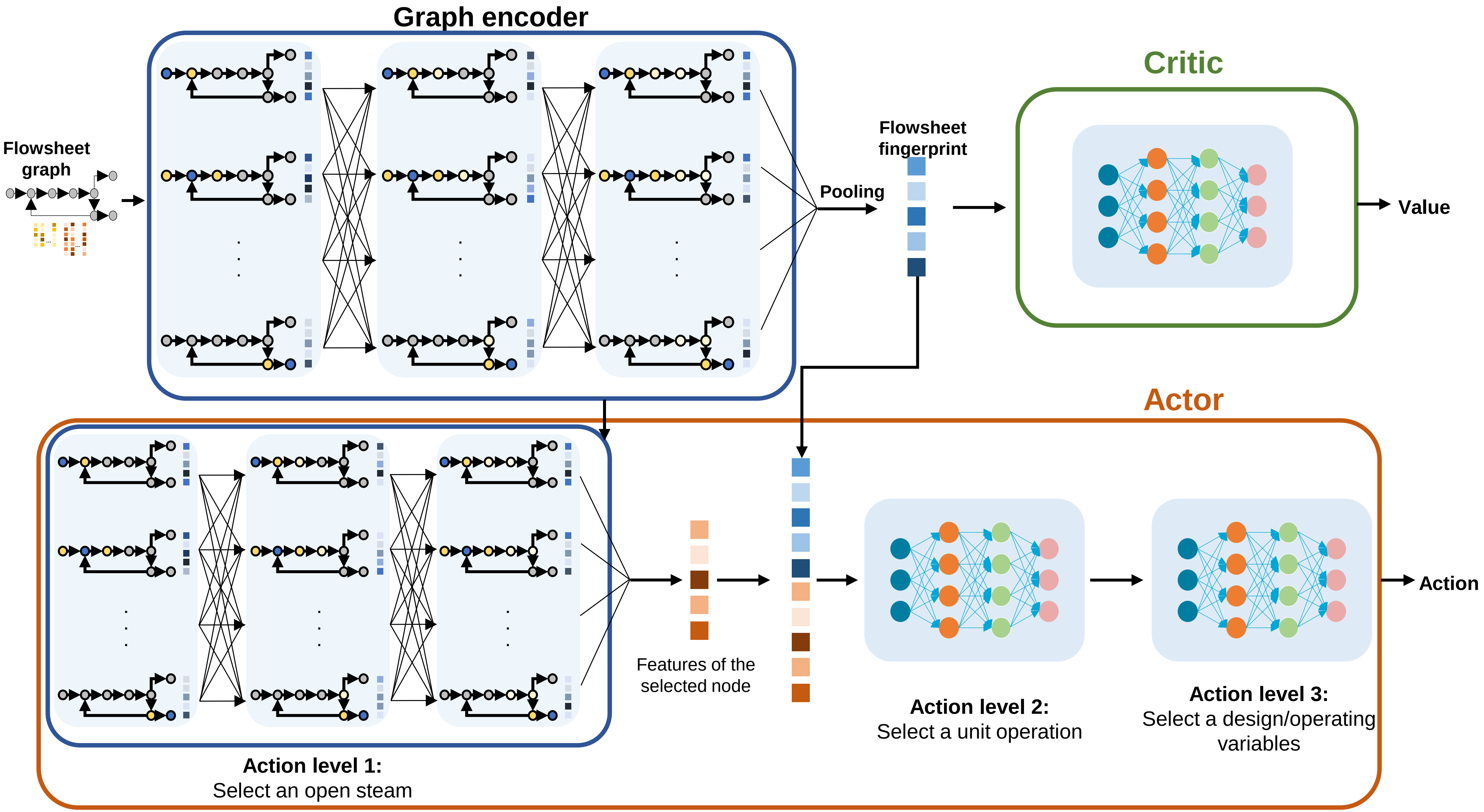
Agent architecture

Action space

Hierarchical hybrid action space



Actor-critic agent structure



Case study

- We use a simple reaction, and for the purpose of illustration, we are assuming ideal mixing behavior.

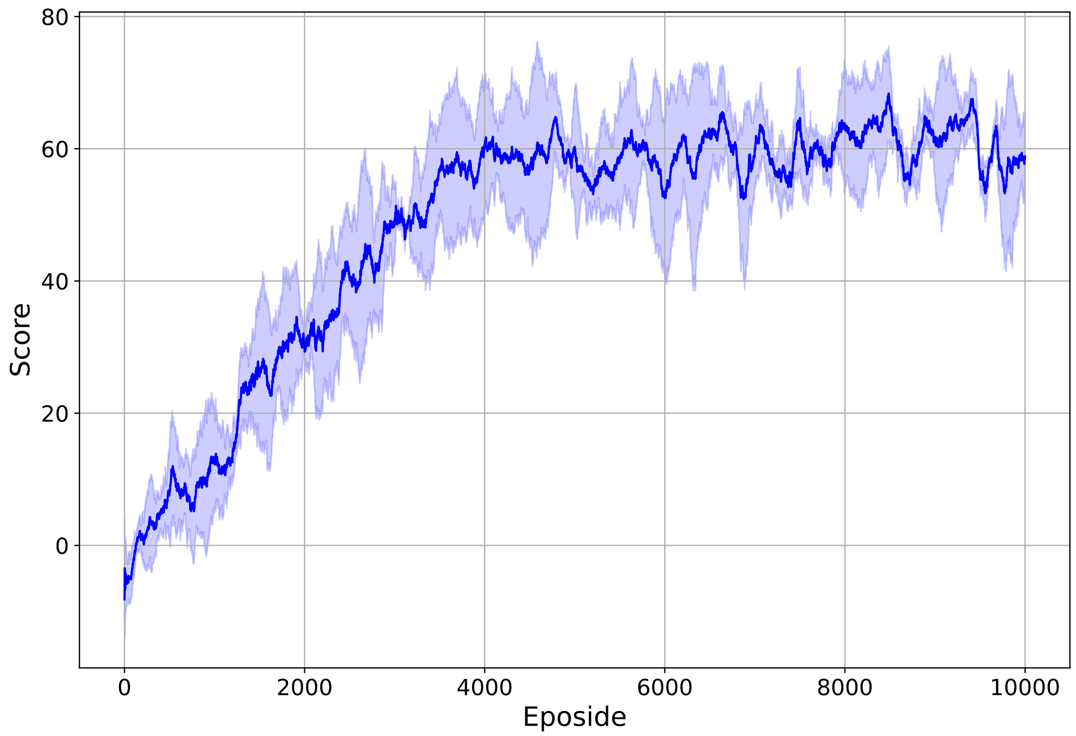
$$A + B \rightleftharpoons C + D$$

  - Feed initialization: 100 mol/s molar flow, 300 K temperature, equimolar mixture of A and B
- DWSIM environment
- Unit operations and design variables
  - Reactor: Length l (0.1m – 20m)
  - Column: Distillate to feed ratio D/F (0.05 - 0.95)
  - Heat exchanger: Water temperature T (278.15K - 326.95K)
  - Recycle: Recycled ratio *r* (0.1 – 0.9)
- Reward: Net cash flow

$$reward = \sum P_{product} - P_{feed} - \sum (I + O)_{unit} - C_{fixed}$$

[1] Cuncun Zuo, Langsheng Pan, Shasha Cao, Chunshan Li, and Suojiang Zhang Industrial & Engineering Chemistry Research 2014 53 (26), 10540-10548 DOI: 10.1021/ie500371c

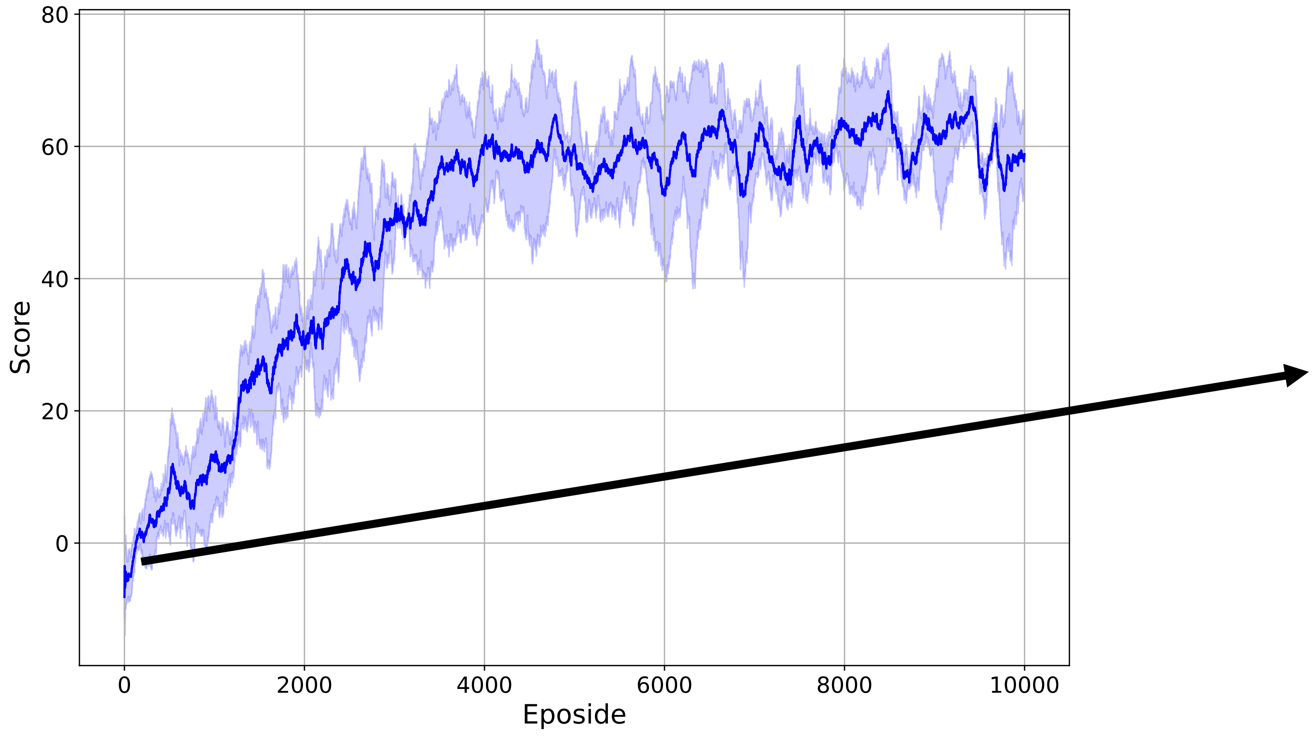
Learning curve of agent



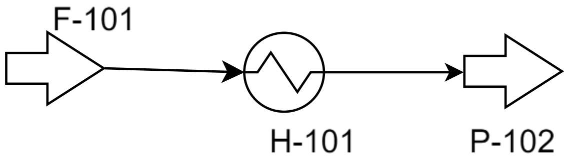
- There are in total 3 parallel runs
- Each run contains 10,000 episodes
- Each episode generate a complete flowsheet
- 10,000 training episodes need 72 hours

[1]

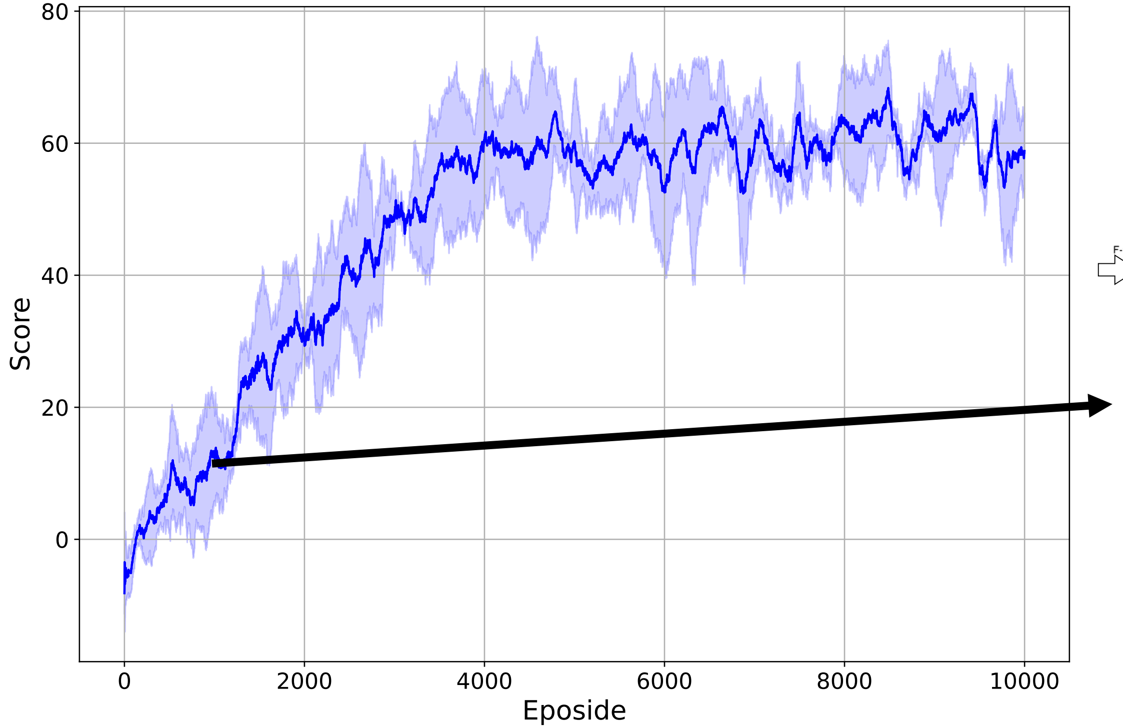
Learning curve of agent



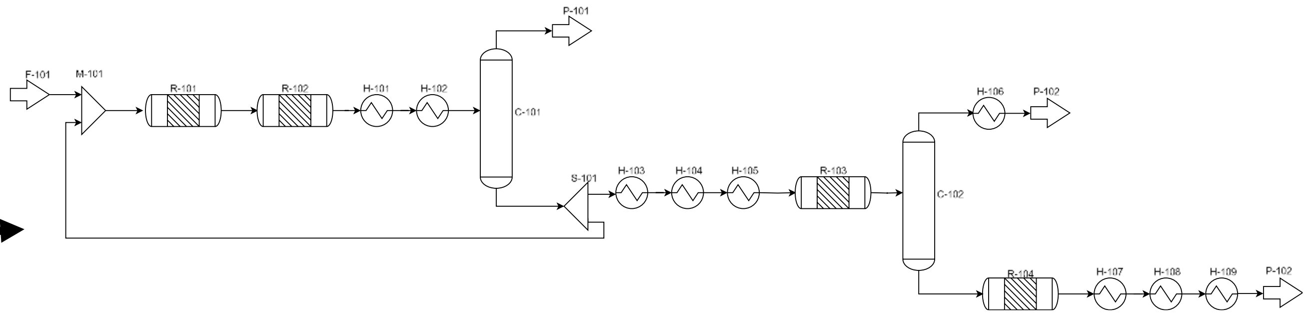
50 episodes



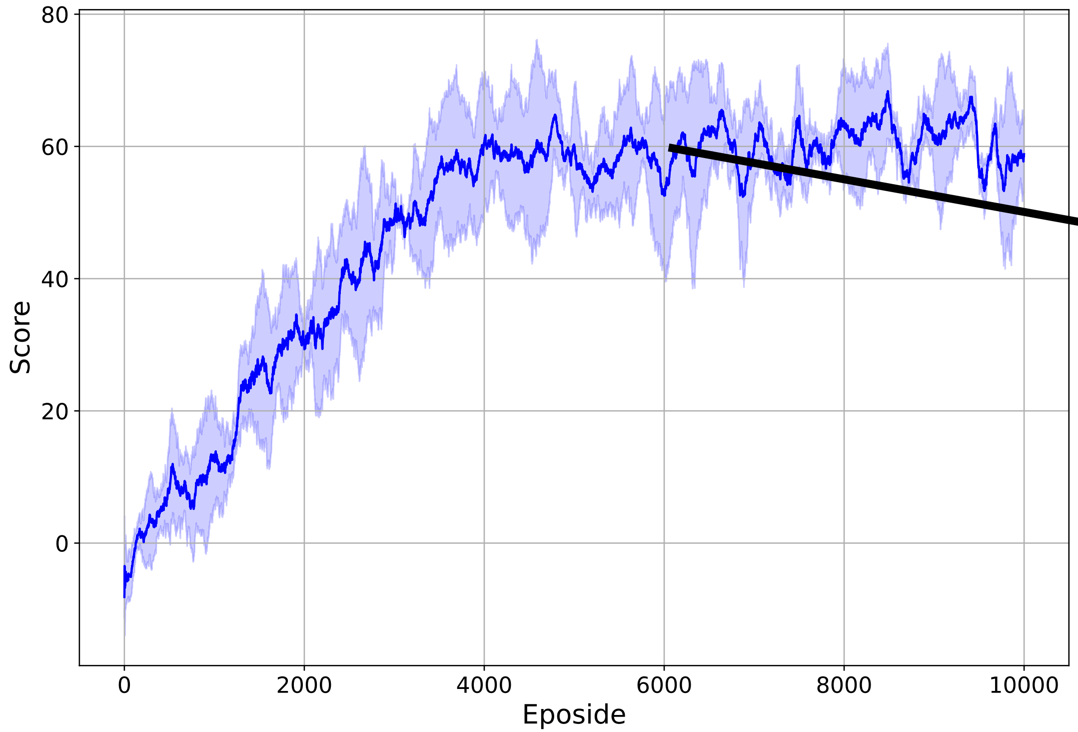
Learning curve of agent



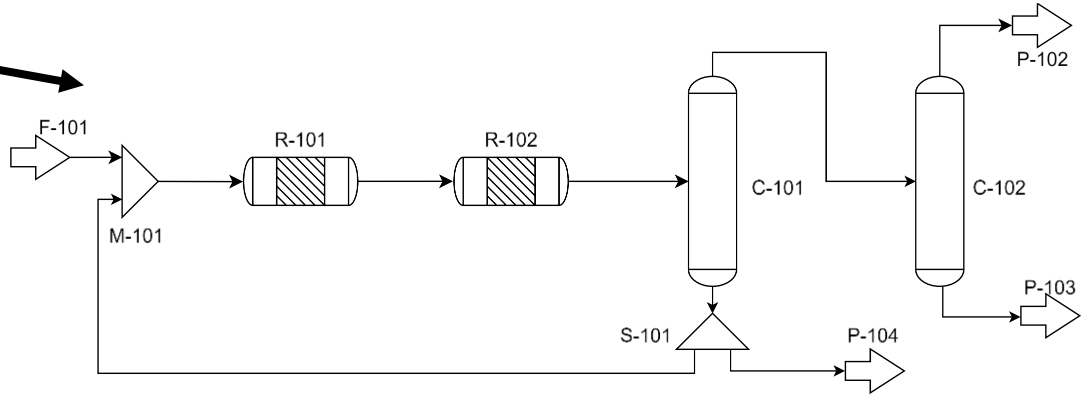
250 episodes



Learning curve of agent

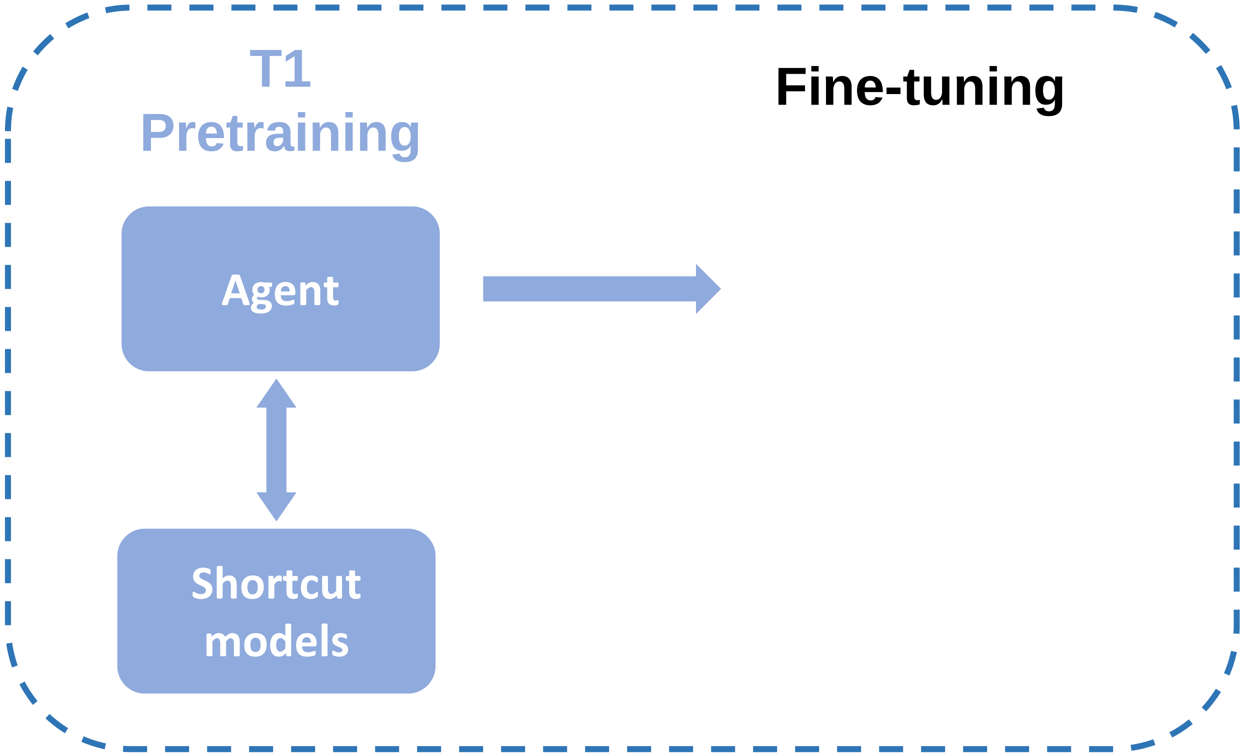


6000 episodes



Limitation: Long simulation time

- 10,000 training episodes need 72 hours
- Can we accelerate the training process?



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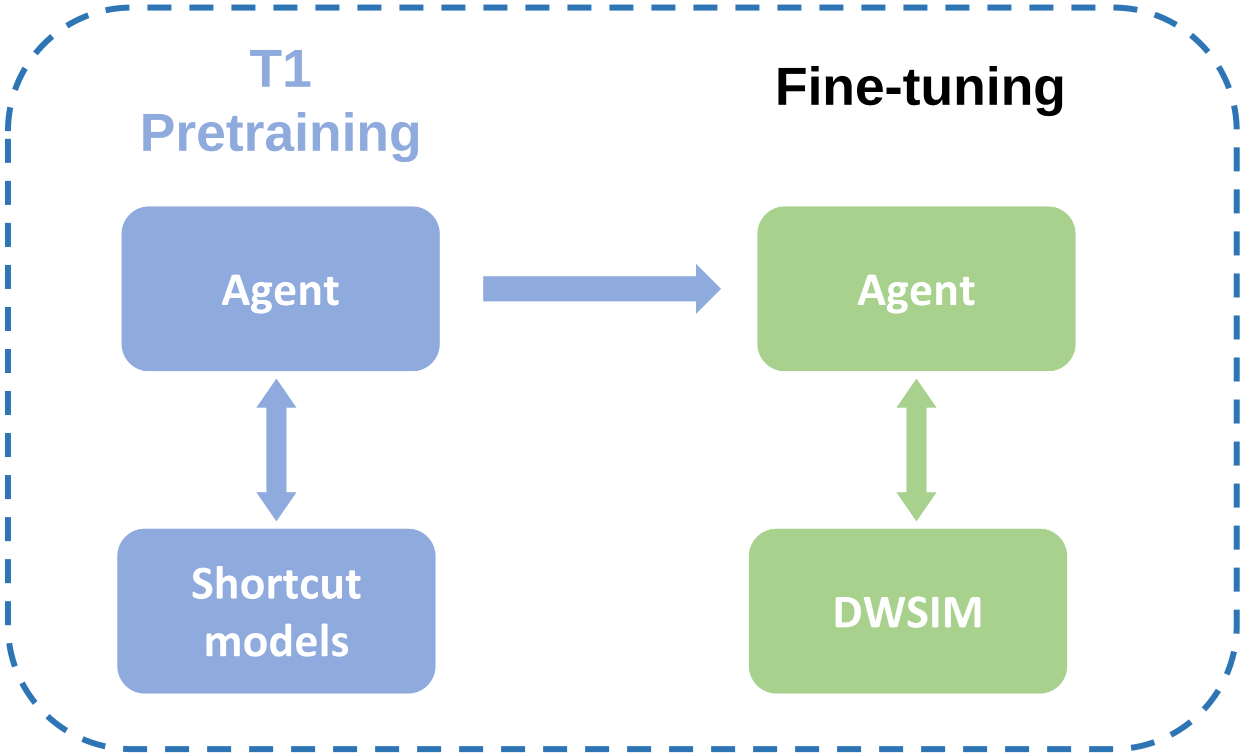
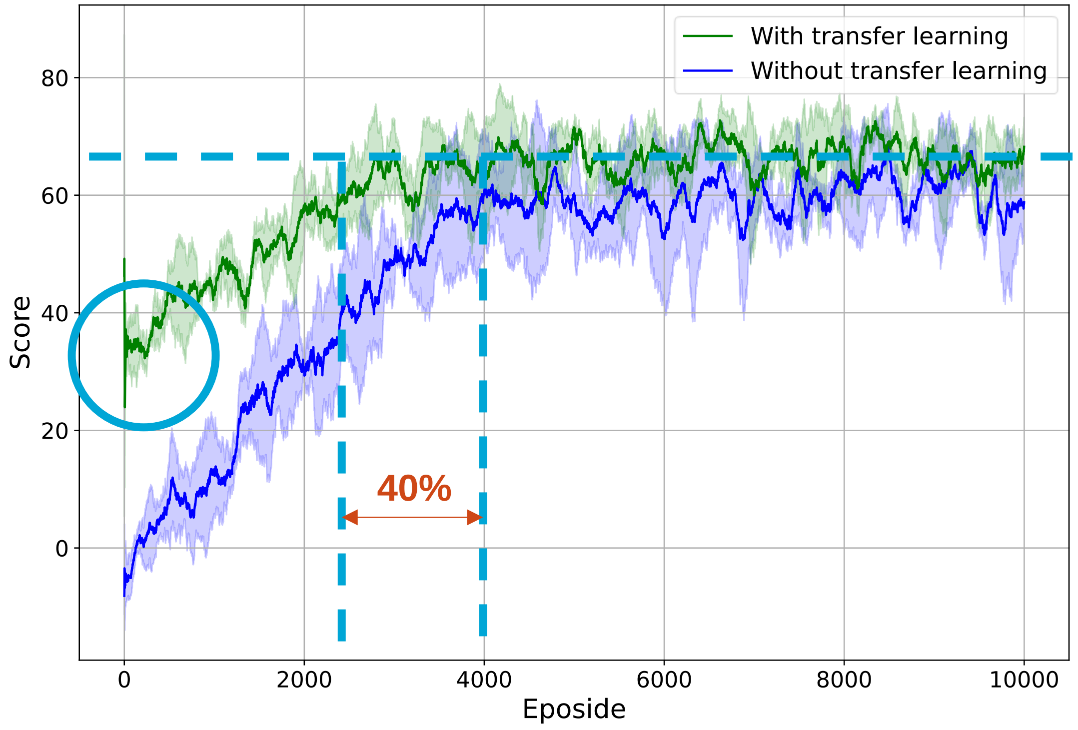


Transfer learning in RL for process synthesis



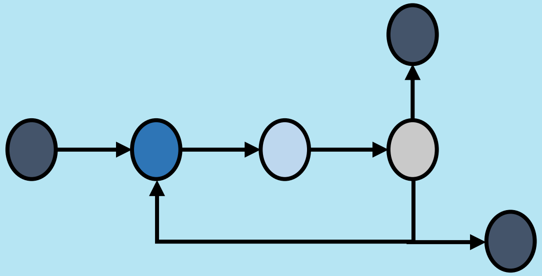
- Faster feasibility
  - The agent with transfer learning can generate feasible flowsheet even in the first episode
- Improved performance
  - The agent with transfer learning reaches even higher convergence score
- Efficiency boost
  - Using score of 60 as reference, the agent with transfer learning decreases by 40% training episodes

[1]Gao, Q., Yang, H., Shanbhag, S. M., & Schweidtmann, A. M. (2023). Transfer learning for process design with reinforcement learning. In Computer Aided Chemical Engineering (Vol. 52, pp. 2005-2010). Elsevier.

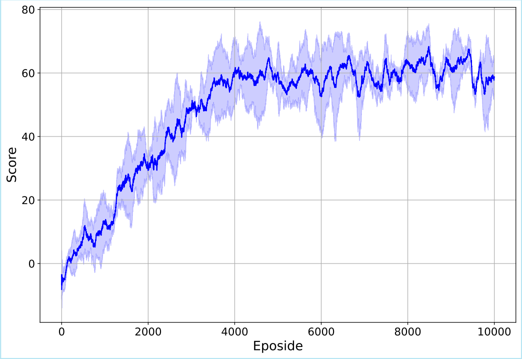
Conclusion

- We propose a reinforcement learning algorithm that

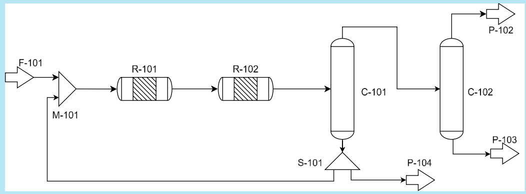
represents flowsheets as graphs



uses graph neural networks to learn



can synthesize new processes



→ Reinforcement learning provides new possibility for process design

Thank you very much for your attention!

Paper link: https://aiche.onlinelibrary.wiley.com/doi/pdf/10.1002/aic.17938