# Generative artificial intelligence for control structure prediction

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Seminar on GraphsData@TUDelft

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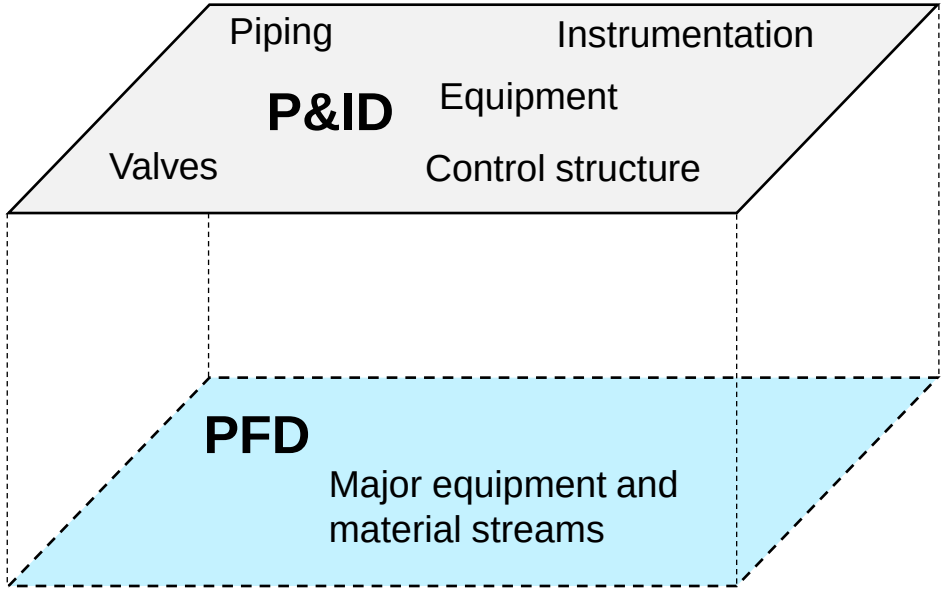
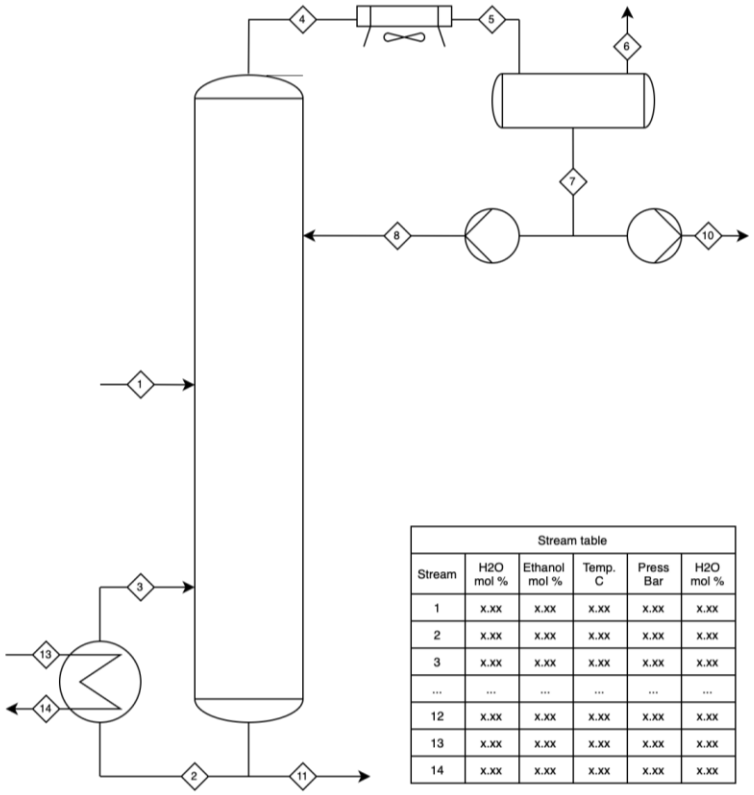
# Piping and Instrumentation Diagram (P&ID)




[1] Toghraei, M. (2019). *Piping and Instrumentation Diagram Development*. Wiley & Sons. ISBN: 9781119329343

# Piping and Instrumentation Diagram (P&ID)

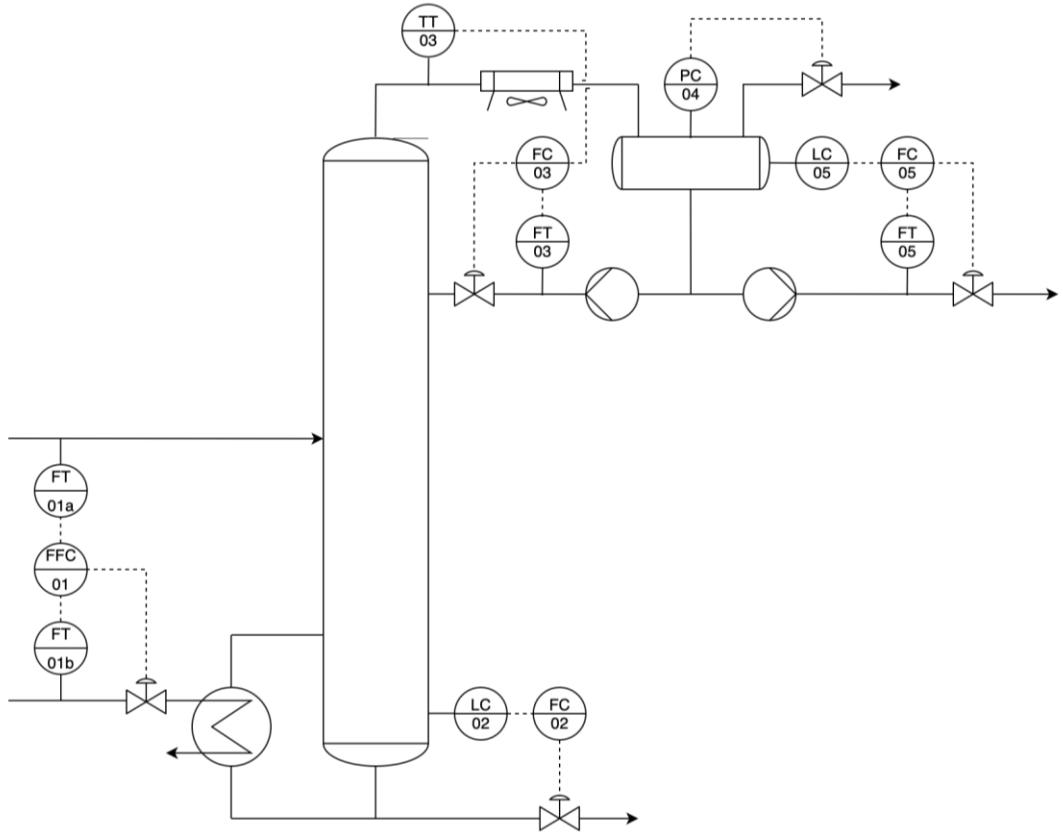
**PFD**




Stream table

| Stream | H2O mol % | Ethanol mol % | Temp. C | Press Bar | H2O mol % |
|---|---|---|---|---|---|
| 1 | x.xx | x.xx | x.xx | x.xx | x.xx |
| 2 | x.xx | x.xx | x.xx | x.xx | x.xx |
| 3 | x.xx | x.xx | x.xx | x.xx | x.xx |
| ... | ... | ... | ... | ... | ... |
| 12 | x.xx | x.xx | x.xx | x.xx | x.xx |
| 13 | x.xx | x.xx | x.xx | x.xx | x.xx |
| 14 | x.xx | x.xx | x.xx | x.xx | x.xx |

**P&ID**



# Piping and Instrumentation Diagram (P&ID)

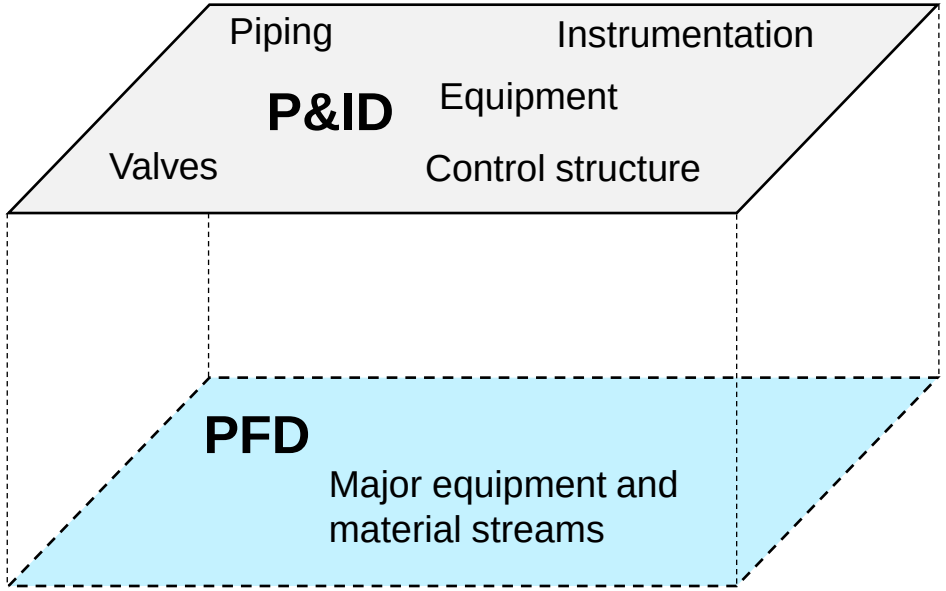
**Deployment of P&IDs[1]:**

- Engineering and design
- HAZOP
- Construction
- Start-up and operation
- Maintenance
- Decommissioning

» Central document for storing, revising, and exchanging information about processes

**Preparation of P&IDs:**

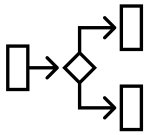
- prior projects, design heuristics, experience, etc.
- tedious, manual, and time-consuming task




[1] Toghraei, M. (2019). *Piping and Instrumentation Diagram Development*. Wiley & Sons. ISBN: 9781119329343

# Previous work on automatic P&ID generation

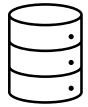
## Rule-based systems[1,2,3]



- Development since the 1990s
- Based on the modularization of chemical plants
- Domain knowledge structured as a decision tree
- Guidance of the user with design questions to generate P&IDs

» Difficult to set-up, maintain, and extend
Little adoption by industry

## (Semi-)automated AI systems

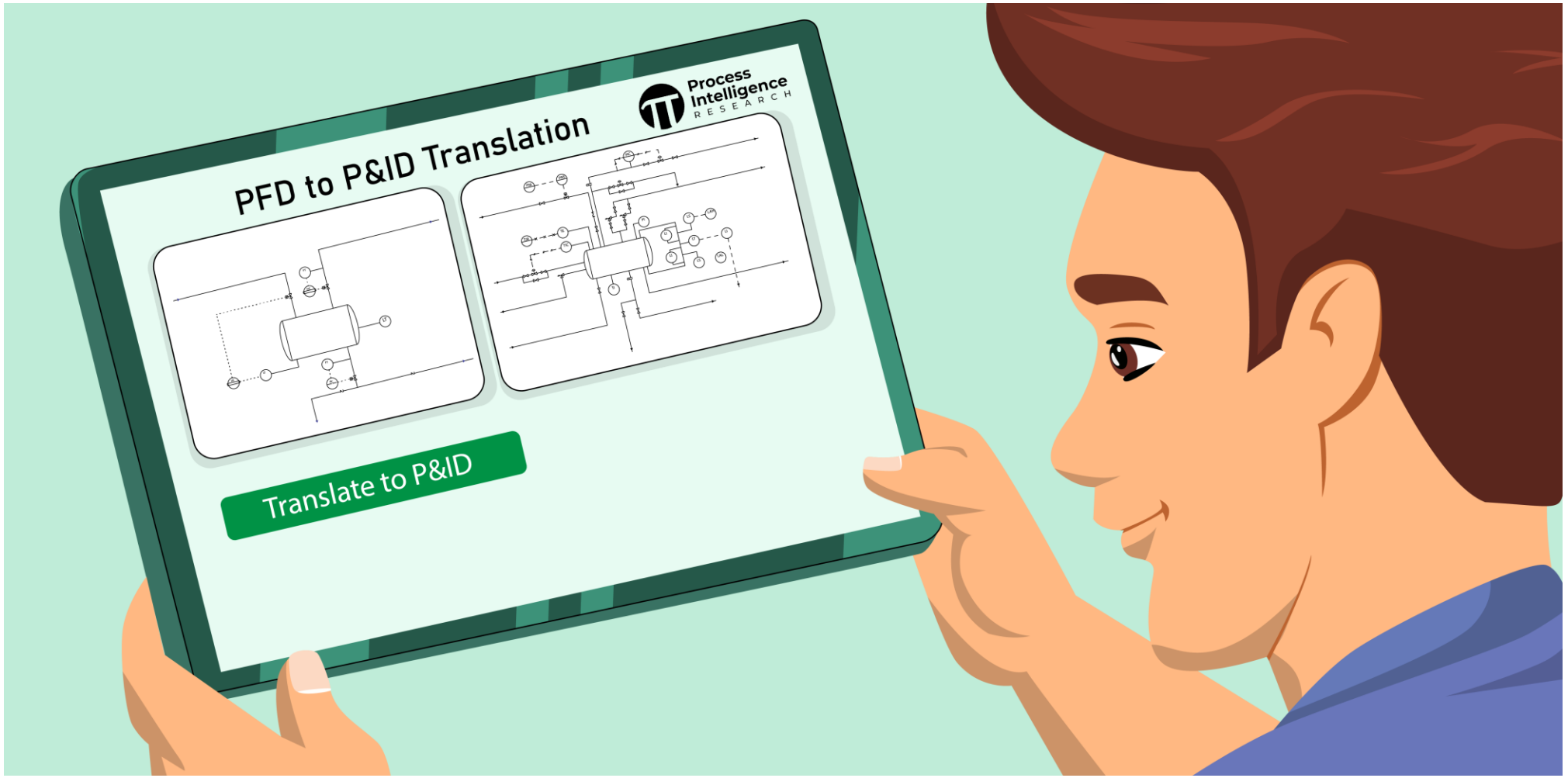


- Recent development
- Methods learn patterns in process diagrams
- Autocompletion of PFDs[4]
- Subsequent equipment prediction[5]

» No method for the direct generation of P&IDs from PFDs


[1] Blitz, H., Engelke, J., Sonnenschein, R., Schmidt-Traub, H. (1994). *Rechnergestützte Konfigurierung von RI-Fließbildern am Beispiel von Pumpen*. CIT. https://doi.org/10.1002/cite.330660404
[2] Uzuner, H., Schembecker, G. (2012). *Wissensbasierte Erstellung von R&I-Fließbildern*. CIT. https://doi.org/10.1002/cite.201100230
[3] Obst, M., Doherr, F., Urbas, L. (2013). *Wissensbasiertes Assistenzsystem für modulares Engineering*. Automatisierungstechnik. https://doi.org/10.1524/auto.2013.0011
[4] Vogel, G., Schulze Balhorn, L., Schweidtmann, A.M. (2022). *Learning from flowsheets: A generative transformer model for flowsheet autocompletion*. Preprint on arXiv. https://doi.org/10.48550/arXiv.2208.00859
[5] Oeing, J., Welscher, W., Krink, N., Jansen, L., Henke, F., Kockmann, N. (2022). *Using artificial intelligence to support the drawing of piping and instrumentation diagrams using DEXPI standard*. Digital Chemical Engineering. https://doi.org/10.1016/j.dche.2022.100038

# PFD to P&ID translation



# What does it take to develop generative AI algorithms?

| | Big data | Information representation | Model architecture |
|---|---|---|---|
| ChatGPT | 57 TB | Text | Transformer |
| Process engineering | ? | ? | ? |

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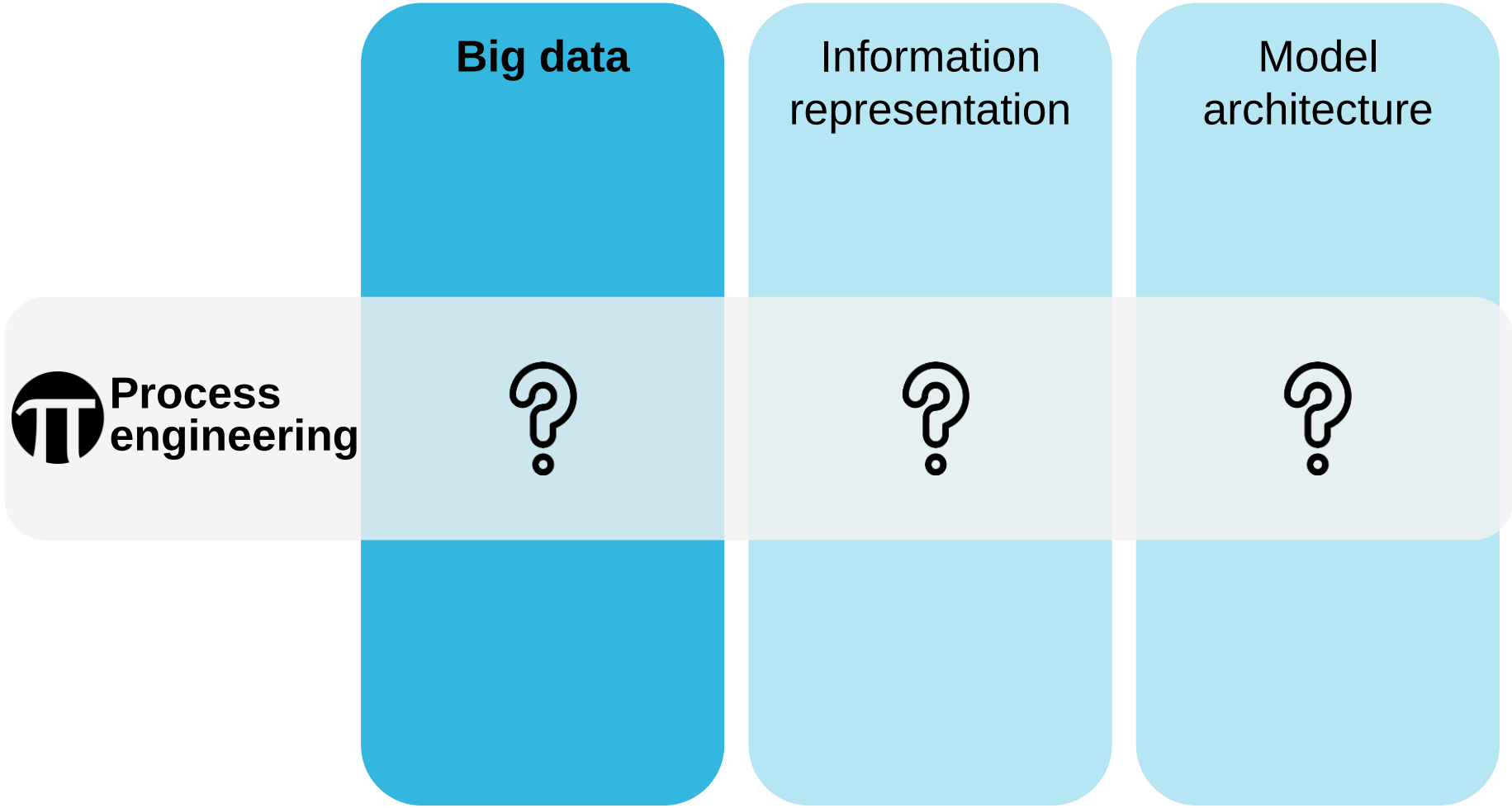
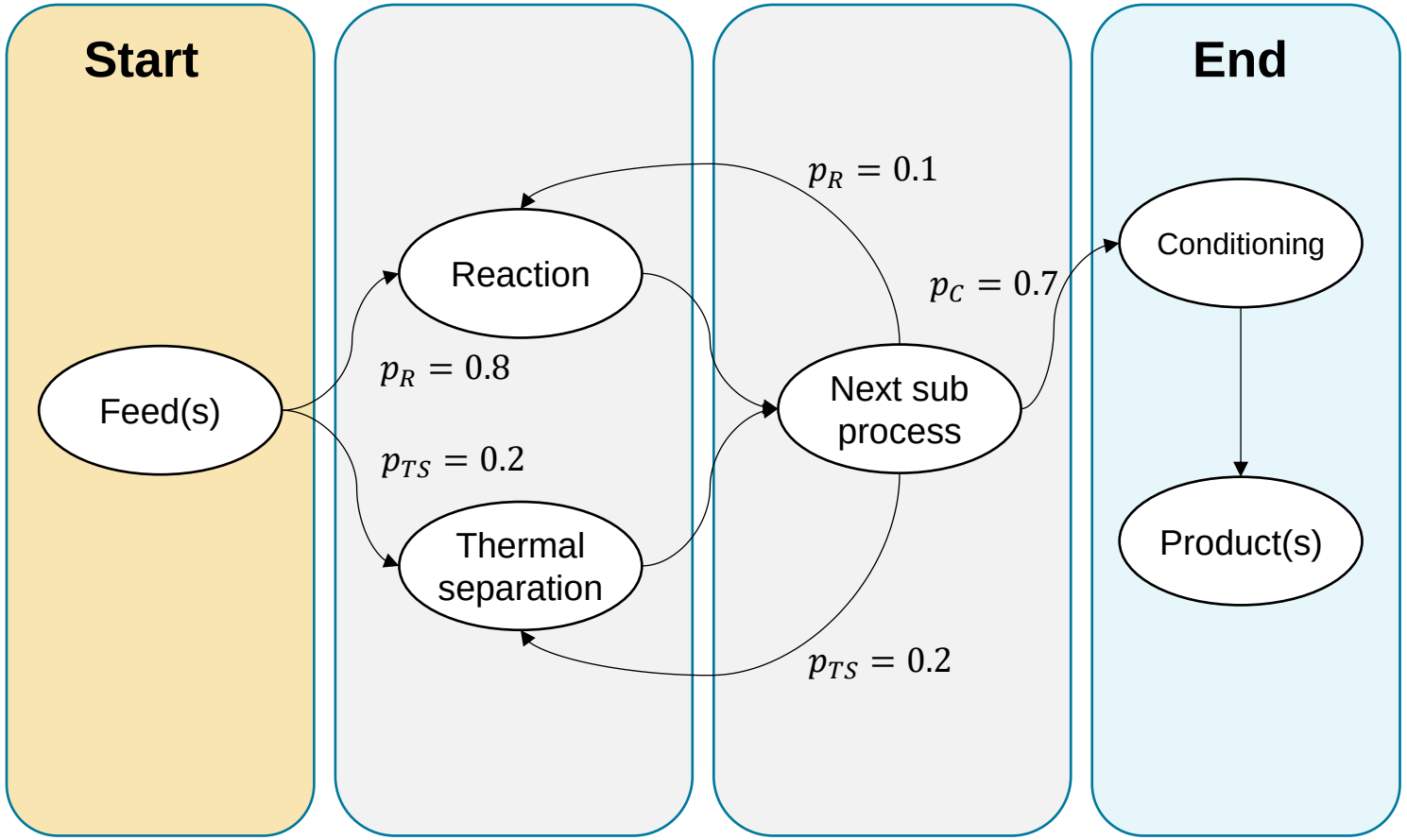


# P&ID generation[1]




**Generated flowsheets**
based on design heuristics and Markov chains

- Generation in graph format

[1] Hirtreiter, E., Schulze Balhorn, L., & Schweidtmann, A. M. (2024). Toward automatic generation of control structures for process flow diagrams with large language models. *AIChE Journal*, *70*(1), e18259.

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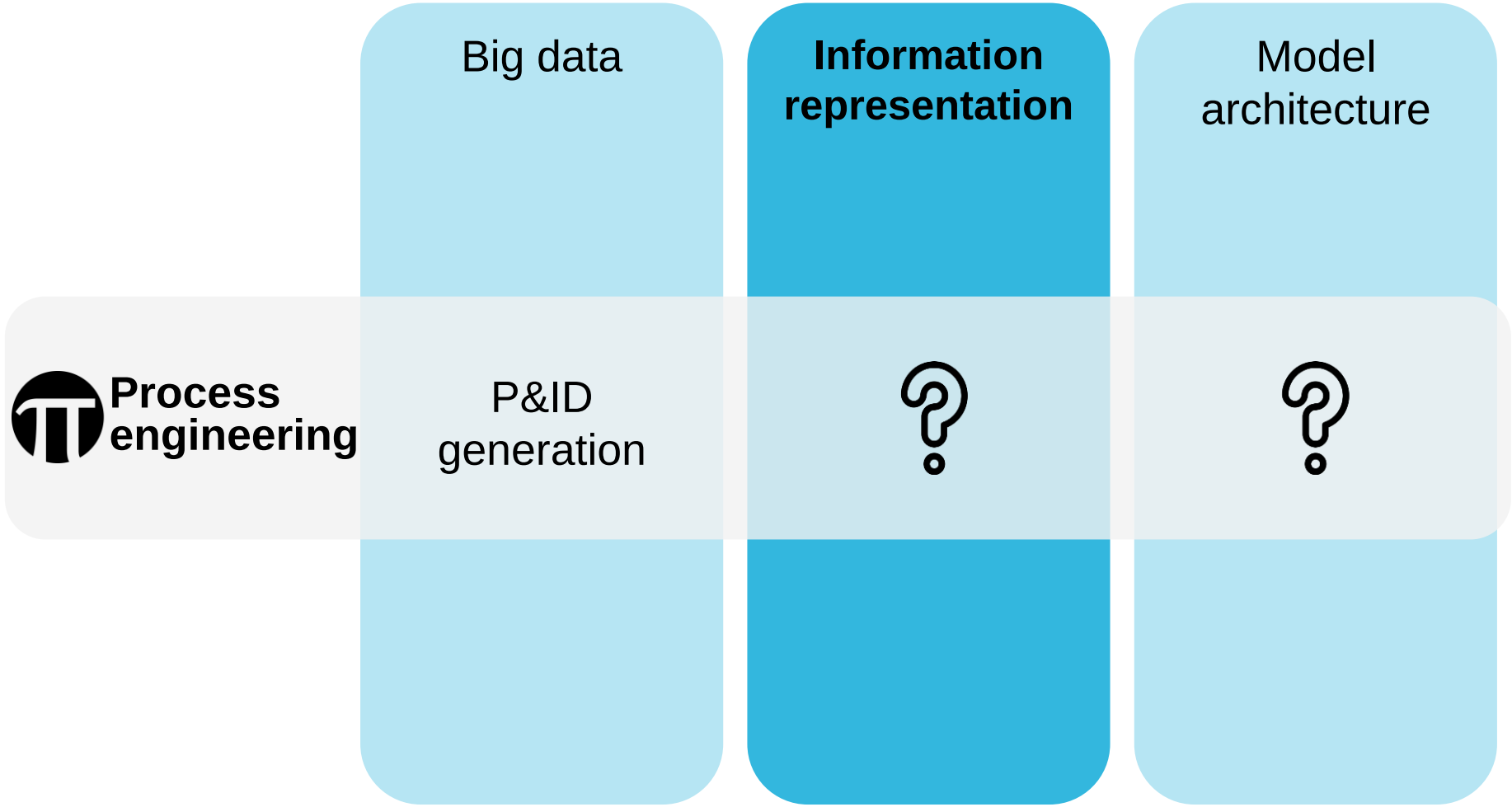
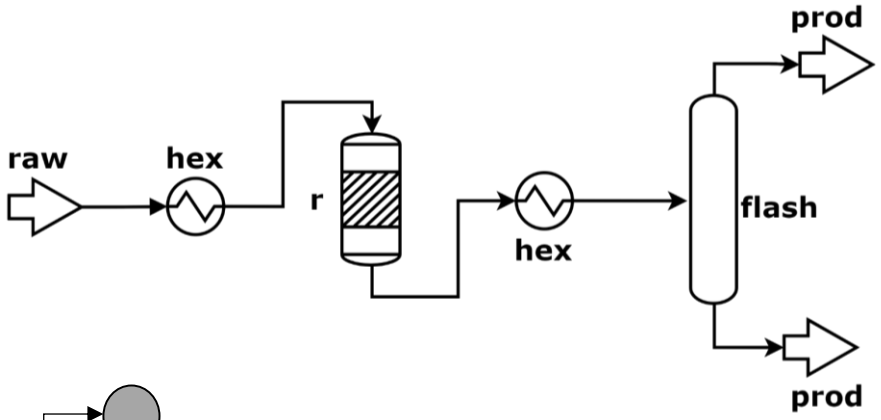
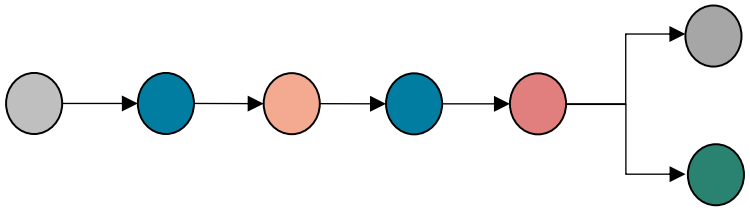


# Information representation of flowsheets



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## Flowsheet graphs[1] *G = (V, E)*

- Unit operations as nodes and streams as edges
- Add. information as feature vectors
- Variations incl. directed, hyper-, knowledge graphs

## SFILES[2-4]

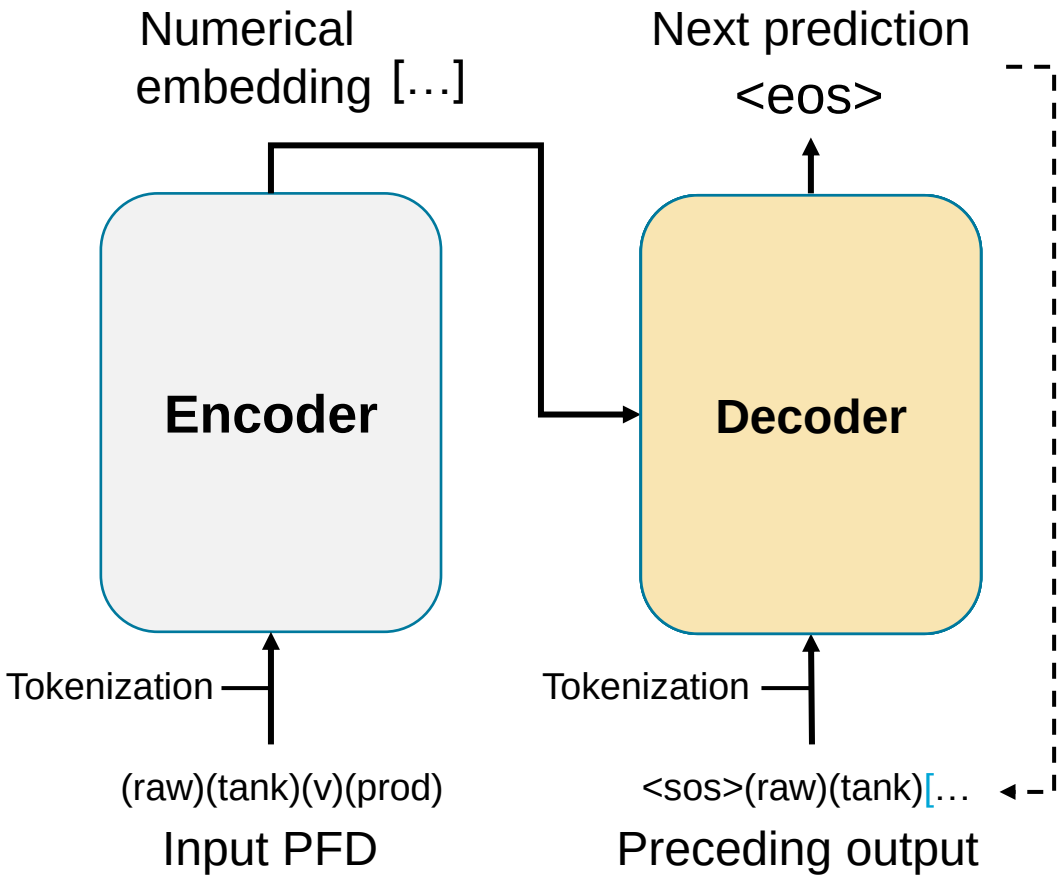
- Unique text representation of flowsheet topology
- Inspired by SMILES for molecules
- Currently limited to topology

[1] 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.
[2] d'Anterroches, L. (2005). *Process Flowsheet Generation & Design through a Group Contribution Approach*. [CAPEC], Department of Chemical Engineering, Technical University of Denmark.
[3] Vogel, G., Hirtreiter, E., Schulze Balhorn, L., & Schweidtmann, A. M. (2023). SFILES 2.0: an extended text-based flowsheet representation. *Optimization and Engineering*, 1-23.
[4] Mann, V., Gani, R., Venkatasubramanian, V. (2023). Intelligent Process Flowsheet Synthesis and Design using Extended SFILES Representation. *ESCAPE33*

# What does it take to develop generative AI algorithms?

| | Big data | Information representation | **Model architecture** |
|---|---|---|---|
| **Process engineering** | P&ID generation | SFILES 2.0 or graphs |  |

# P&ID prediction model – SFILES-to-SFILES




**Applied model for control structure prediction:**

T5[1] (based on transformer architecture[2])

**Final P&ID:**

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[1] Raffel, C., Shazeer, N., Roberts, N., Lee, K., Narang, S., Matena, M., Zhou, Y., Li, W., Liu, P.J. (2020). *Exploring the Limits of Transfer Learning with a Unified Text-to-Text Transformer.* arXiv. https://doi.org/10.48550/arxiv.1910.10683
[2] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L., Polosukhin, I. (2017). *Attention is All you Need.* arXiv. https://doi.org/10.48550/arxiv.1706.03762

# Illustrative example

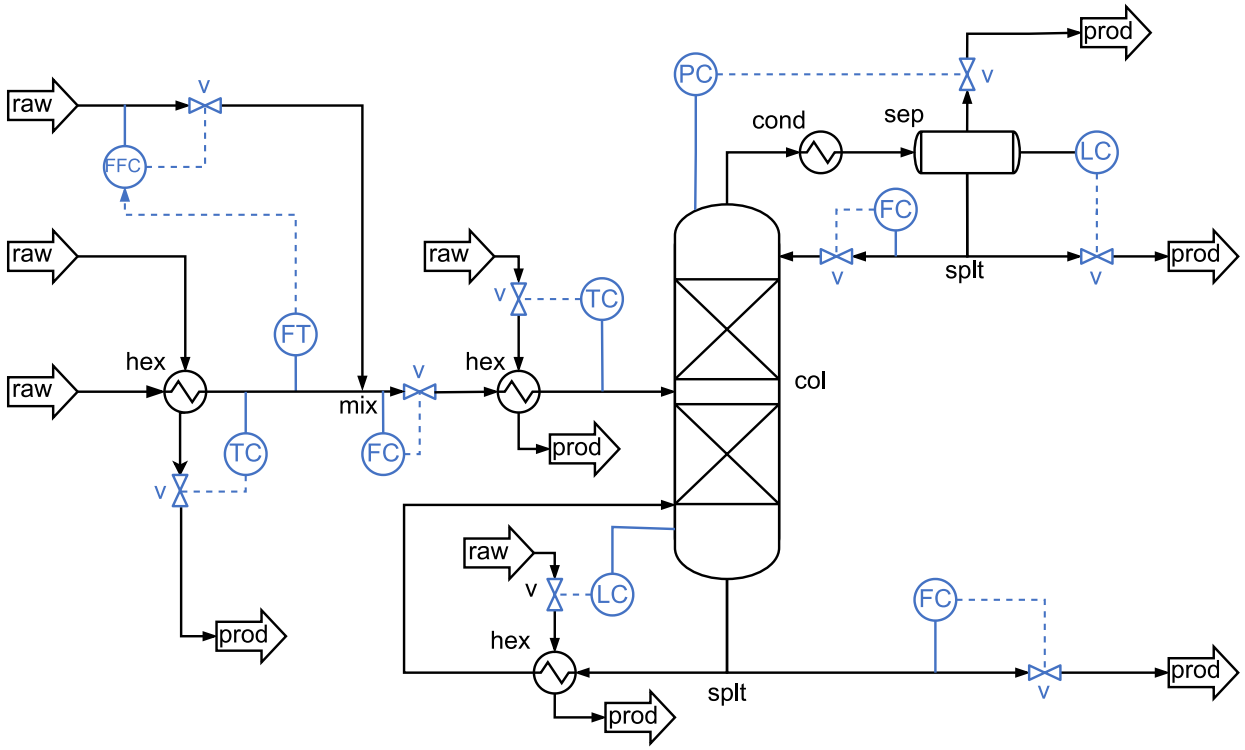
**Proof of concept**
Limited to topology information, training bias, potential errors in prediction…

## Model

- SFILES-to-SFILES model (7.9M param)
- **In**: PFD; **Out**: PFD w/ control structure

## Dataset

- 100,000 synthetic flowsheets with control structure
- 53 different building blocks




[1] Hirtreiter, E., Schulze Balhorn, L., & Schweidtmann, A. M. (2024). Toward automatic generation of control structures for process flow diagrams with large language models. *AIChE Journal*, *70*(1), e18259.

# Thank you very much for your attention!