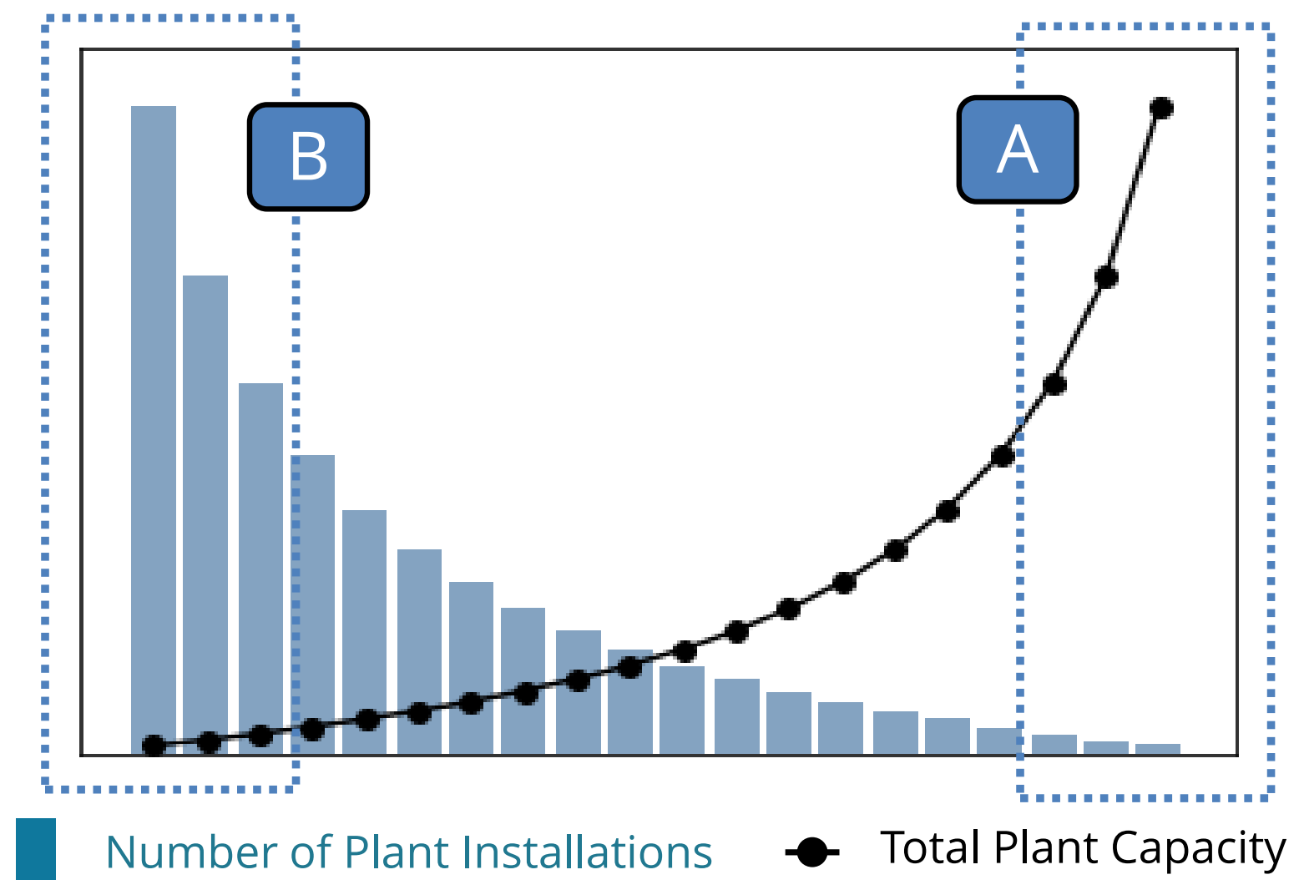
Advances in Process Family Design for Rapid Deployment of Chemical Processes

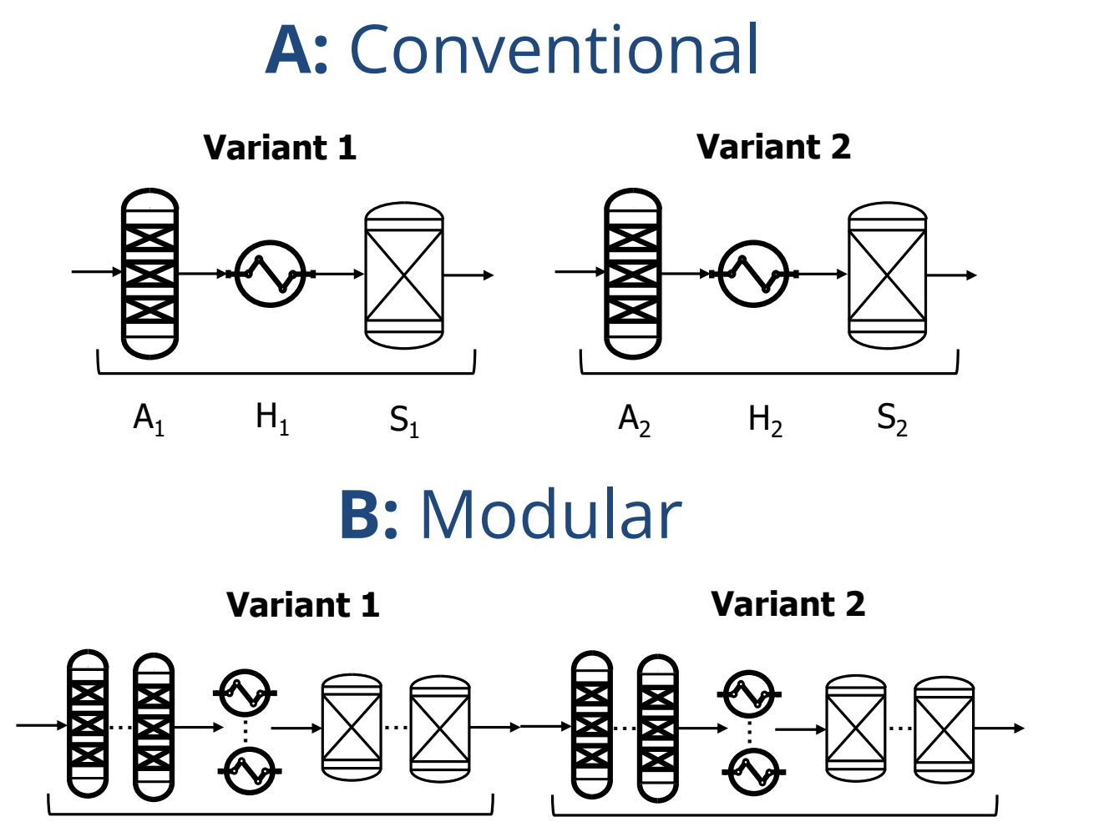
Georgia Stinchfield[a], Sherzoy Jan[a], Miguel Zamarripa[b,c], Joshua C. Morgan[b,c], Jean-Paul Watson[d], Carl D. Laird[a]

[a] Carnegie Mellon University, [b] National Energy and Technology Laboratory, [c] NETL Support Contractor, [d] Lawrence Livermore National Laboratory

Motivation[1]

Optimally deploy a **process system** across **decentralized sites** with **different** geographical, environmental & operating requirements

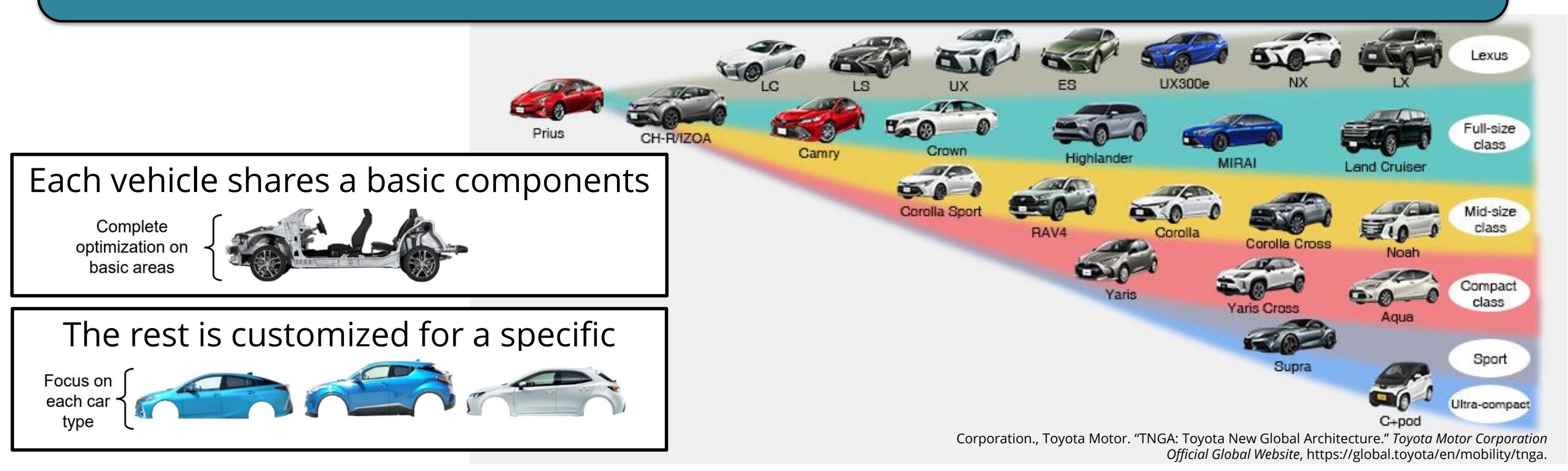




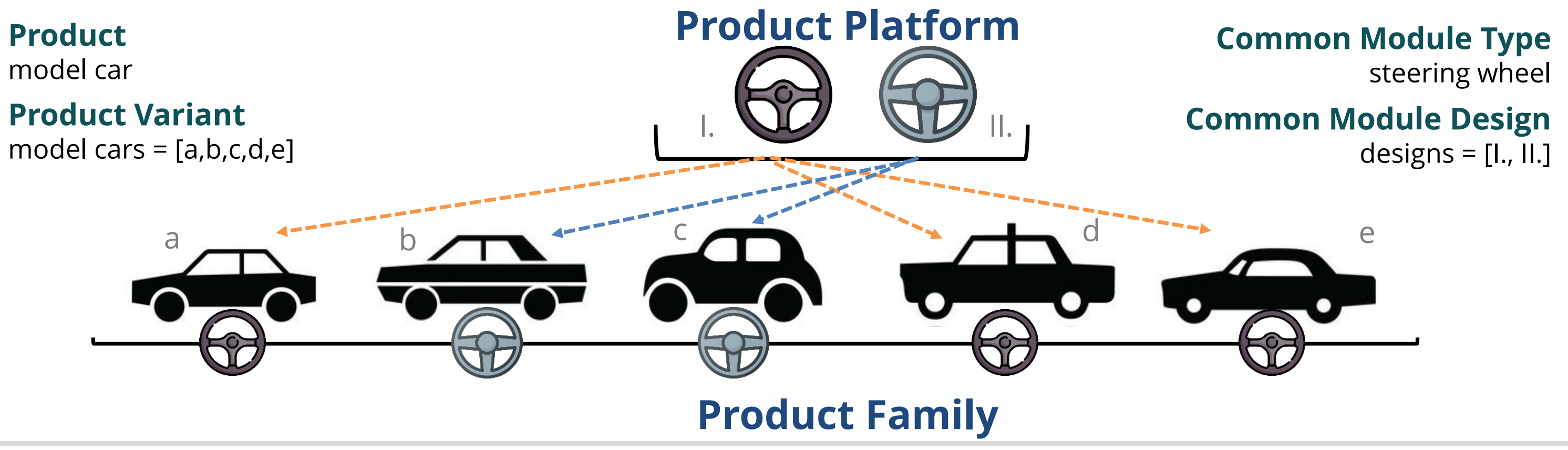
Process Family Design **includes** the **benefits of both**

Product Family Design[2]

A **set of products** that **share** one or more **common "element(s)"** yet target a variety of **different market segments**



Corporation., Toyota Motor. "TNGA: Toyota New Global Architecture." *Toyota Motor Corporation Official Global Website*, https://global.toyota/en/mobility/tnga.



Product
model car

Product Variant
model cars = [a,b,c,d,e]

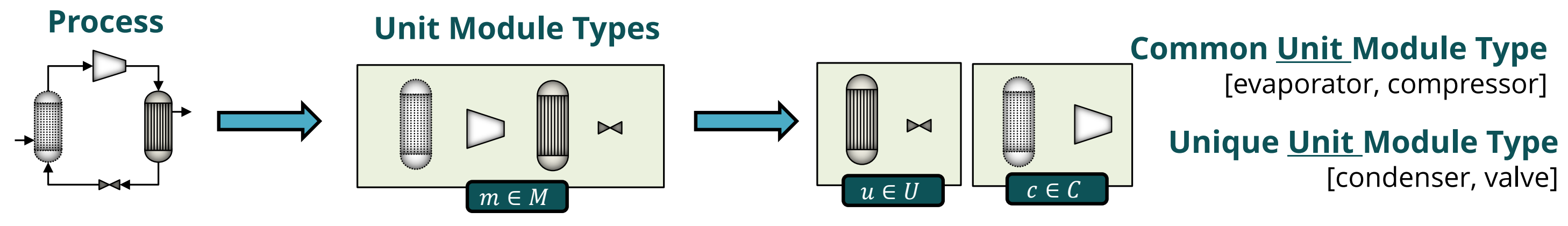
Product Platform

Common Module Type
steering wheel

Common Module Design
designs = [I., II.]

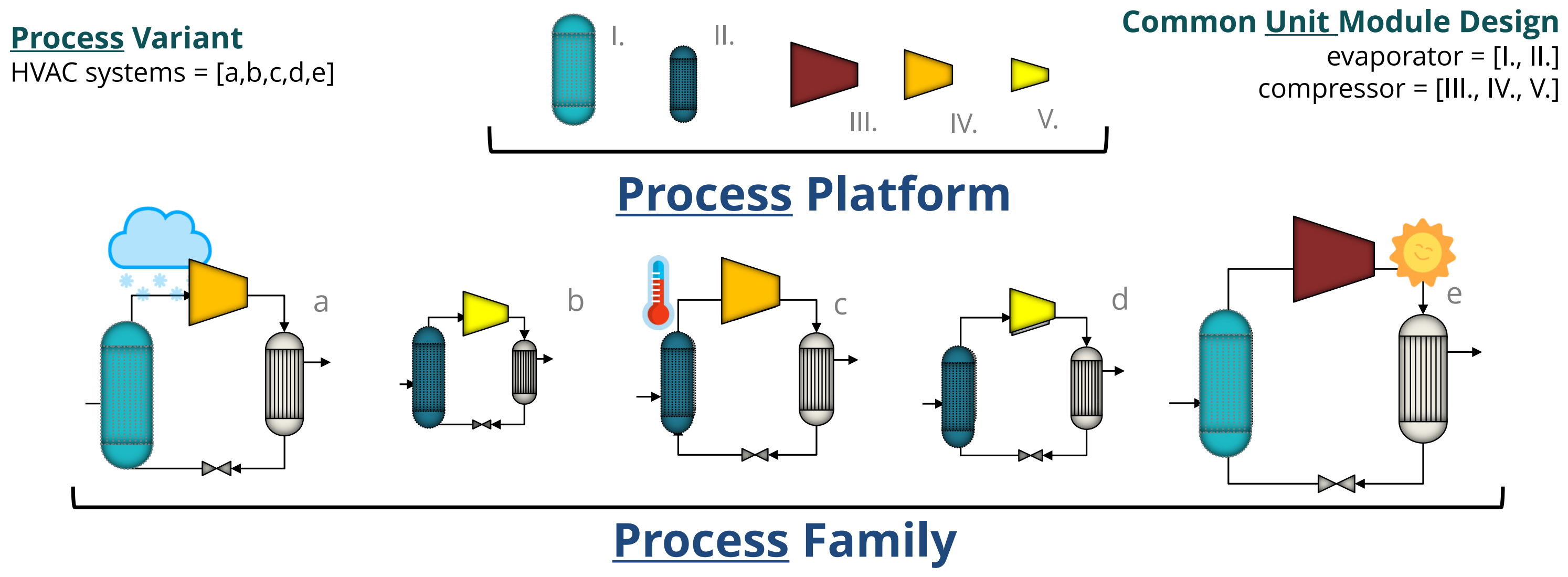
Product Family

Mapping to PSE



Common Unit Module Type
[evaporator, compressor]

Unique Unit Module Type
[condenser, valve]



Process Variant
HVAC systems = [a,b,c,d,e]

Common Unit Module Design
evaporator = [I., II.]
compressor = [III., IV., V.]

Process Platform

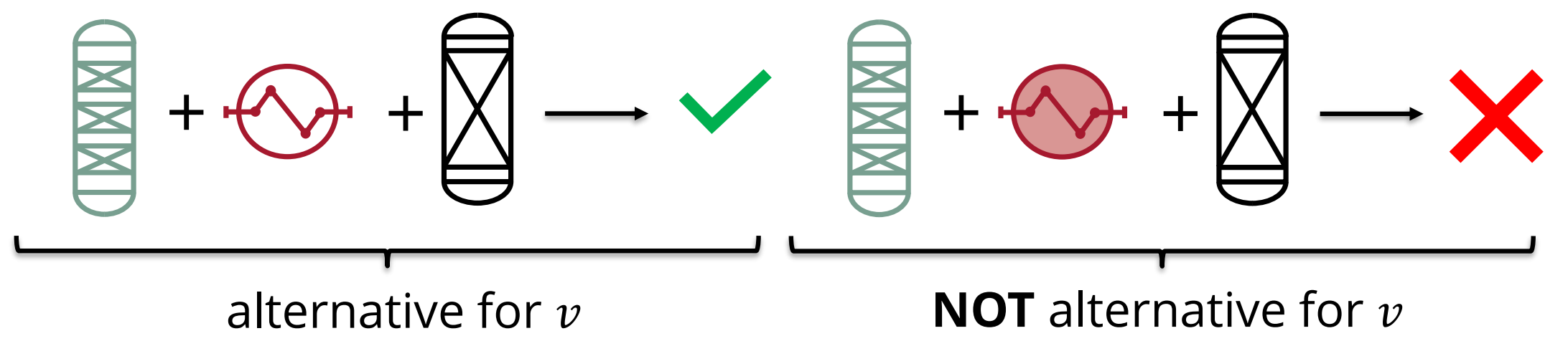
Process Family

(1) Discretization[3]

V: Set of **process variants** identified by unique **performance targets** & **feed conditions**

C: Set of **unit module types** considered for shared design for all variants in the **process family**

A_v: Set of **feasible** alternatives (i.e. combination of **designs** $d_{c,l}$) for a **variant** $v \in V$



$$\min. \sum_{v\in V} w_v \sum_{a\in A_v} p_{v,a} x_{v,a} \qquad (1.1)$$

Minimize the total weighted cost of **all variants** in the process family

$$\text{s.t.} \quad \sum_{l\in L_c} z_{c,l} \le N_c \qquad \forall\, c \in C \qquad (1.2)$$

→ Select units for manufacture

$$\sum_{a\in A_v} x_{v,a} = 1 \qquad \forall\, v \in V \qquad (1.3)$$

→ Select 1 alternative

$$x_{v,a} \le z_{c,l} \qquad \forall\, v \in V, a \in A_v, (c,l) \in Q_a \qquad (1.4)$$

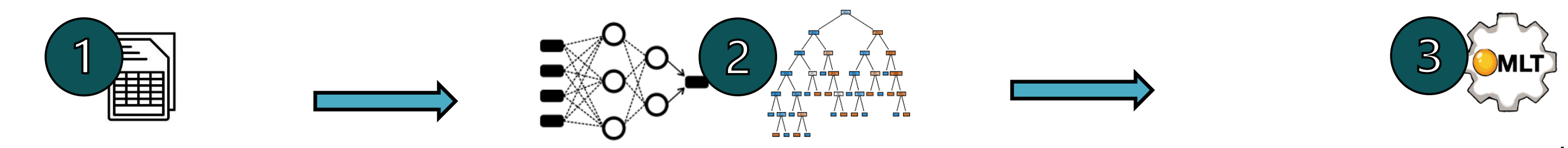
→ Alternative *must be* manufactured

$$z_{c,s} \in \{0,1\} \qquad \forall\, c \in C, l \in L_c \qquad (1.5)$$

$$0 \le x_{v,a} \le 1 \qquad \forall\, v \in V, a \in A_v \qquad (1.6)$$

At optimality, the **solution will converge to binary** under mild assumptions
ReVelle, Charles S., and Ralph W. Swain. "Central facilities location." *Geographical analysis* 2.1 (1970): 30-42.

(2) ML Surrogates[4]



Reduced data set → Train PWL performance & cost surrogate → Import MIP-represented PWL surrogate into formulation

$$\min. \sum_{v\in V} w_v p_v \qquad (2.1)$$

→ Objective

$$\text{s.t.} \quad p_v = g_v^p(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}) \qquad \forall\, v \in V \qquad (2.2)$$

→ Cost surrogate

$$i_v = g_v^i(\mathbf{r}_v, \mathbf{d}_{v,1}, \dots, \mathbf{d}_{v,m}) \qquad \forall\, v \in V \qquad (2.3)$$

→ Performance surrogate

$$\bigvee_{l \in L_c} \begin{bmatrix} Y_{v,c,l} \\ \mathbf{d}_{v,c} = \hat{\mathbf{d}}_{c,l} \end{bmatrix} \qquad \forall\, v \in V, c \in C \qquad (2.4)$$

→ Assignment of unit designs

$$\hat{\mathbf{d}}_c^{\mathrm{LB}} \le \hat{\mathbf{d}}_{c,l} \le \hat{\mathbf{d}}_c^{\mathrm{UB}} \qquad \forall\, c \in C, l \in L_c \qquad (2.5)$$

→ Design boundaries

$$\mathbf{i}_v^{\mathrm{LB}} \le \mathbf{i}_v \le \mathbf{i}_v^{\mathrm{UB}} \qquad \forall\, v \in V \qquad (2.6)$$

→ Performance boundaries

$$\hat{\mathbf{d}}_{c,l-1} \le \hat{\mathbf{d}}_{c,l} \qquad \forall\, c \in C, l \in L_c : l > 1 \qquad (2.7)$$

→ Ordering constraints

$$Y_{v,c,l} \in \{\text{True}, \text{False}\} \qquad \forall\, v \in V, c \in C, l \in L_c \qquad (2.8)$$

Advances

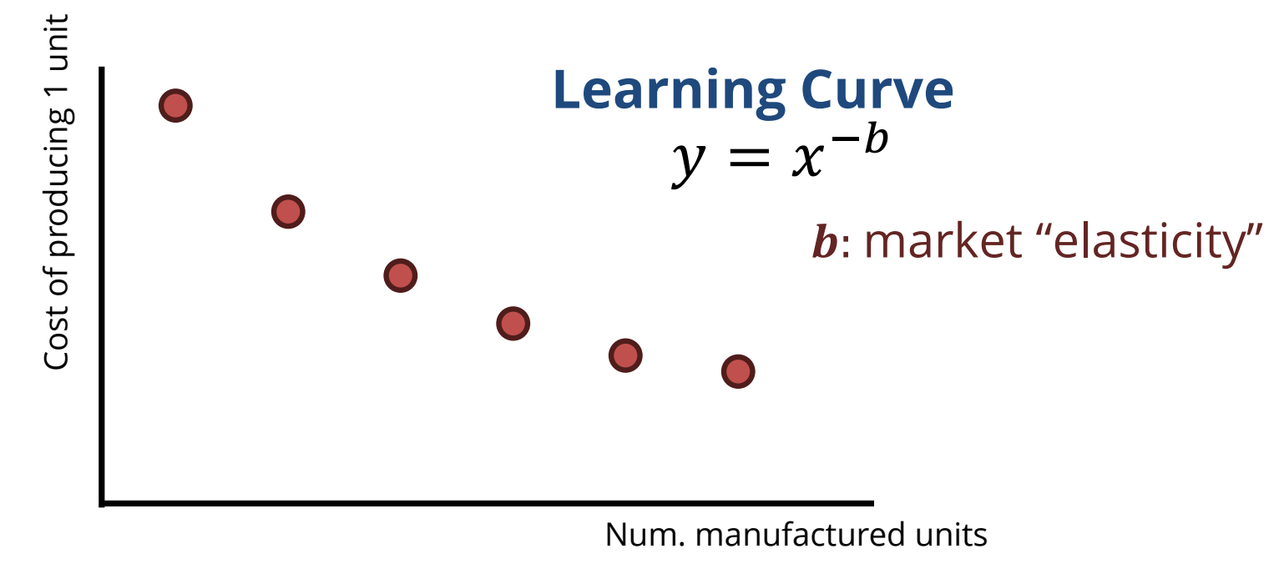
(3) Discretized + Economies of Numbers[5,6]

Challenge

(1.2) requires us to **specify size** of the **platform a priori**.

Approach

Include EoN savings *within* formulation.



Adapted Gazzaneo et al.'s (2022) piece-wise learning curve to include a "smooth" asymptotic behavior.

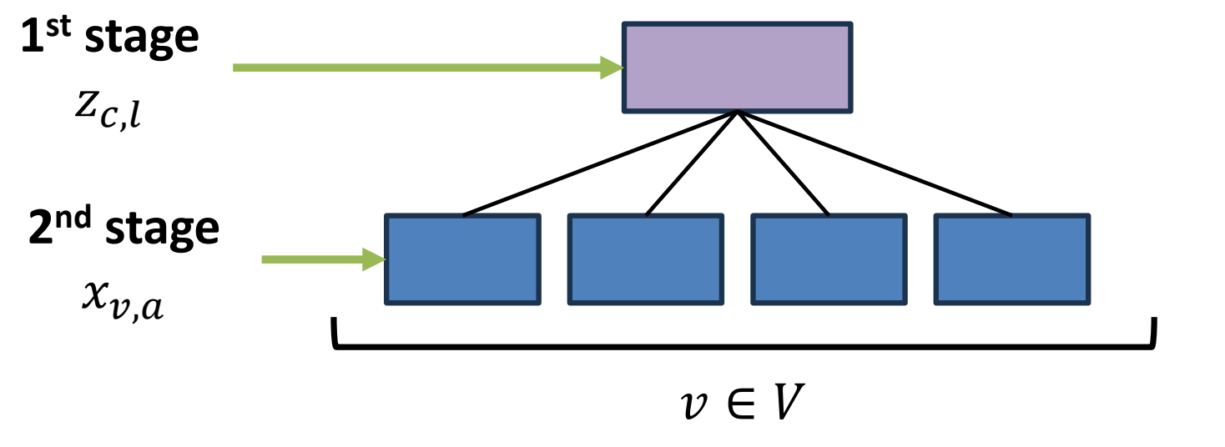
(4) Discretized + Decomposition[7]

Challenge

More variants & **candidate designs** lead to **large-scale problems**.

Approach

Decompose by *variant;* exploit similar structure exhibited by stochastic programs



Used `mpi-sppy` [7] to solve using Progressive Hedging in parallel

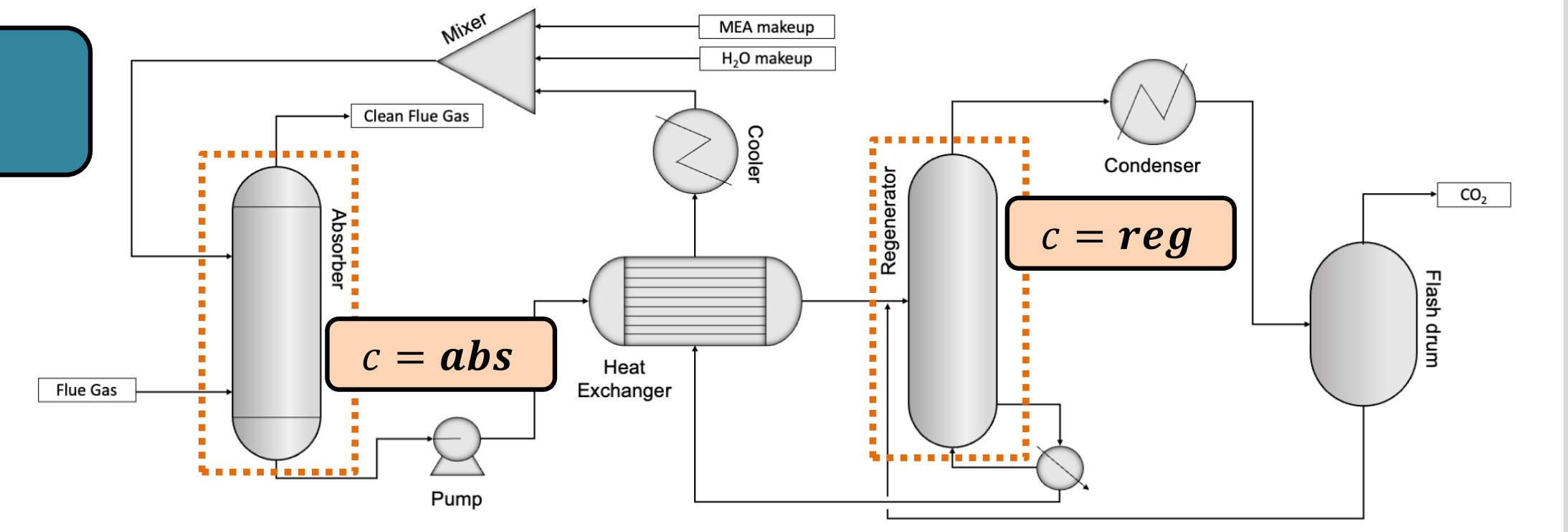
Case Study[8]

Carbon Capture
Monoethanolamine (MEA)

Common Units

1) Diam. of the Absorber
2) Diam. of the Regenerator

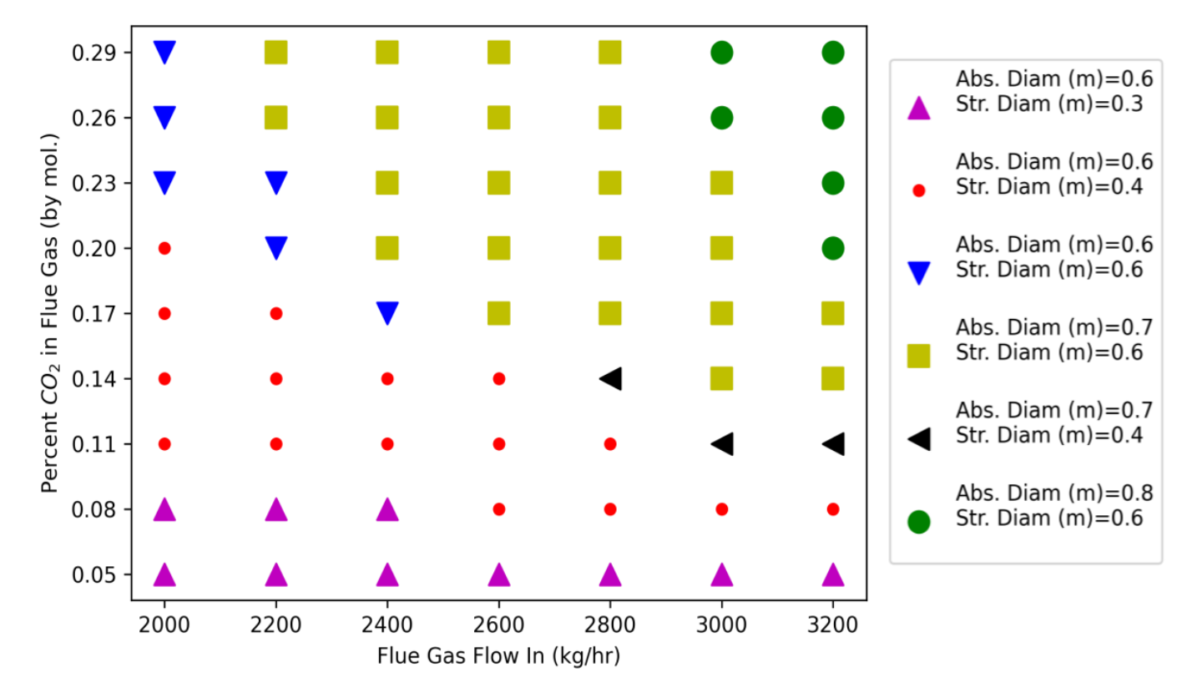
$C = [\boldsymbol{abs}, \boldsymbol{reg}]$



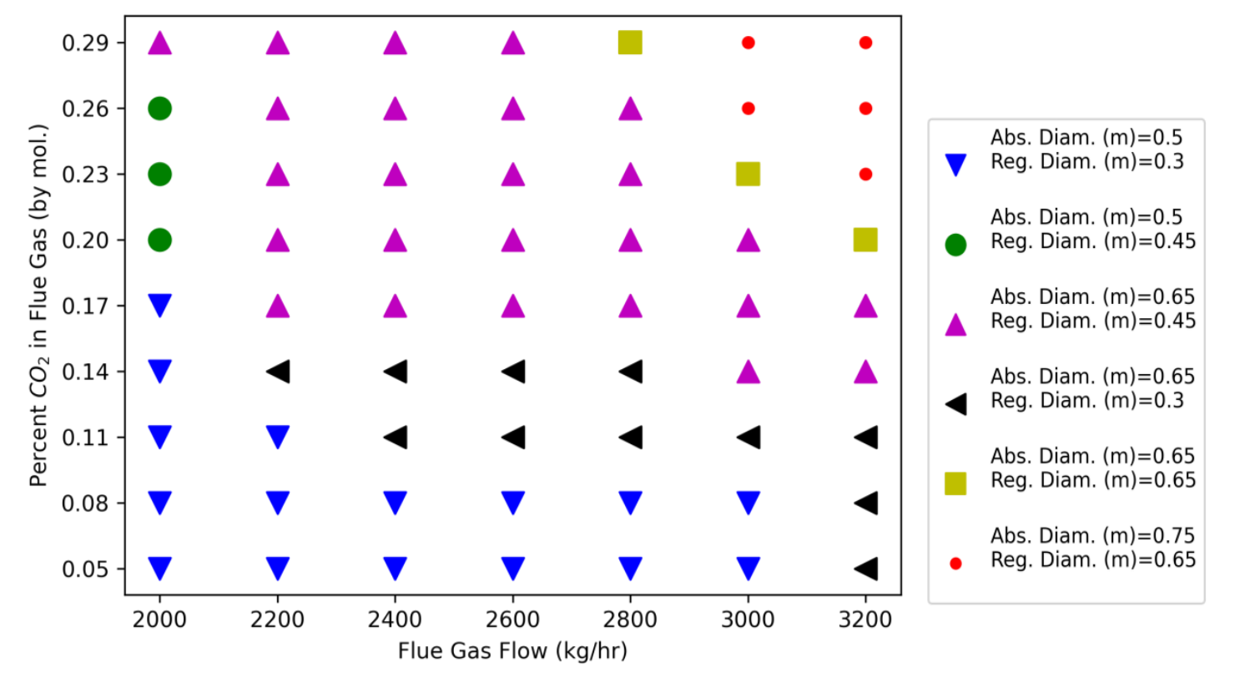
Results

(1) Discretization[4]

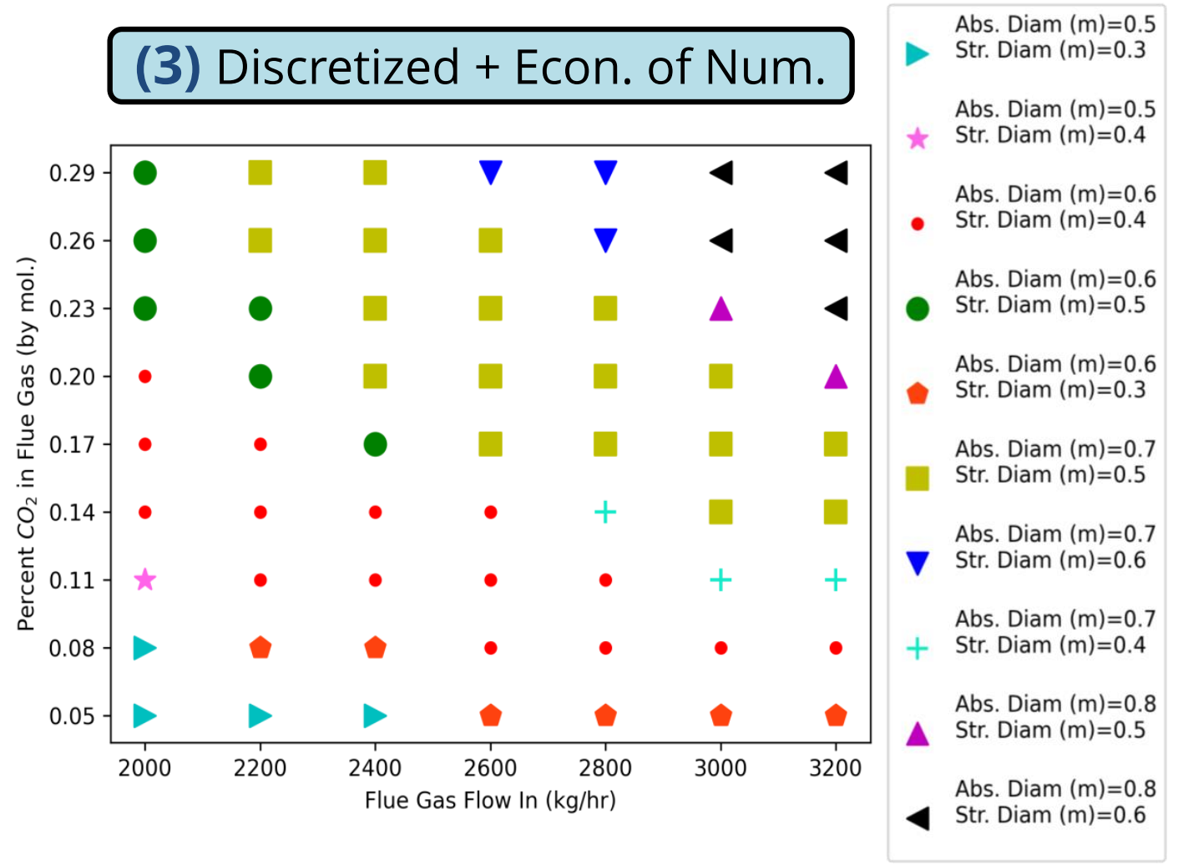
(4) Discretized + Decomposition



(2) ML Surrogates[5]



(3) Discretized + Econ. of Num.



Formulation Comments

	(1)	(2)
Sim.	~ 252 *hr.*	~ 200 *hr.*
Train	-	~ 10 *min.*
Gurobi	< 1 s	~ 100 s
Total	~ 252 *hr.*	**~ 200 *hr.***

***(1)** has major bottlenecks with simulation time*
⇩
(2) reduces data requirement via embedded surrogates

	(1)	(3)
Obj.	\$75.35 *M*	**\$73.96 *M***

***(1)** must specify N_c*
⇩
(3) determines N_c & has lower overall cost

Conclusions

- ✓ Reduced manufacturing costs
  - ○ Economies of numbers (modular concepts at unit level)
  - ○ Economies of scale (customization to design range)
- ✓ Multiple scalable optimization formulations
- ✓ **(2)** reduces data requirement[5]
- ✓ **(3)** adds cost savings & determines size of platform.
- ✓ **(4)** demonstrates decomposability of larger problems.

Future Work

- ❑ Perform a rigorous costing analysis for each design approach.
- ❑ Incorporate Econ. Of Num. and decomposition for ML Surrogates.

References

[1] Baldea, M., Edgar, T. F., Stanley, B. L. & Kiss, A. A. (2017), 'Modular manufacturing processes: Status, challenges, and opportunities', AIChE journal 63(10), 4262–4272.
[2] Simpson, Timothy & Siddique, Zahed & Jiao, Roger. (2006). Product Platform and Product Family Design: Methods and Applications. 10.1007/978-1-4614-7937-6.
[3] Zhang, C., et al. (2021). Optimization-based Design of Product Families with Common Components. 14th International Symposium on Process Systems Engineering.
[4] Stinchfield, G., et al., "Optimization-based Approaches for Design of Chemical Process Families Using Machine Learning Surrogates" In proceedings, FOCAPO\CPC 2023.
[5] Gazzaneo, V., Watson, M., Ramsayer, C. B., Kilwein, Z. A., Alves, V., Lima, F. V., *J. Adv. Manuf. Process.* 2022, e10115. https://doi.org/10.1002/amp2.10115
[6] Weber, Robert S., and Lesley J. Snowden-Swan. "The economics of numbering up a chemical process enterprise." *Journal of Adv. Manuf. & Processing* 1.1-2 (2019): e10011.
[7] Knueven, Bernard, et al. "A parallel hub-and-spoke system for large-scale scenario-based optimization under uncertainty." *Mathematical Programming Computation* (2023): 1-29.
[8] Carbon capture simulation for industry impact (CCSI2), v3.2.1. MEA Steady state model. https://github.com/CCSI-toolset/MEA/ssm/realeases/tag/23.2.1 (2022).

Contact: Georgia Stinchfield, gstinchf@andrew.cmu.edu