Optimal Design Approaches for Rapid, Cost-Effective Manufacturing and Deployment of Chemical Processes

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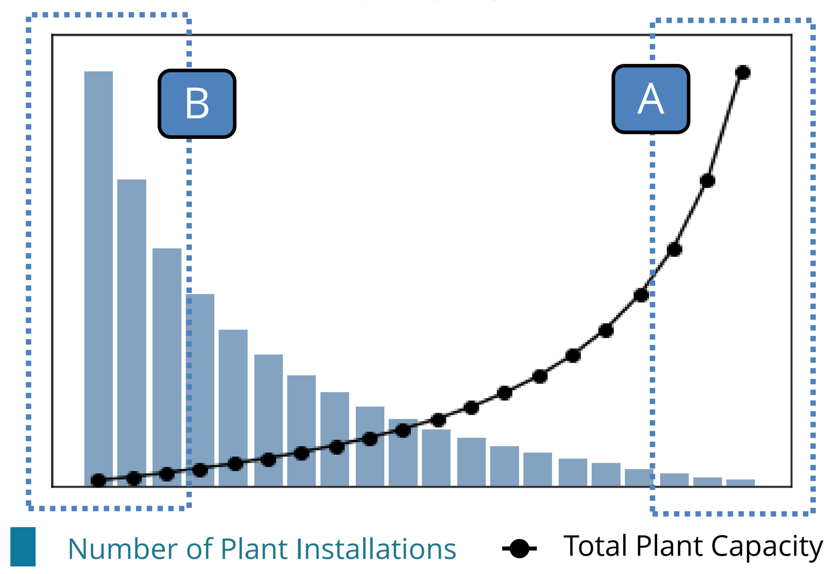
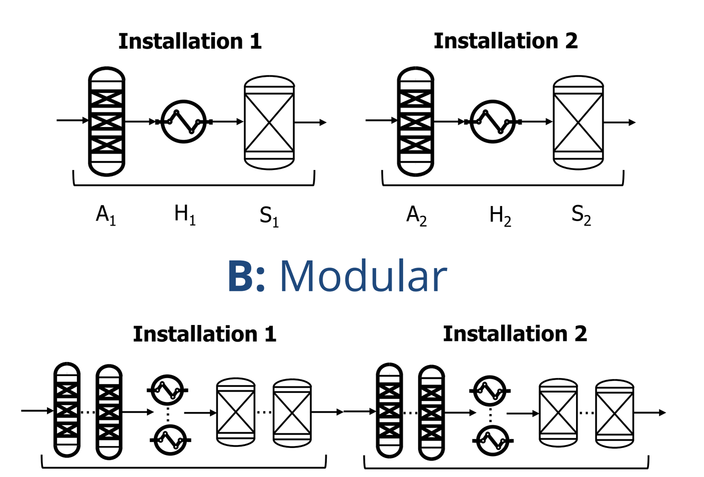
Motivation[1]

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

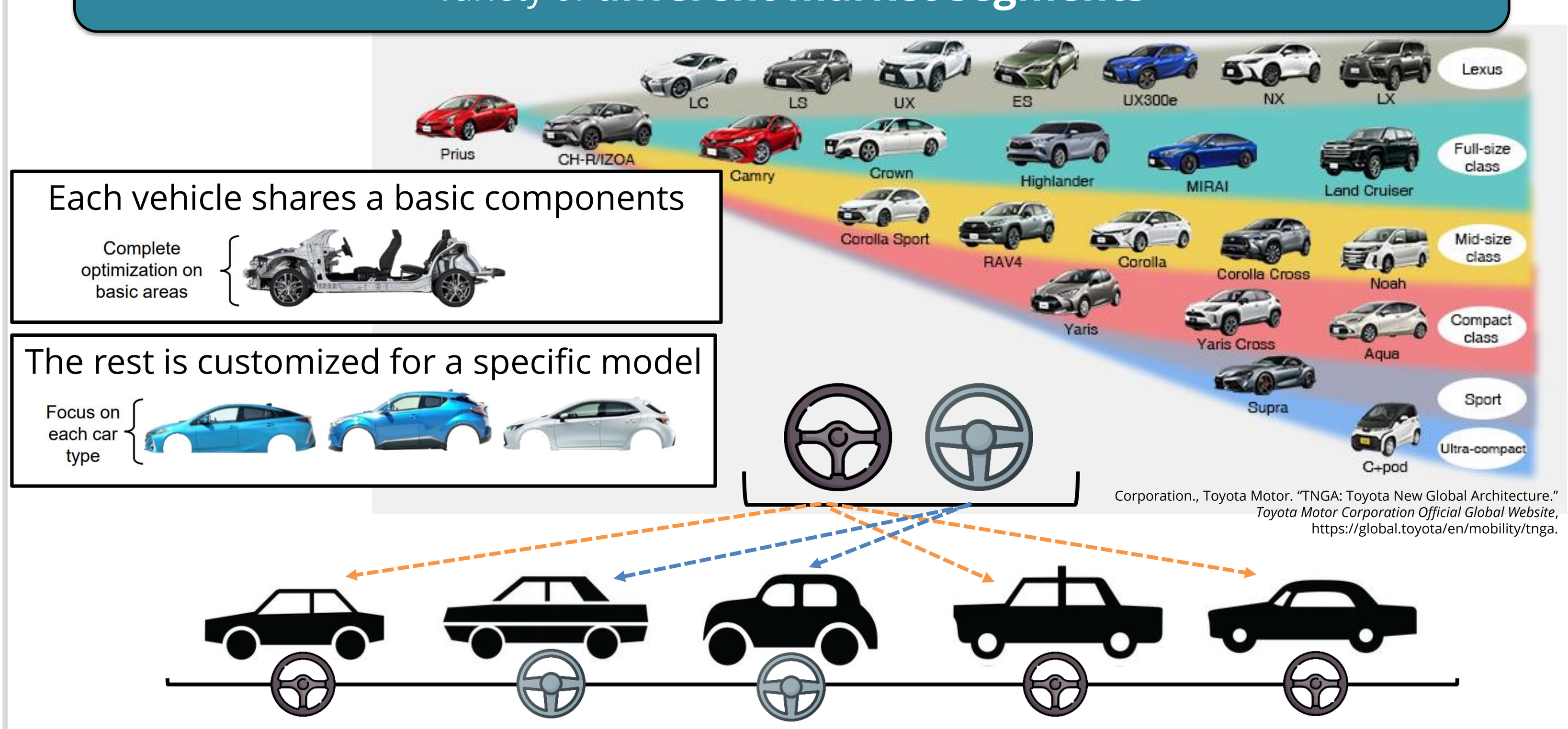




Process Family Design **includes** the **benefits of both**

Background: Product Family Design[2,3]

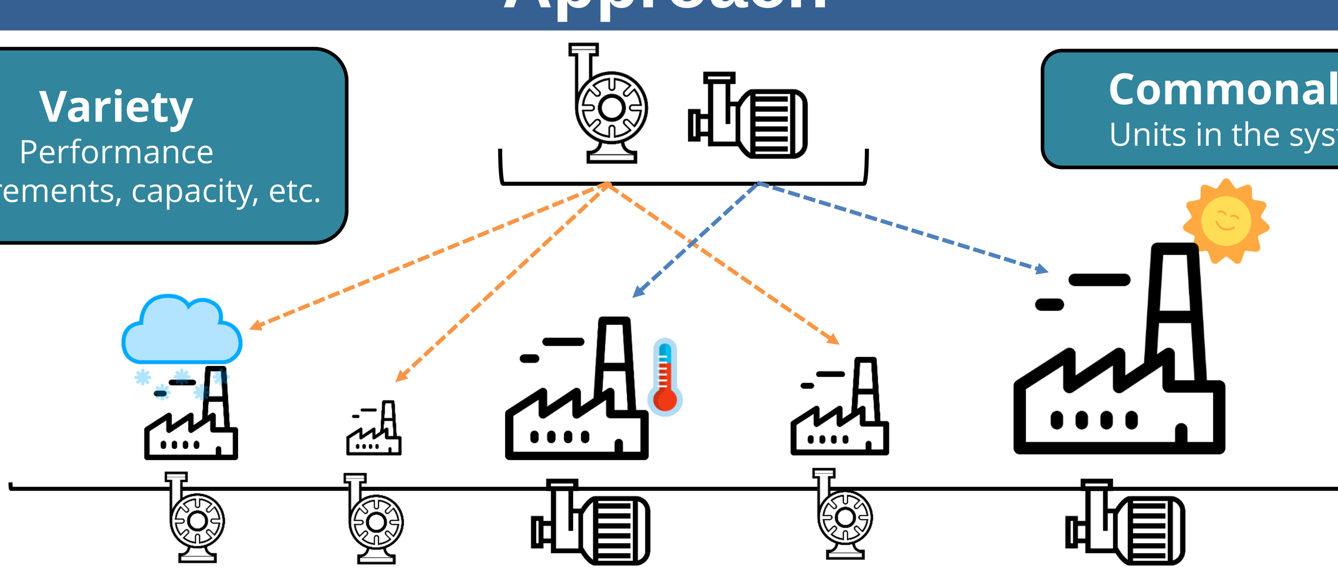
A **set of products** that **share** one or more **common "element(s)"** yet target a variety of **different market segments**



Approach

Variety
Performance requirements, capacity, etc.

Commonality
Units in the system



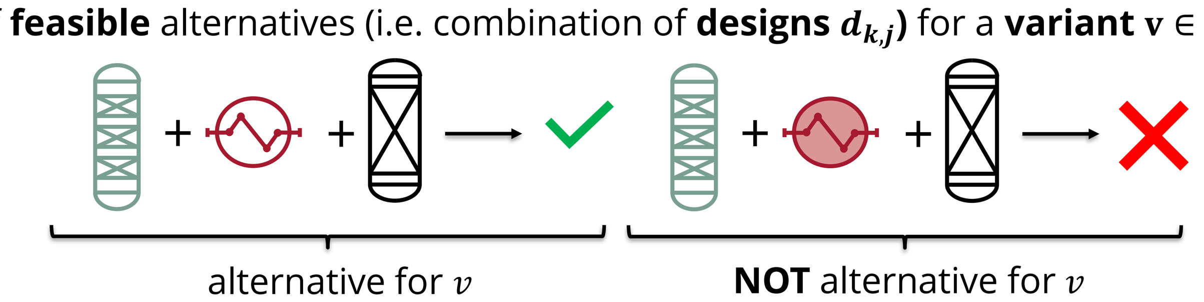
- ✓ Identify factors affecting system design
- ✓ Identify unit types to share
- ✓ Optimally **design each unit & allocation** to installations **simultaneously**

Formulation 1: Discretization Approach[4]

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

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

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



$$\min. \sum_{v \in V} w_v \sum_{a \in A_v} c_{v,a} x_{v,a}$$

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

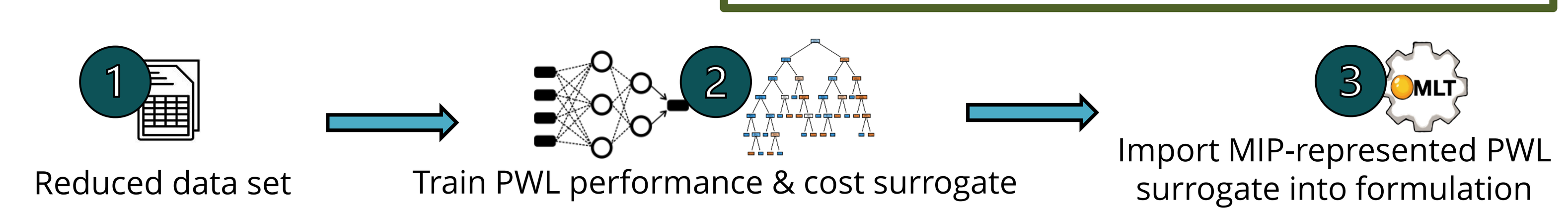
s.t.

$\sum_{j \in J_k} z_{k,j} \le N_k$	$\forall k \in K$	Select units for manufacture
$\sum_{a \in A_v} x_{v,a} = 1$	$\forall v \in V$	Select 1 alternative
$x_{v,a} \le z_{k,j}$	$\forall v \in V, a \in A_v, (k,j) \in Q_a$	Alternative *must be* manufactured
$z_{k,j} \in \{0,1\}$	$\forall k \in K, j \in S_j$	
$0 \le x_{v,a} \le 1$	$\forall v \in V, a \in A_v$	

At optimality, the **solution will converge to binary** under mild assumptions

Formulation 2: Piecewise Linear Surrogates[5]

Formulation 1	Formulation 2
☒ Computational expensive simulations.	☑ Order of magnitude less data required.
☒ Discrete sets limit optimal design decisions.	☑ Approx. continuous design space.



$$\min. \sum_{i \in I} w_i c_i$$

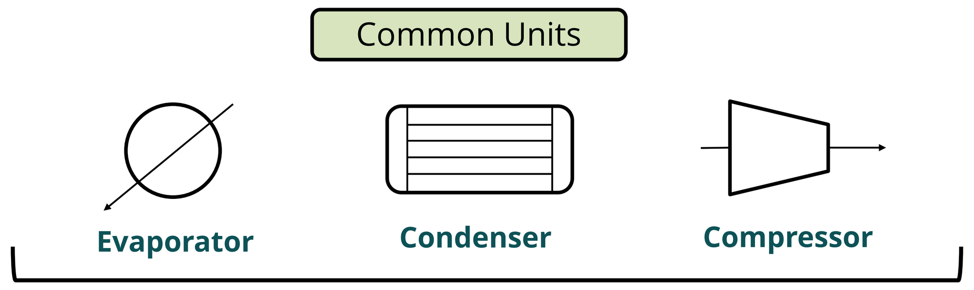
s.t.

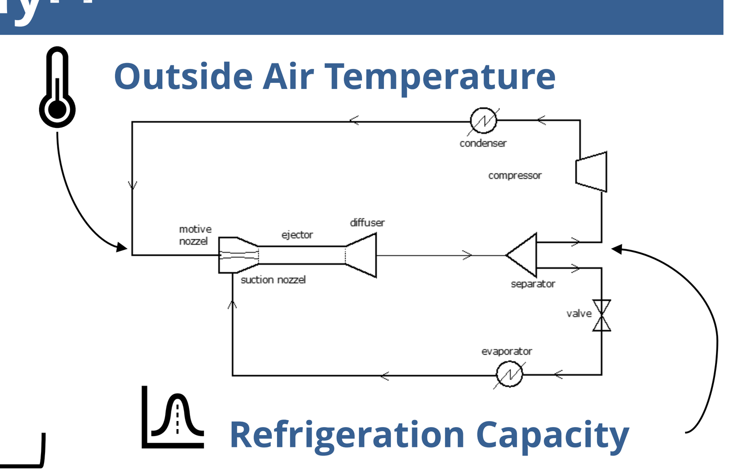
$c_i = g^c(b_i, d_{i,1}, \dots, d_{i,k})$	$\forall i \in I$	Cost surrogate
$p_i = g^p(b_i, d_{i,1}, \dots, d_{i,k})$	$\forall i \in I$	Performance surrogate
$\bigvee_{j \in J_k} \begin{bmatrix} Y_{i,k,j} \\ d_{i,k} = \hat{d}_{k,j} \end{bmatrix}$	$\forall i \in I, k \in K$	Assignment of unit designs to variant
$\hat{d}^{LB}_{k,j} \le \hat{d}_{k,j} \le \hat{d}^{UB}_{k,j}$	$\forall k \in K, j \in J_k$	Design boundaries
$p^{LB}_i \le p_i \le p^{UB}_i$	$\forall i \in I$	Performance boundaries
$\hat{d}_{k,j-1} \le \hat{d}_{k,j}$	$\forall k \in K, j \in J_k : j > 1$	
$Y_{i,k,j} \in \{\text{True}, \text{False}\}$	$\forall i \in I, k \in K, j \in J_k$	

Case Study[6]

Refrigeration System
Transcritical CO_2

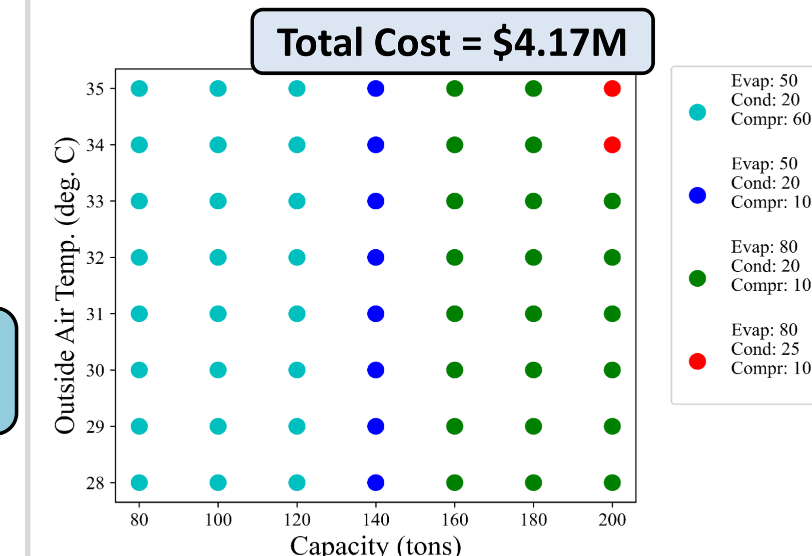
Common Units

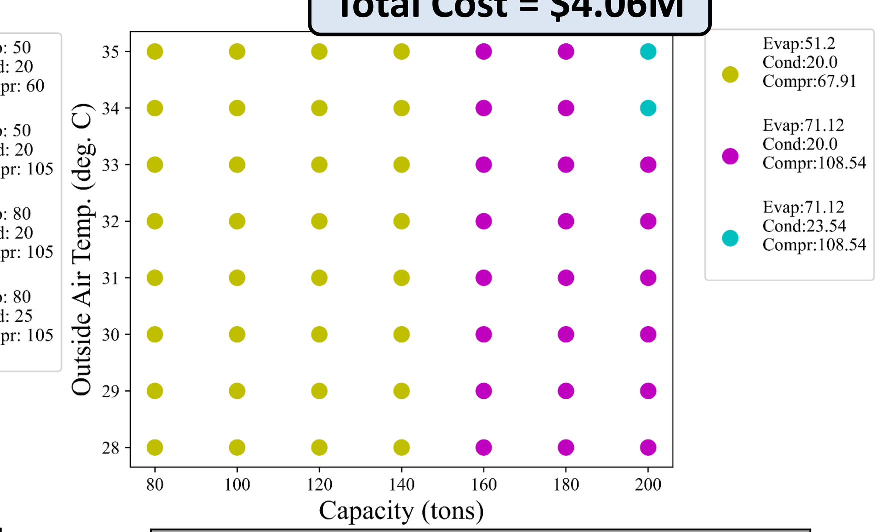




Results[5]

	Formulation 1		Formulation 2	
Evaporator Designs	$50\ m^2$	$80\ m^2$	$51.2\ m^2$	$71.12\ m^2$
Condenser Designs	$20\ m^2$	$25\ m^2$	$20.0\ m^2$	$23.54\ m^2$
Compressor Designs	$60\ \frac{mol}{s}$	$105\ \frac{mol}{s}$	$67.91\ \frac{mol}{s}$	$108.54\ \frac{mol}{s}$
	Total Cost = $4.17M		**Total Cost = $4.06M**	





Formulation 1	
Simulation Time	~67,200s
Gurobi© Solve Time	14.66s
Total Time	**~18.7hrs**

Formulation 2	
Simulation Time	~6,700s
Gurobi© Solve Time	71.70s
Total Time	**~2hrs**

Conclusions

- ✓ Reduced manufacturing costs
  - Economies of numbers (modular concepts at unit level)
  - Economies of scale (customization to design range)
- ✓ Reduced engineering design costs
- ✓ Multiple scalable optimization formulations[4,5]
- ✓ **Order of magnitude reduction** in data requirements[5]
- ✓ Economies of numbers yields **approx. 8% savings** of projected **total annualized cost**[7,8]

Future Work

- ❑ Incorporate economies of numbers savings into formulation
- ❑ Expand to more large-scale industrial case studies (decomposition)

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] Corporation., Toyota Motor. "TNGA: Toyota New Global Architecture." *Toyota Motor Corporation Official Global Website*, https://global.toyota/en/mobility/tnga.
[4] Zhang, C., et al. (2021). Optimization-based Design of Product Families with Common Components. 14th International Symposium on Process Systems Engineering.
[5] Stinchfield, G., et al., "Optimization-based Approaches for Design of Chemical Process Families Using Machine Learning Surrogates" In proceedings, FOCAPO\CPC 2023.
[6] Li, D. & Groll, E. A. (2005), 'Transcritical co2 refrigeration cycle with ejector-expansion device', International Journal of refrigeration 28(5), 766–773.
[7] 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
[8] 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.

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