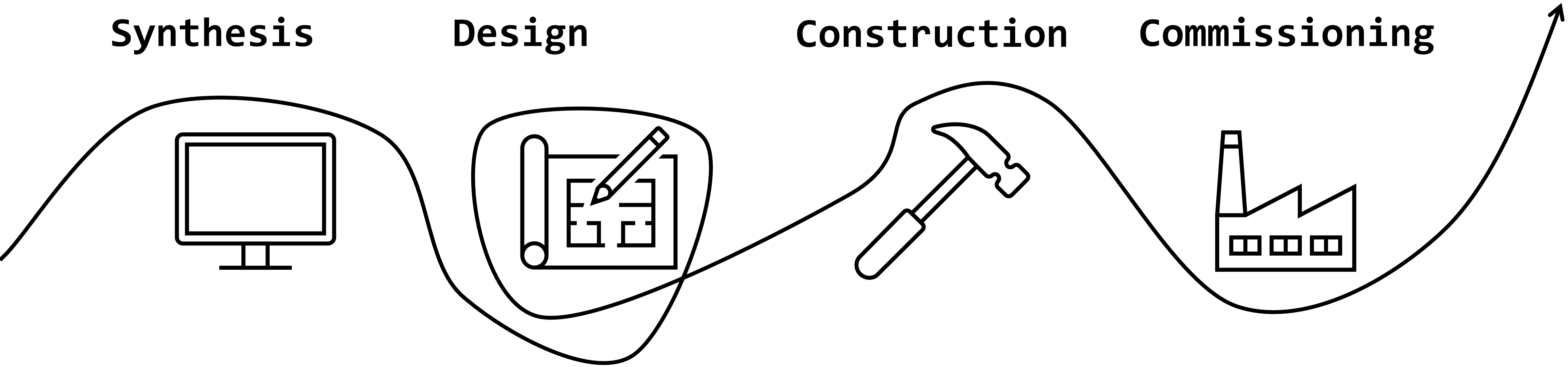
Process Dynamics and Operations Group

CAPE-OPEN and the Future of Superstructure Optimization

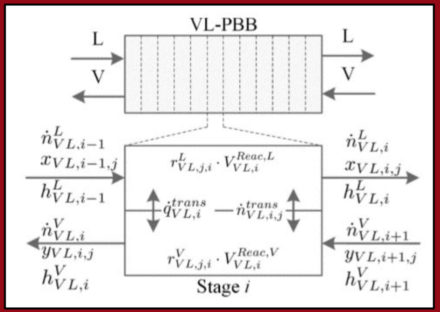
CAPE-OPEN 2024 Annual Meeting | 08.10.2024

Lukas Scheffold, Erik Esche, Jens-Uwe Repke

Motivation and Background



Motivation and Background



GENERALITY

PBB formulation in MOSAICmodeling

FIDELITY

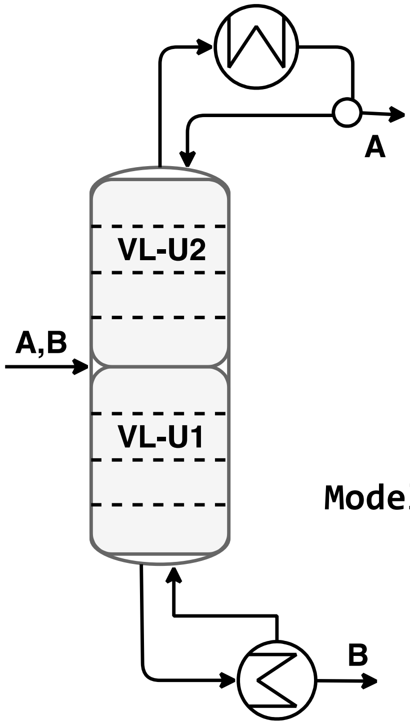
Rigorous thermodynamic and kinetic models

TRACTABILITY

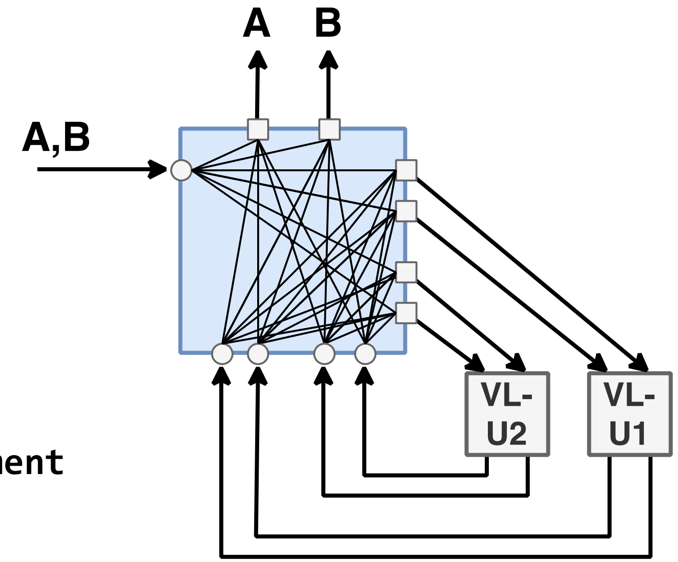
Structural screening

Previous Work

[1]



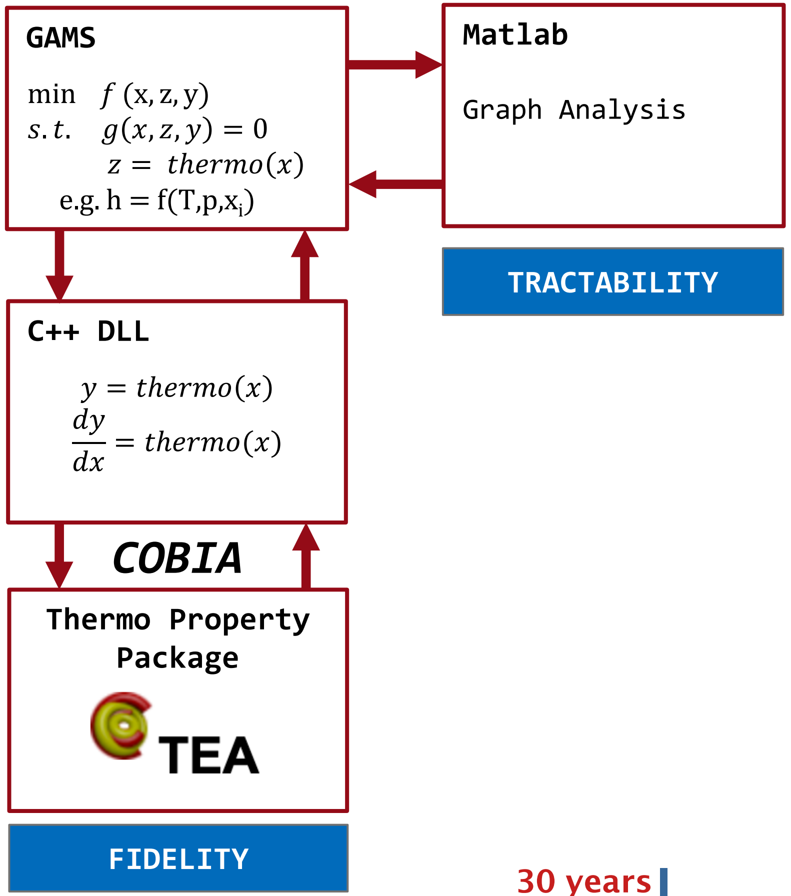
Model development



MOSAICmodeling

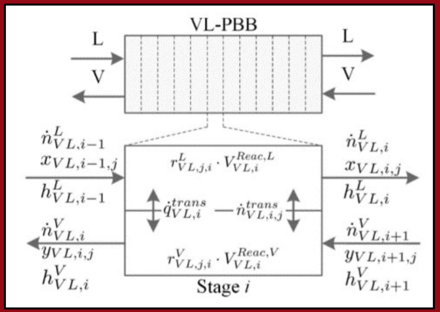
GENERALITY

Code export



[1] D. Krone, E. Esche, N. Asprion, M. Skiborowski und J.-U. Repke, „Enabling optimization of complex distillation configurations in GAMS with CAPE-OPEN thermodynamic models," *Computers & Chemical Engineering*, Bd. 157, p. 107626, 2022.

Challenges



Strong Nonlinearities

Dedicated Initialization Procedures

Solution Time

Improvements ?

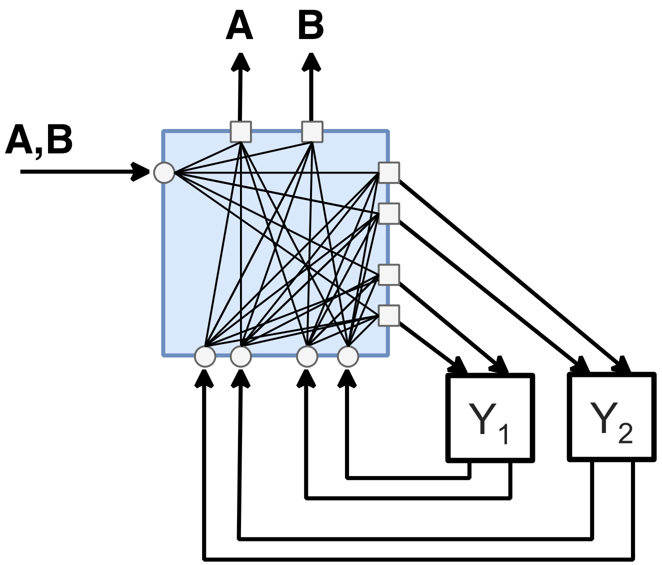
Tractability

Improvements ?

GDP Problem Formulation

[2]

$\min z =$	$f(x)$		Objective Function
$s.t.$	$r(x) \leq 0$		Global Constraints
	$\bigvee_{j \in J_i} \begin{bmatrix} Y_{ij} \\ g_{ij}(x) \leq 0 \end{bmatrix}$	$\forall i \in I$	Disjunctions
	$\Xi(1, Y_{ij}\ \forall j \in J_i)$	$\forall i \in I$	
	$\Omega(Y)$		Logic Propositions
	$x^{LB} \leq x \leq x^{UB}$		Variable Bounds
	$x \in \mathbb{R}^n$		
	$Y_{ij} \in \{True, False\}$	$\forall i \in I, j \in J_i$	

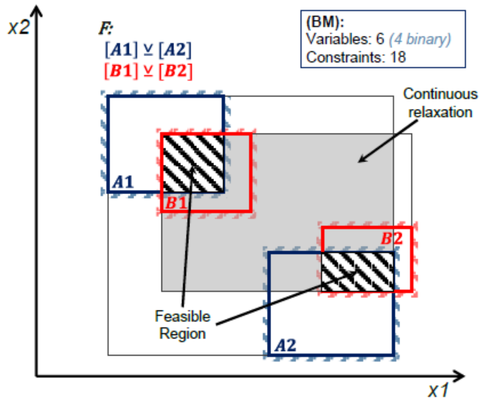


[2] Grossmann, I. E., F. Trespalacios. 2013. Systematic modeling of discrete-continuous optimization models through generalized disjunctive programming. AIChE Journal 59 3276{3295. doi:10.1002/aic.14088. URL http://dx.doi.org/10.1002/aic.14088.

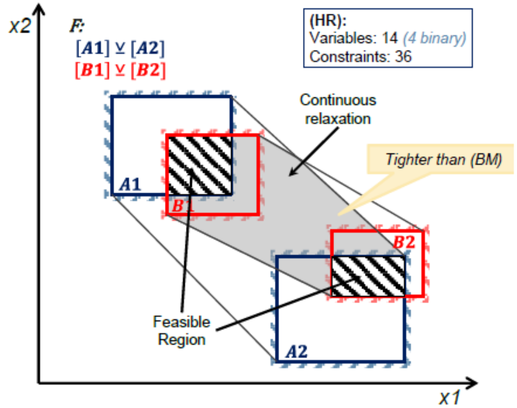
GDP Solution

[2]

Traditionally, Big M relaxation is apply **by hand** in MINLP formulation



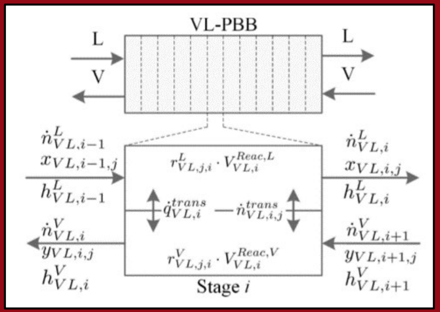
Relaxations that provide **tighter bounds exist** (i.e. Convex Hull relaxation).



By retaining the logical structure of the optimiza-tion problem, **GDP** algorithms can **automatically** generate/ **use tighter relaxations.**

[2] Grossmann, I. E., F. Trespalacios. 2013. Systematic modeling of discrete-continuous optimization models through generalized disjunctive programming. AIChE Journal 59 3276{3295. doi:10.1002/aic.14088. URL http://dx.doi.org/10.1002/aic.14088.

Possible GDP Improvements



Strong Nonlinearities

Dedicated Initialization Procedures

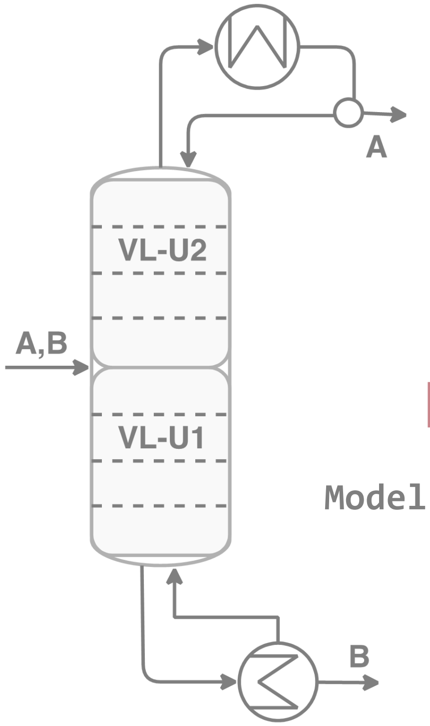
Solution Time

Stronger GDP Relaxations

Tractability

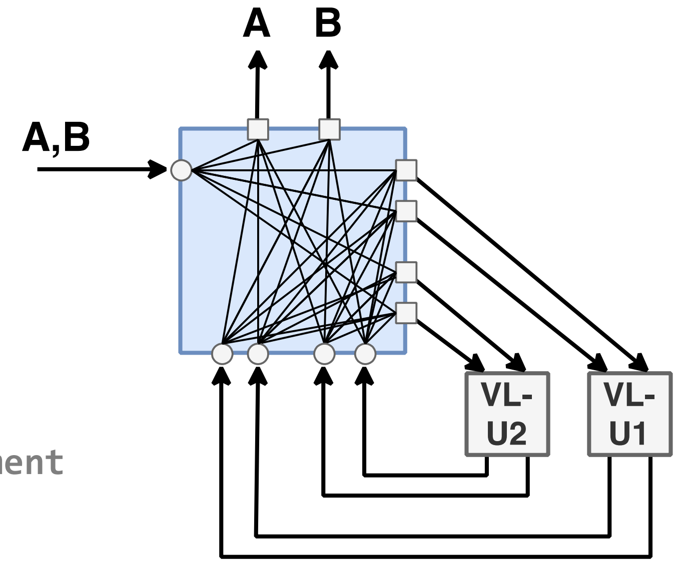
Additional GDP formulation

GDP Formulation in MOSAICmodeling



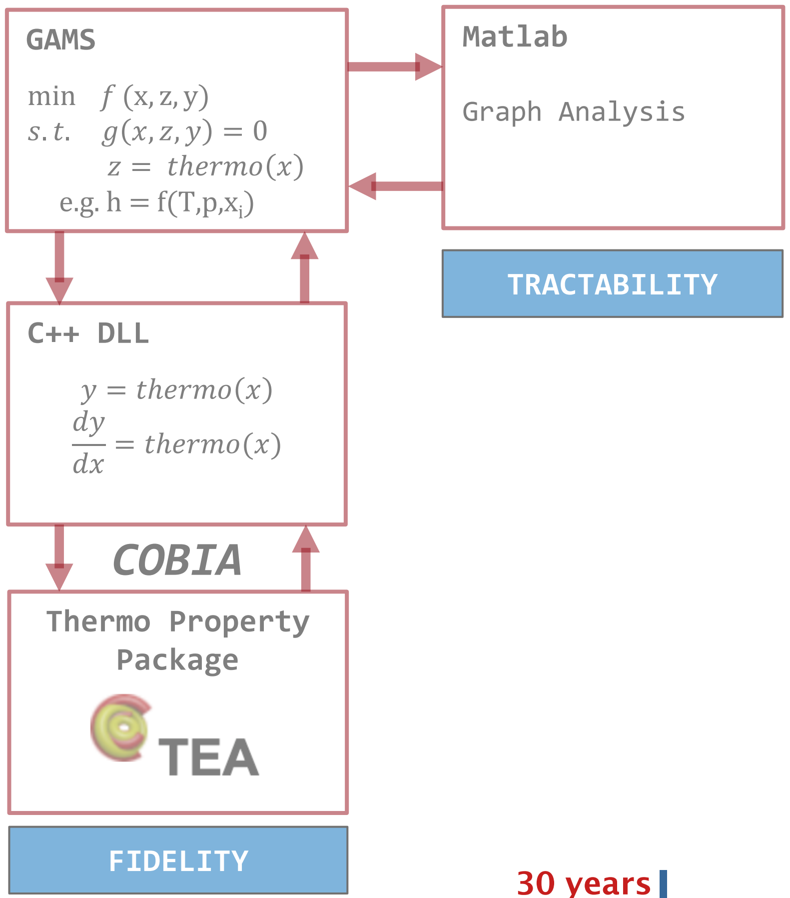
GENERALITY

Model development



MOSAICmodeling

Code export



GDP Formulation in MOSAICmodeling

Minimize $c + 2x_1 + x_2$ — Objective Function

subject to

$$\begin{bmatrix} Y_1 \\ -x_1 + x_2 + 2 \leq 0 \\ c < 5 \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ 2 - x_2 \leq 0 \\ c < 7 \end{bmatrix}$$

$$\begin{bmatrix} Y_3 \\ x_1 - x_2 \leq 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_3 \\ x_1 \leq 1 \end{bmatrix}$$

Disjunctions [Equations]

$$Y_1 \wedge \neg Y_2 \Rightarrow \neg Y_3$$
$$Y_2 \Rightarrow \neg Y_3$$
$$Y_3 \Rightarrow \neg Y_2$$

Logic Propositions

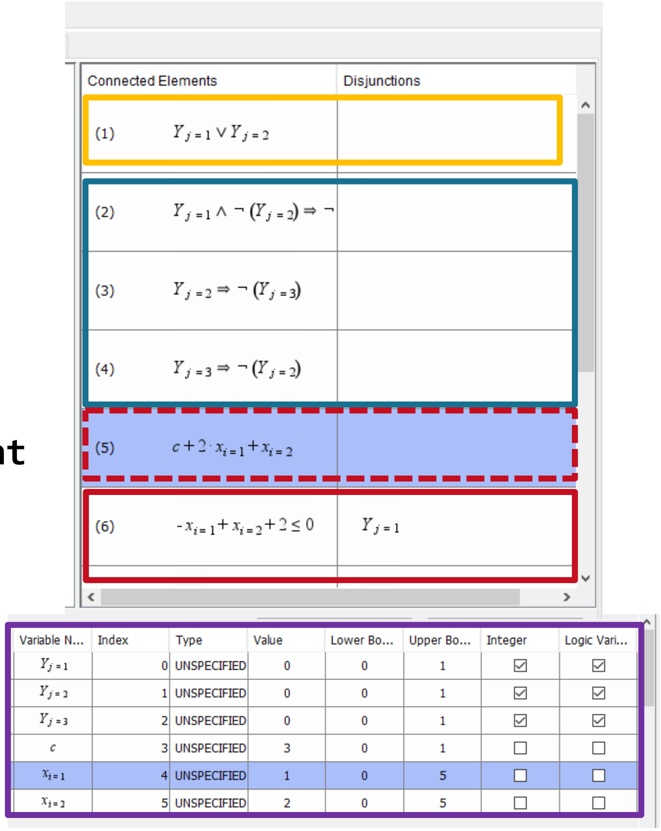
$$0 \leq x_1 \leq 5$$
$$0 \leq x_2 \leq 5$$
$$c \geq 0$$

Continuous Variables

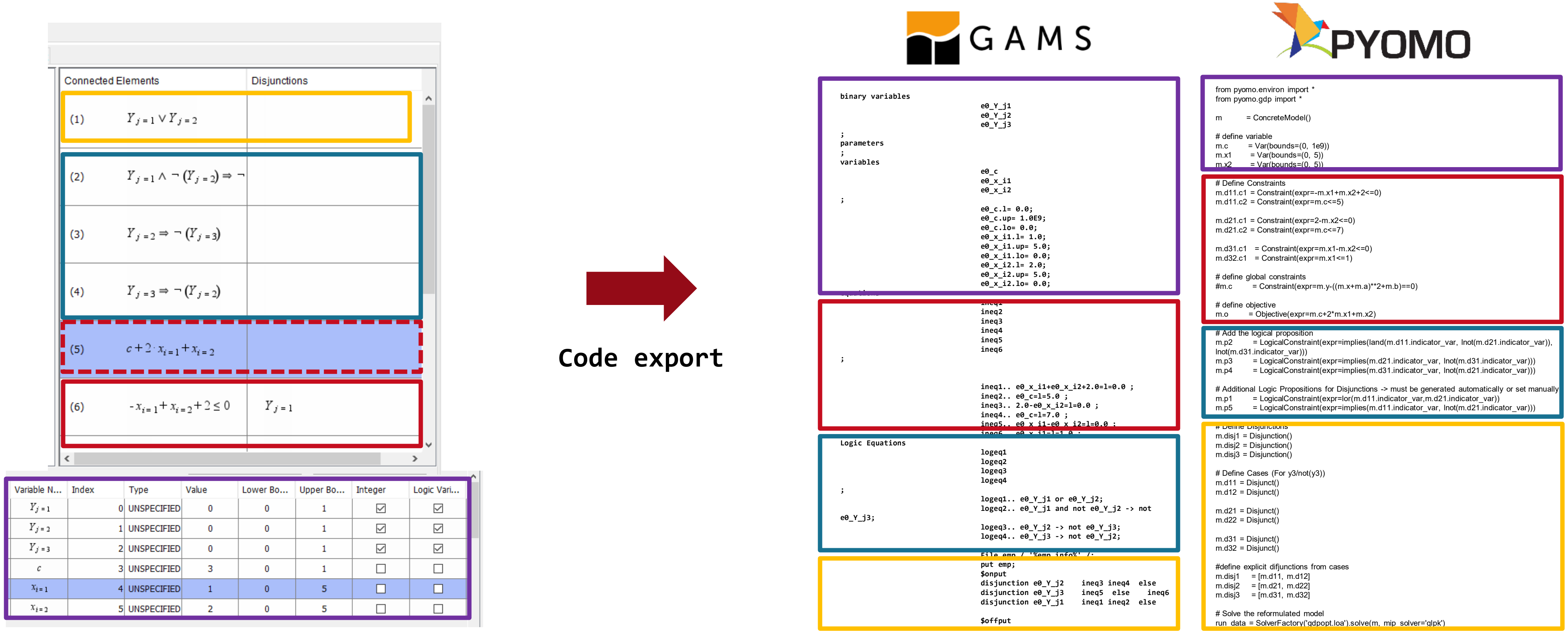
$$Y_j \in \{\text{True}, \text{False}\}, \ j = 1, 2, 3$$

Boolean Variables

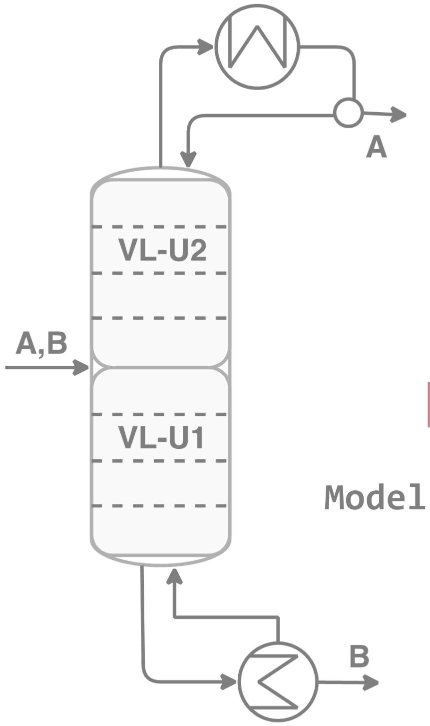
Model development



Code Export from MOSAICmodeling

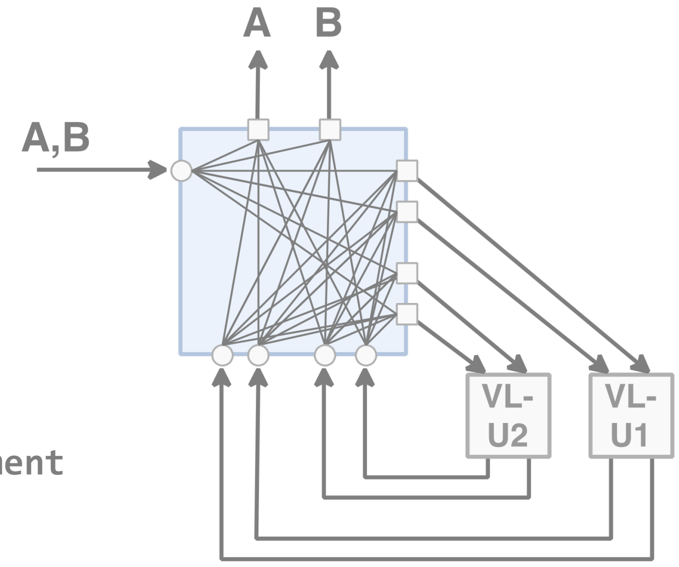


Current and Future Work



GENERALITY

Model development



Code export

~~GAMS~~ → Pyomo

$$\min \; f(x,z,y)$$
$$s.t. \; g(x,z,y) = 0$$
$$z = thermo(x)$$
e.g. $h = f(T,p,x_i)$

Matlab

Graph Analysis

TRACTABILITY

C++ DLL

$$y = thermo(x)$$
$$\frac{dy}{dx} = thermo(x)$$

COBIA

Thermo Property Package

TEA

FIDELITY

Thank You For Your Attention, Questions ?

Acknowledgements

DFG

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