

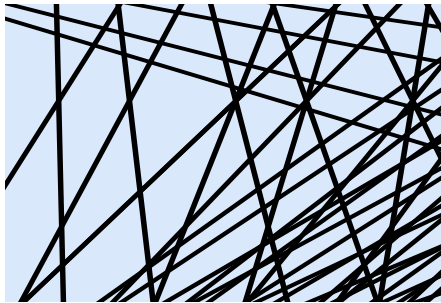
dibltla

Process Dynamics and Operations Group

 **BASF**
We create chemistry

 **tu** technische universität
dortmund


Technische
Universität
Berlin



Mixed-Integer Optimization in GAMS using
CAPE-OPEN Thermodynamics via
MOSAICmodeling and COBIA
for Conceptual Design

CAPE-OPEN 2019 Annual Meeting | 22.10.2019

David Krone, Erik Esche, Norbert Asprion, Jens-Uwe Repke, Mirko Skiborowski

Motivation

Optimization with thermodynamic calculations

1. Formulate all thermo functions explicitly

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

→ Inflated model

- Complex initialization necessary
- No easy changes in thermo calculations (e.g. change from ideal to non-ideal liquid phase)



2. Function calls to thermo property packages

$$\begin{aligned} \min \quad & f(x, y) \\ \text{s.t.} \quad & g(x, y) = 0 \\ & y = \text{thermo}(x) \end{aligned}$$

→ Lean models with thermo flexibility



Problem: optimization tools do not usually provide integrated thermo packages

Motivation

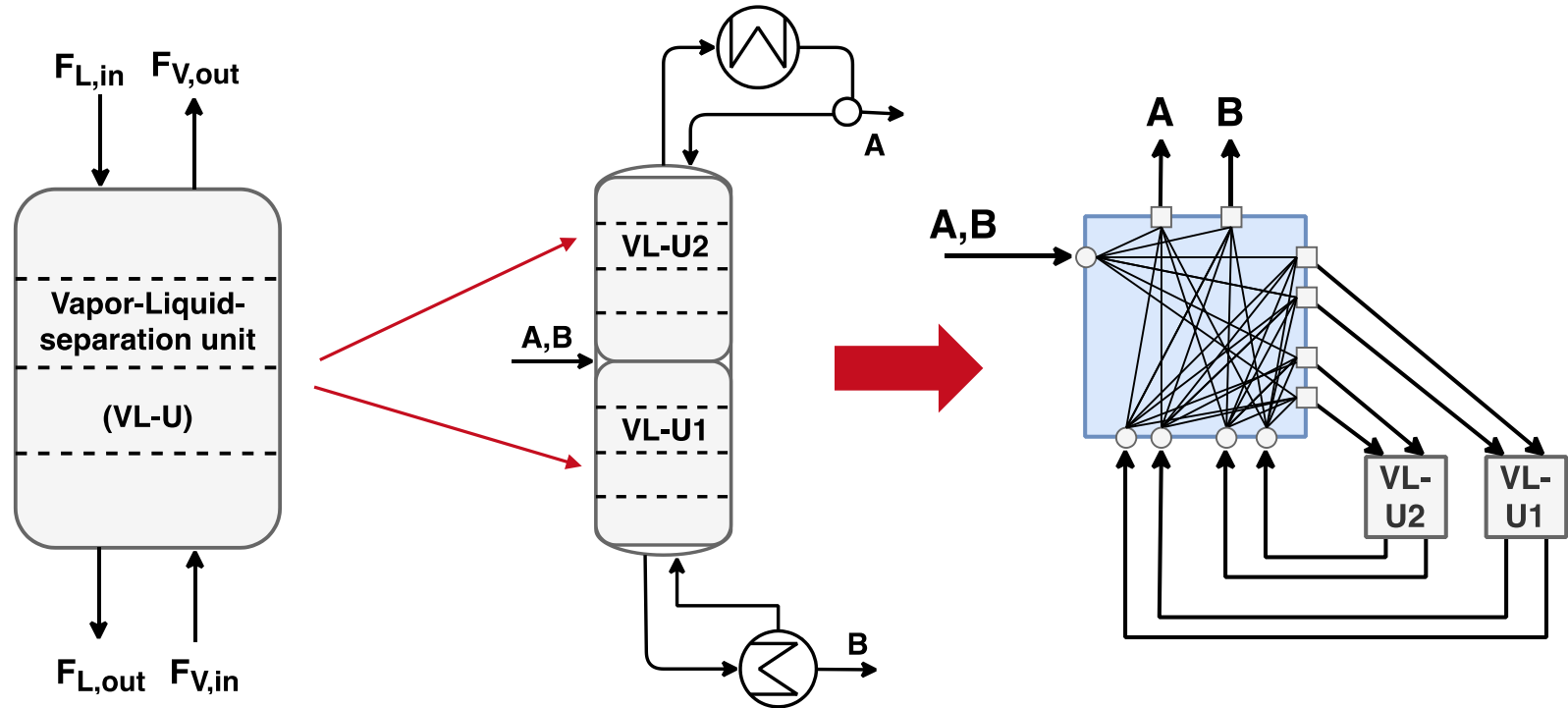
Development Goal

Generate the **interface between**
GAMS and CAPE-OPEN thermo property packages
for **fast thermo calculations**

3 Mixed-Integer Optimization in GAMS using CO Thermodynamics via MOSAICmodeling and COBIA for Conceptual Design

D. Krone | CAPE-OPEN 2019 Annual Meeting | 22.10.2019

I. Mixed-Integer(MI) Optimization for Conceptual Design



4 Mixed-Integer Optimization in GAMS using CO Thermodynamics via MOSAICmodeling and COBIA for Conceptual Design

D. Krone | CAPE-OPEN 2019 Annual Meeting | 22.10.2019

I. MI Optimization for Conceptual Design

The necessity of calculation speed

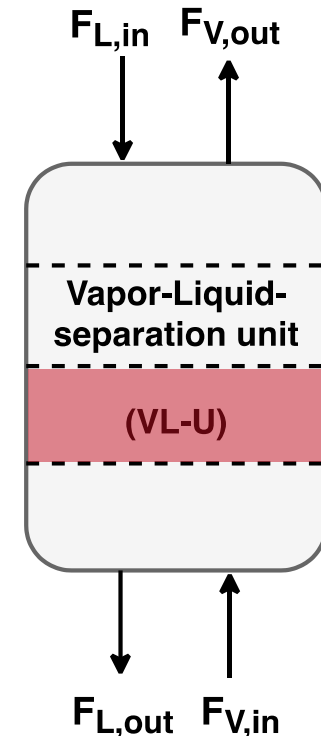
Number of thermo calls per equilibrium stage (ternary mixture)

property	Calls in GAMS program file	Calls to thermo package (C++)
single phase enthalpies (h^L and h^V)	2	8
distribution coefficients K_c	3	18

→ 26 calls/stage

For four equilibrium stages per unit:

→ 104 calls/separation unit



I. Optimization-based Conceptual Design

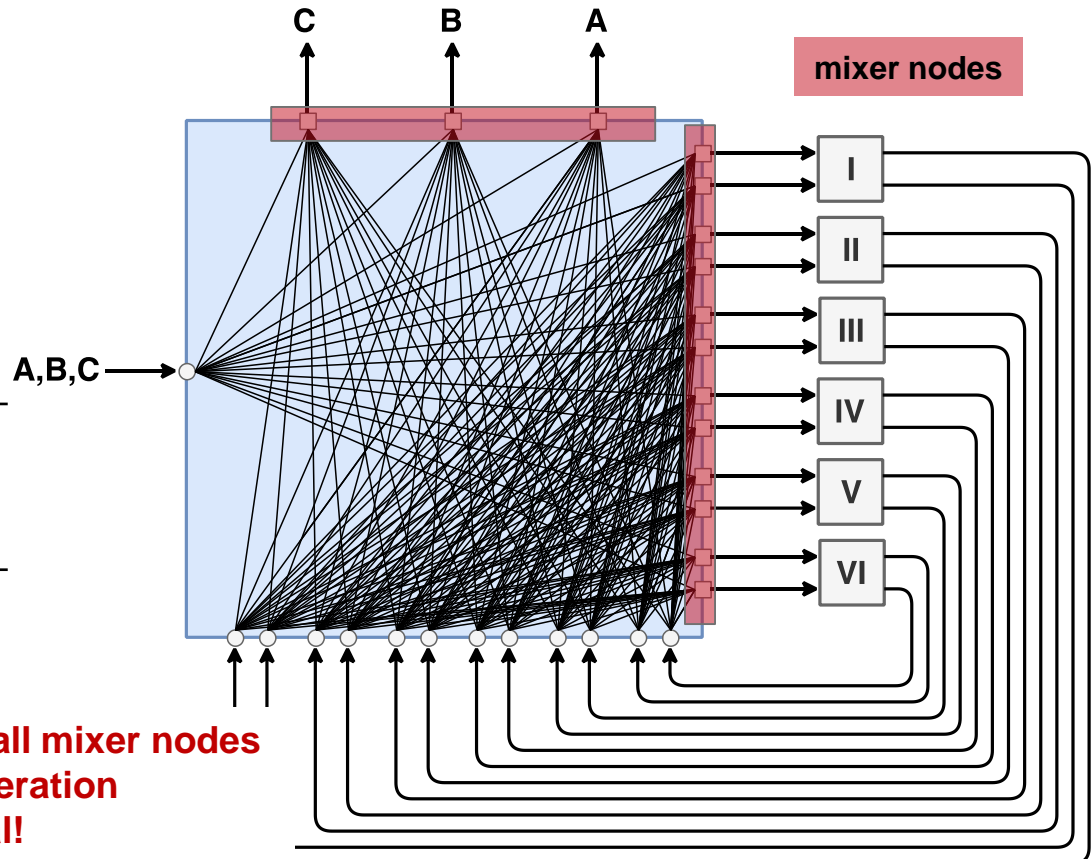
The necessity of calculation speed

→ 624 calls/all separation units

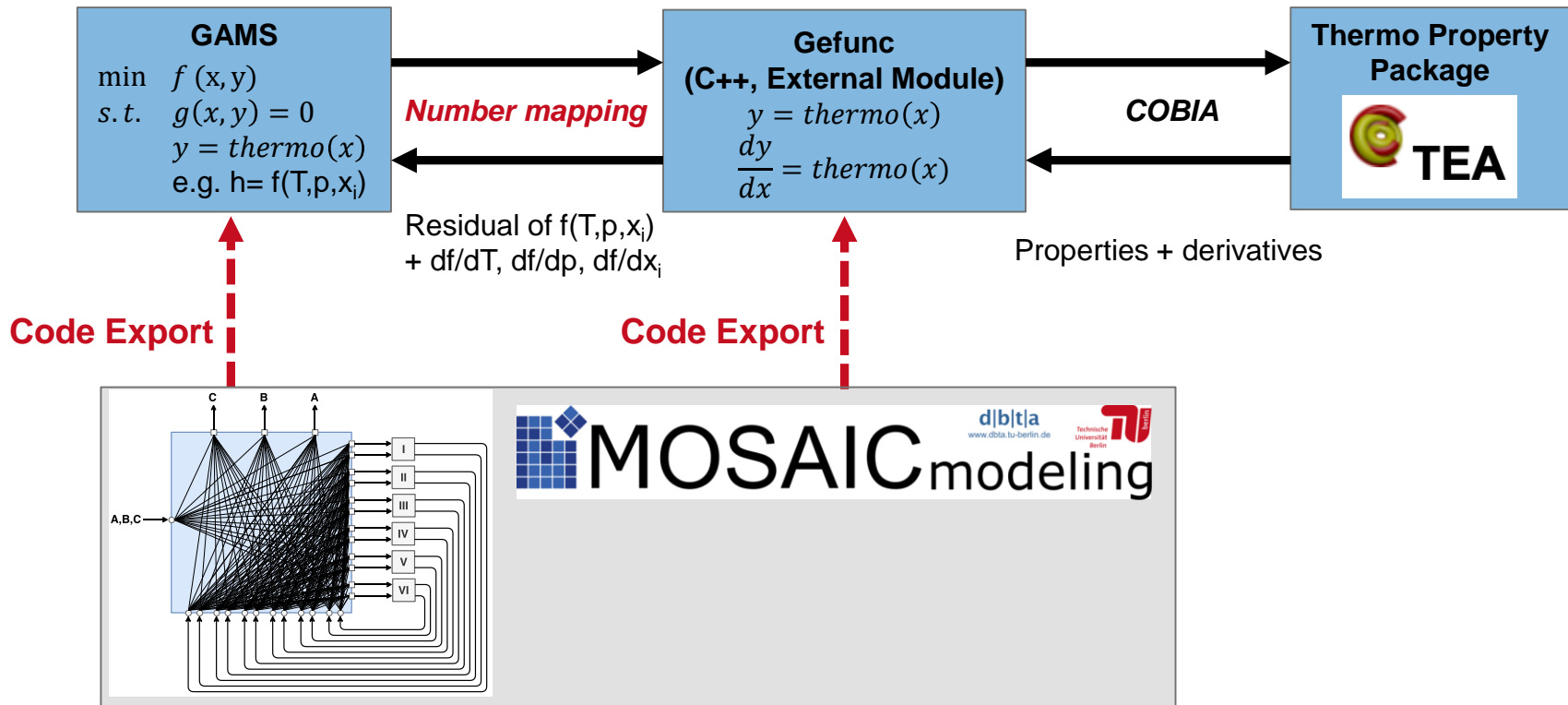
Number of thermo function calls
per mixer node

property	Calls to thermo package (C++)
single phase enthalpies (h^L and h^V)	8
distribution coefficients K_c	18

→ 26 calls/mixer node → 390 calls/all mixer nodes
 → 1014 thermo function calls per iteration
 Calculation speed is vital!



II. Thermo function interface

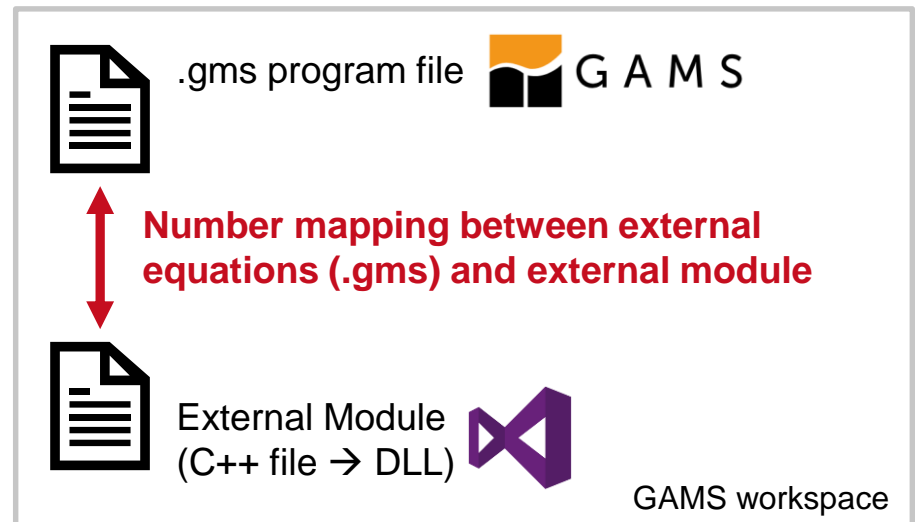
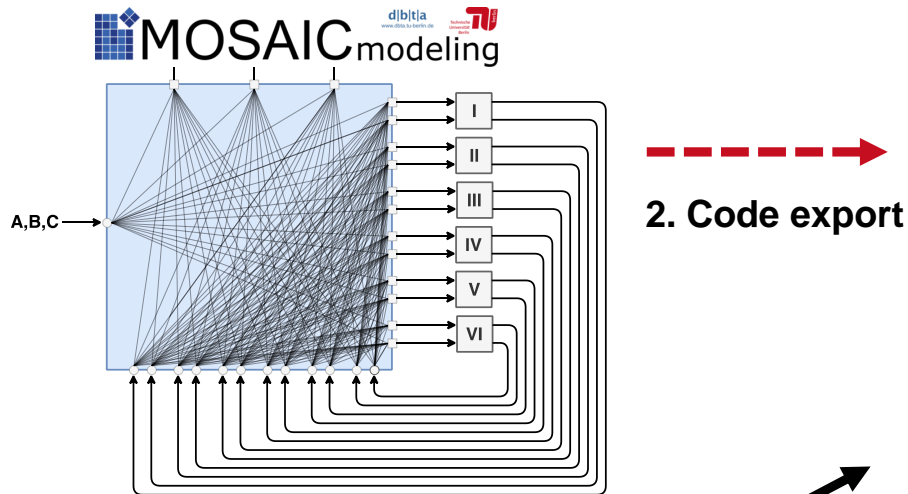


7 Mixed-Integer Optimization in GAMS using CO Thermodynamics via MOSAICmodeling and COBIA for Conceptual Design

D. Krone | CAPE-OPEN 2019 Annual Meeting | 22.10.2019

III. Optimization Workflow Overview

1. Model development



Thermo property package (manager)



3. Thermo calls via COBIA

III. Optimization Workflow

1. Model Development – Equation System

Equation System
Notation

Hierarchy
Equations
Functions
Flowsheet

124220: EQS_6&VL-PBBs [with cc

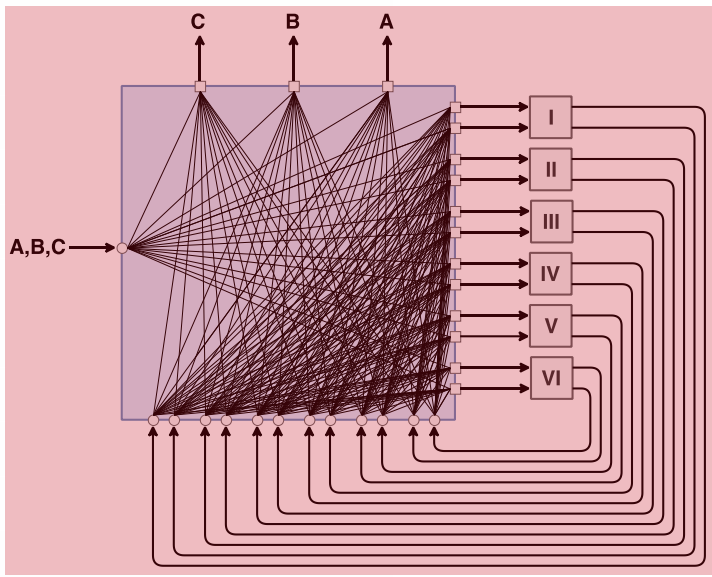
- 0 - [s] 124221: EQS_VL_PBB (
 - 0 - [s] 124222: EQS evap
 - 1 - [s] 124217: EQS conde
 - 2 - [s] 120149: EQS_relax
 - 1 - [s] 124221: EQS_VL_PBB (
 - 2 - [s] 124221: EQS_VL_PBB (
 - 3 - [s] 124221: EQS_VL_PBB (
 - 4 - [s] 124221: EQS_VL_PBB (
 - 5 - [s] 124221: EQS_VL_PBB (
 - 6 - [s] 123506: EQS_DN&flash

All Subsystems of
the Superstructure

Connected Elements

- (1) $y_{VL,i,j} = \beta_i \cdot K_{VL,i,j}^{VLE} \cdot x_{VL,i,j}$
- (2) $F_{VL,i-1}^L \cdot h_{VL,i-1}^L + Q_{VL,i}^{trans} = F_{VL,i}^L \cdot h_{VL,i}^L$
- (3) $F_{VL,i-1}^L \cdot x_{VL,i-1,j} + F_{VL,i,j}^{trans} = F_{VL,i}^L \cdot x_{VL,i,j}$
- (4) $F_{VL,i+1}^V \cdot h_{VL,i+1}^V - Q_{VL,i}^{trans} = F_{VL,i}^V \cdot h_{VL,i}^V$
- (5) $F_{VL,i+1}^V \cdot y_{VL,i+1,j} - F_{VL,i,j}^{trans} = F_{VL,i}^V \cdot y_{VL,i,j}$
- (6) $\sum_{i=1}^{nc} x_{VL,i,j} = 1$
- (7) $\sum_{i=1}^{nc} y_{VL,i,j} = 1$
- (8) $p_{VL}^{PBB} = p_{VL}$
- (9) $\beta_i - 1 = s_i^V - s_i^L$
- (10) $(s_i^L + t_{tol,i}) \cdot (F_{VL,i}^L + t_{tol,i}) - (t_{tol,i})^{2.0} \geq 0$

System equations
all equations defined generically!
→ instantiated before initialization



III. Optimization Workflow

1. Model Development – Thermo Functions

Equation System Notation

Hierarchy Equations Functions Flowsheet

Function

Location: 112801: fun_KValues.mosfun

$$K_{VL}^{VLE}(T_{VL}, p_{VL}, x_{VL, j}) = ?$$

Description: empty function for distribution coefficients (vapor–liquid equilibrium)
No. of usages: 6

Location: 111441: fun_enthalpy_vapor.mosfun

$$h^V(P, T, y_j) = ?$$

Description: function enthalpy vapor
No. of usages: 1

Location: 120080: fun_enthalpy_vapor_with_composition&miniscular_pre

v

Function Applications

Output Variable		Input Variables		
Generic	Applied	Generic ▲	Namespace	Applied
K_{VL}^{VLE}	$K_{VL, i, j}^{VLE}$	p_{VL}	e0e0e2	p_{VL}
		T_{VL}	e0e0e2	$T_{VL, i}$
		$x_{VL, j}$	e0e0e2	$x_{VL, i, j}$

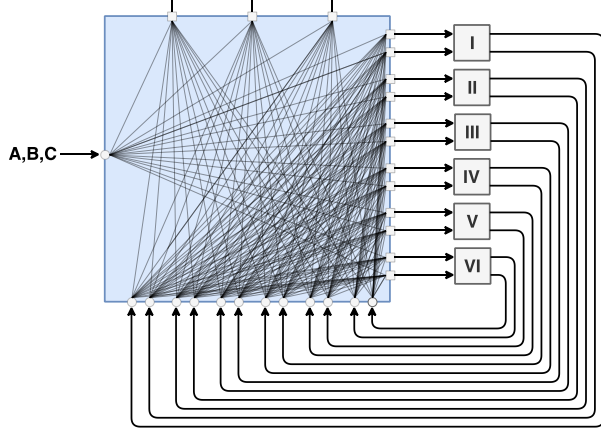
Output Variable		Input Variables		
Generic	Applied	Generic ▲	Namespace	Applied
K_{VL}^{VLE}	$K_{VL, i, j}^{VLE}$	p_{VL}	e0e1e2	p_{VL}
		T_{VL}	e0e1e2	$T_{VL, i}$
		$x_{VL, j}$	e0e1e2	$x_{VL, i, j}$

III. Optimization Workflow

2. Code Export

1. Model development 

MOSAIC modeling



2. Code export



.gms program file



G A M S

Number mapping between external equations (.gms) and external module



External Module
(C++ file → DLL)



GAMS workspace

Thermo property package (manager)



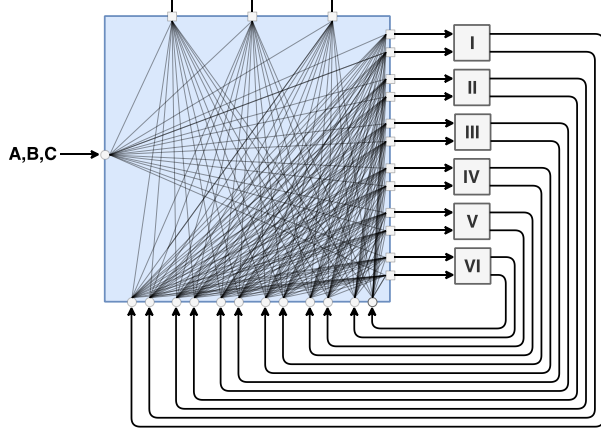
3. Thermo calls via COBIA

III. Optimization Workflow

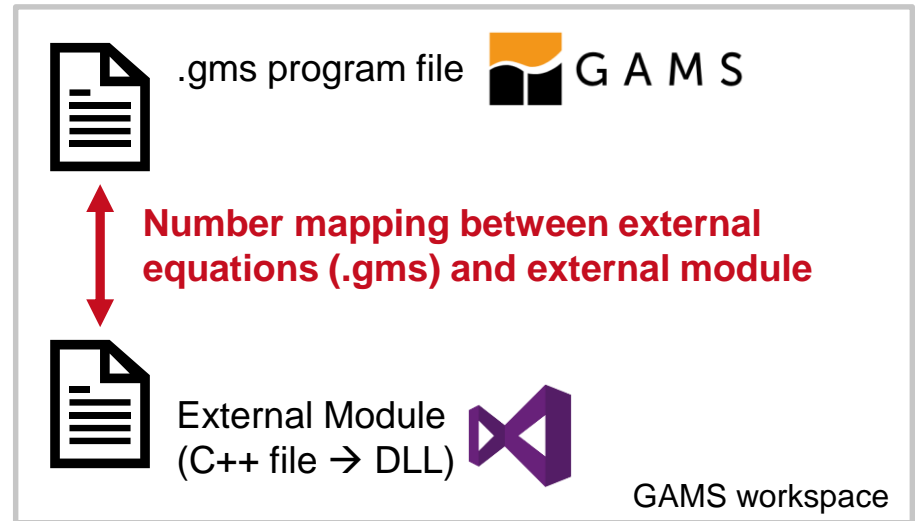
2. Code Export

1. Model development 

MOSAIC modeling 



2. Code export 



Thermo property package (manager)



3. Thermo calls via COBIA

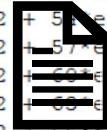
III. Optimization Workflow

Mapping of external equations and external module

```

1 =x= 1*e0e6_h_outL_mix_k1 + 43*e0e6_x_outL_mix_k1_j1 + 44*e0e6_x_outL_mix_k1_j2 + 45*e0e6_x_outL_mix_k1_j3 + 31*e0s0_T + 37*e0s0_p;
2 =x= 2*e0e6_h_outL_mix_k2 + 46*e0e6_x_outL_mix_k2_j1 + 47*e0e6_x_outL_mix_k2_j2 + 48*e0e6_x_outL_mix_k2_j3 + 32*e0s1_T + 38*e0s1_p;
3 =x= 3*e0e6_h_outL_mix_k3 + 49*e0e6_x_outL_mix_k3_j1 + 50*e0e6_x_outL_mix_k3_j2 + 51*e0e6_x_outL_mix_k3_j3 + 33*e0s2_T + 39*e0s2_p;
4 =x= 4*e0e6_h_outL_mix_k4 + 52*e0e6_x_outL_mix_k4_j1 + 53*e0e6_x_outL_mix_k4_j2 + 54*e0e6_x_outL_mix_k4_j3 + 34*e0s3_T + 40*e0s3_p;
5 =x= 5*e0e6_h_outL_mix_k5 + 55*e0e6_x_outL_mix_k5_j1 + 56*e0e6_x_outL_mix_k5_j2 + 57*e0e6_x_outL_mix_k5_j3 + 35*e0s4_T + 41*e0s4_p;
6 =x= 6*e0e6_h_outL_mix_k6 + 58*e0e6_x_outL_mix_k6_j1 + 59*e0e6_x_outL_mix_k6_j2 + 60*e0e6_x_outL_mix_k6_j3 + 36*e0s5_T + 42*e0s5_p;
7 =x= 7*e0e6_h_outV_mix_k1 + 61*e0e6_x_outV_mix_k1_j1 + 62*e0e6_x_outV_mix_k1_j2 + 63*e0e6_x_outV_mix_k1_j3 + 37*e0s6_T + 43*e0s6_p;
8 =x= 8*e0e6_h_outV_mix_k2 + 64*e0e6_x_outV_mix_k2_j1 + 65*e0e6_x_outV_mix_k2_j2 + 66*e0e6_x_outV_mix_k2_j3 + 38*e0s7_T + 44*e0s7_p;

```



.gms program file



GAMS

Referencing by numbers, e.g. for: $h^L = f(p, T, X_1, X_2, X_3)$

```

if (icntr[I_Eqno] == 1) { //for the first function
  std::vector<double> composition_liquid = { x[42], x[43], x[44] };
  //External Function for liquid enthalpy calculation
  mylocalThermoObj.setSinglePhasePropResult(enthalpyF, x[30], x[36] * 100000.0, liquid, composition_liquid);
  f[0] = (x[0] - mylocalThermoObj.getSinglePhasePropResult(0));
  //Derivatives
  //dh/dh
  d[0] = 1.0;
  //dh/dy_j
  mylocalThermoObj.setSinglePhasePropResult(enthalpyF_DmolFraction, x[30], x[36] * 100000.0, liquid, composition_liquid);
  d[42] = -mylocalThermoObj.getSinglePhasePropResult(0);
  d[43] = -mylocalThermoObj.getSinglePhasePropResult(1);
  d[44] = -mylocalThermoObj.getSinglePhasePropResult(2);
  //dh/dp
  mylocalThermoObj.setSinglePhasePropResult(enthalpyF_Dpressure, x[30], x[36] * 100000.0, liquid, composition_liquid);
  d[36] = -mylocalThermoObj.getSinglePhasePropResult(0)*100000.0; //[1/bar]*|
  //dh/dT
  mylocalThermoObj.setSinglePhasePropResult(enthalpyF_Dtemperature, x[30], x[36] * 100000.0, liquid, composition_liquid);
  d[30] = -mylocalThermoObj.getSinglePhasePropResult(0); //[1/K]
}

```



External Module
(C++ file → DLL)

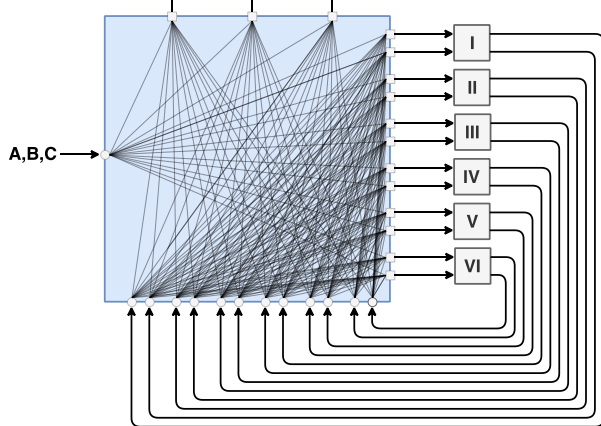


III. Optimization Workflow

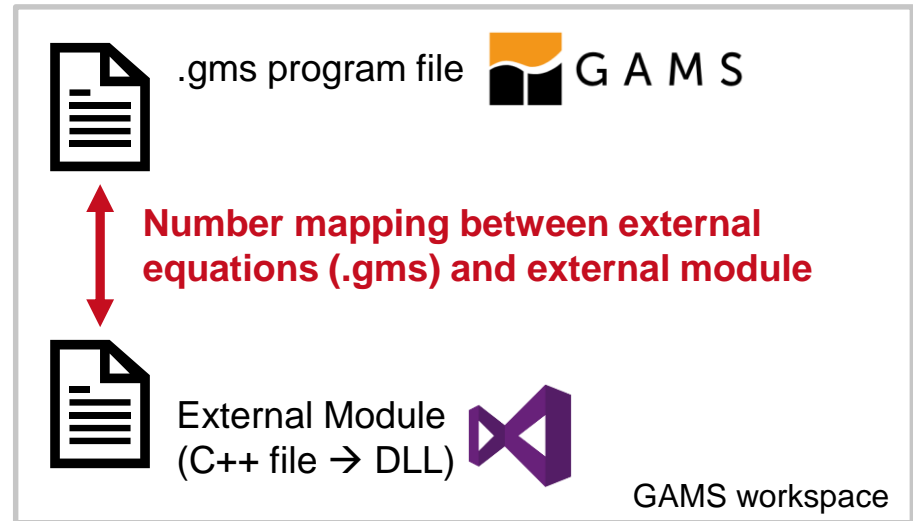
3. Thermo calls to Thermo package via COBIA

1. Model development 

MOSAIC modeling 




2. Code export 



Thermo property package (manager)



3. Thermo calls via COBIA 

IV. Case Studies – Separation of ternary mixture via a dividing wall column (DWC)

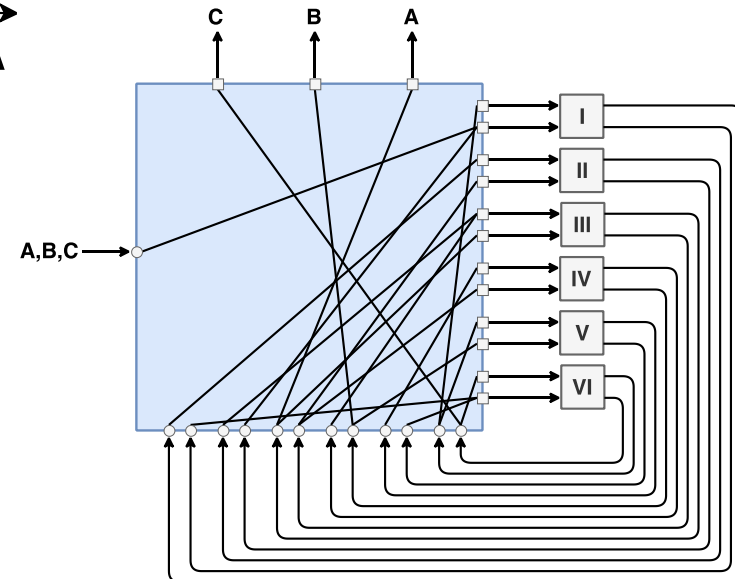
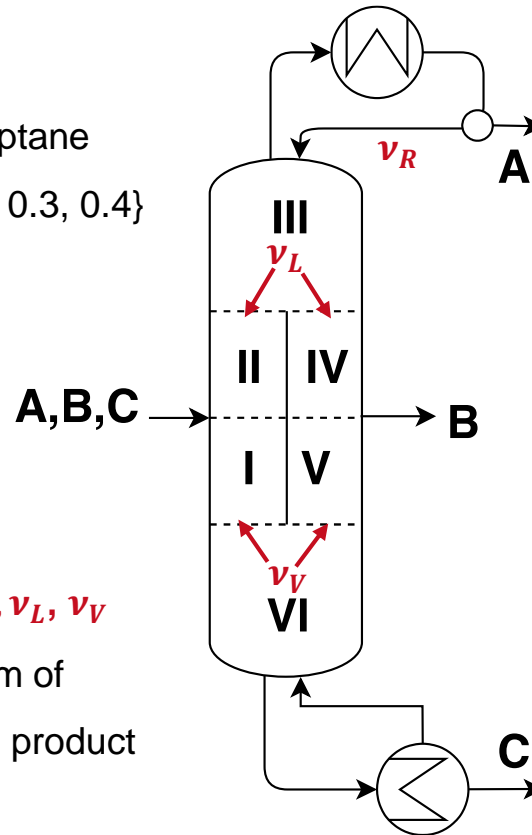
- **Feed specifications:**

- n-pentane/n-hexane/n-heptane
- Molar composition = {0.3, 0.3, 0.4}
- $T = 325 \text{ K}$
- $p = 1 \text{ bar}$
- $F = 1 \text{ kmol/s}$

- **Optimization task:**

find optimal split ratios: v_R, v_L, v_V

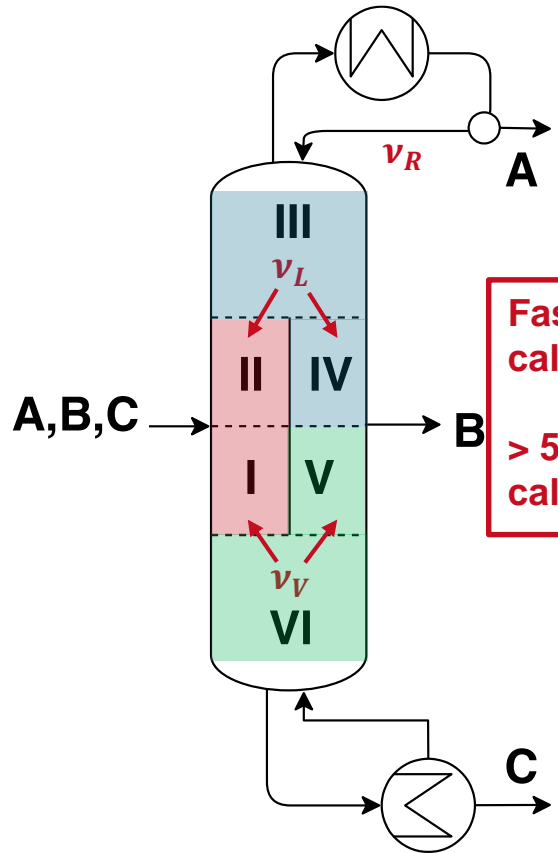
- **Maximizing objective:** sum of desired product qualities in product streams



Only showing active superstructure connections

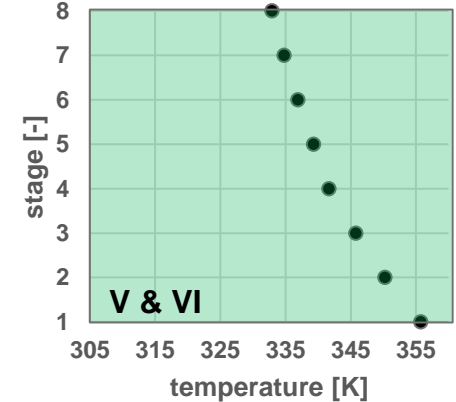
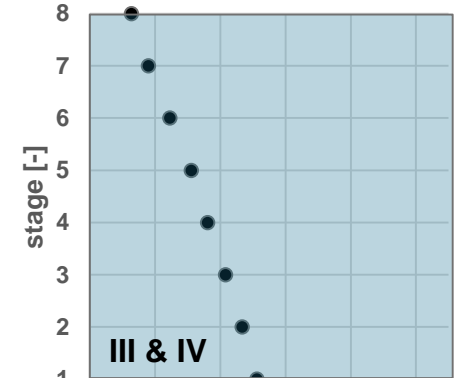
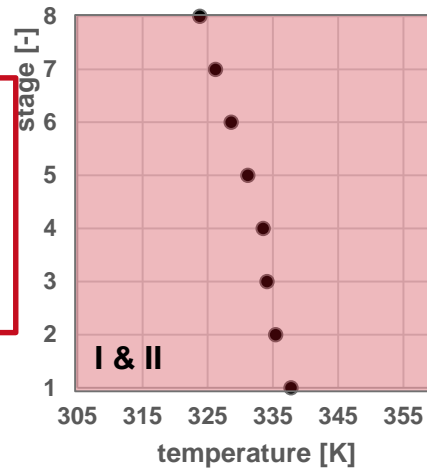
IV. Case Studies – Separation of ternary mixture

Speed of thermo calculations and profiles



Fast thermo calculations
> 500 thermo calculations/second

$v_R = 0.4$
 $v_L = 0.69,$
 $v_V = 0.45$



V. Summary

**Functioning interface between
GAMS and CAPE-OPEN thermo property packages**

For fast thermo calculations

**Reducing modelling effort by automatic code generation
with MOSAICmodeling**

Acknowledgements

Jasper van Baten

for his code examples and help with COBIA

Questions and answers



II. Results – separation of ternary mixture

ii. Optimization of the superstructure in DWC configuration

Product flows and qualities:

Destillate:

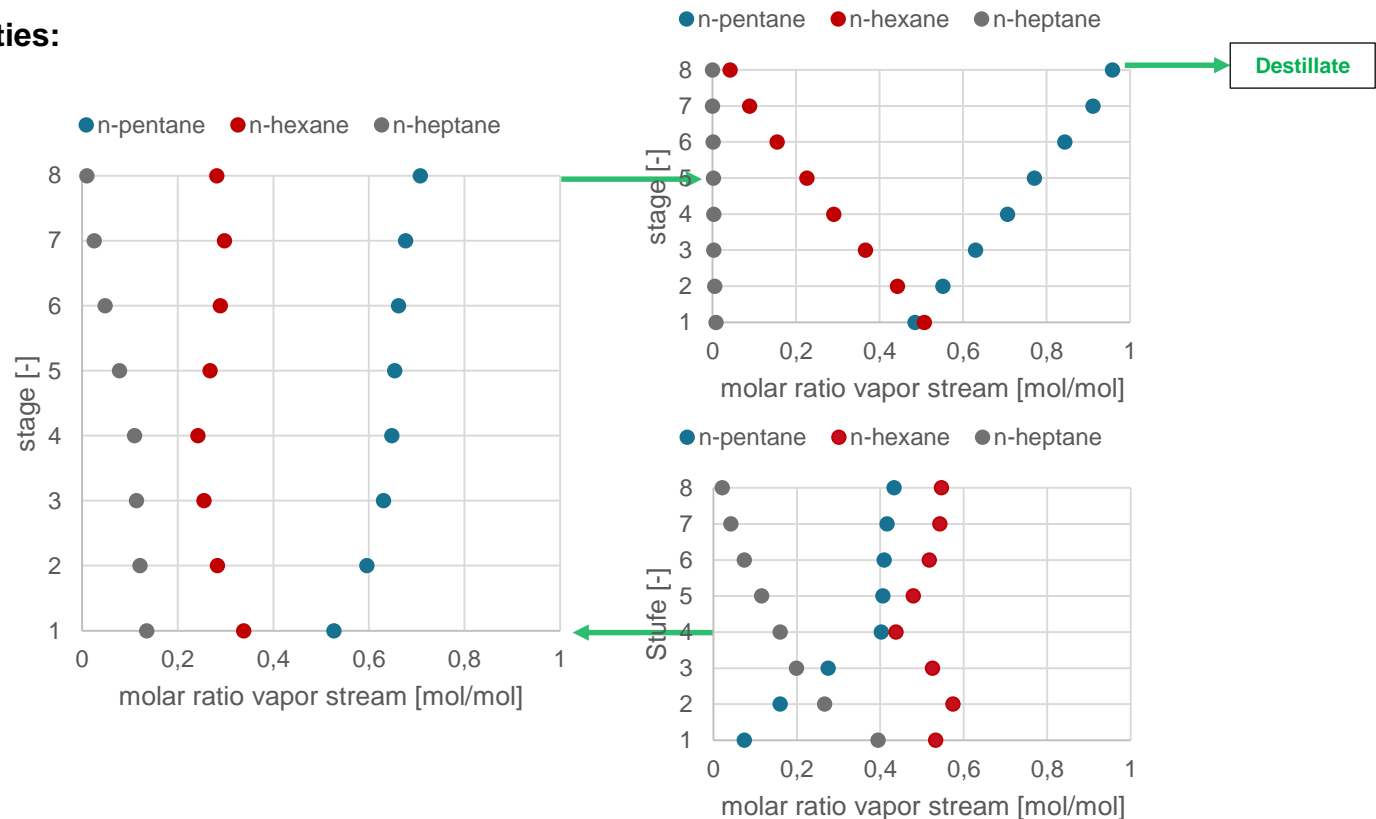
- $F = 0,2752 \text{ kmol/s}$
- Composition =
{**0.958**, 0.042, 0.000}

Middle draw:

- $F = 0,1 \text{ kmol/s}$
- Composition =
{0.241, **0.726**, 0.032}

Bottom draw:

- $F = 0,6236 \text{ kmol/s}$
- Composition =
{0.019, 0.345, **0.636**}



II. Results – separation of ternary mixture

ii. Optimization of the superstructure in DWC configuration

Product flows and qualities:

Destillate:

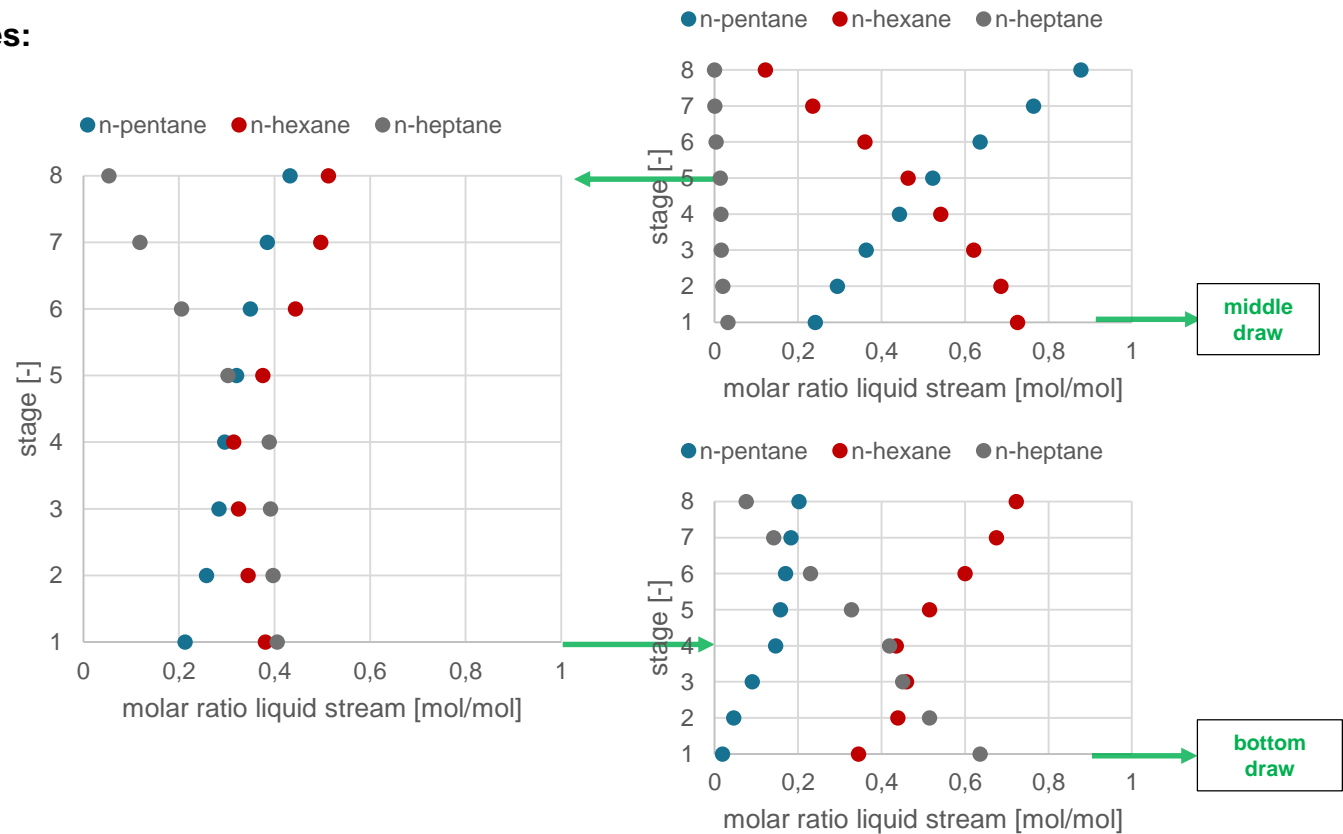
- $F = 0,2752$ kmol/s
- Composition =
{**0.958**, 0.042, 0.000}

Middle draw:

- $F = 0,1$ kmol/s
- Composition =
{0.241, **0.726**, 0.032}

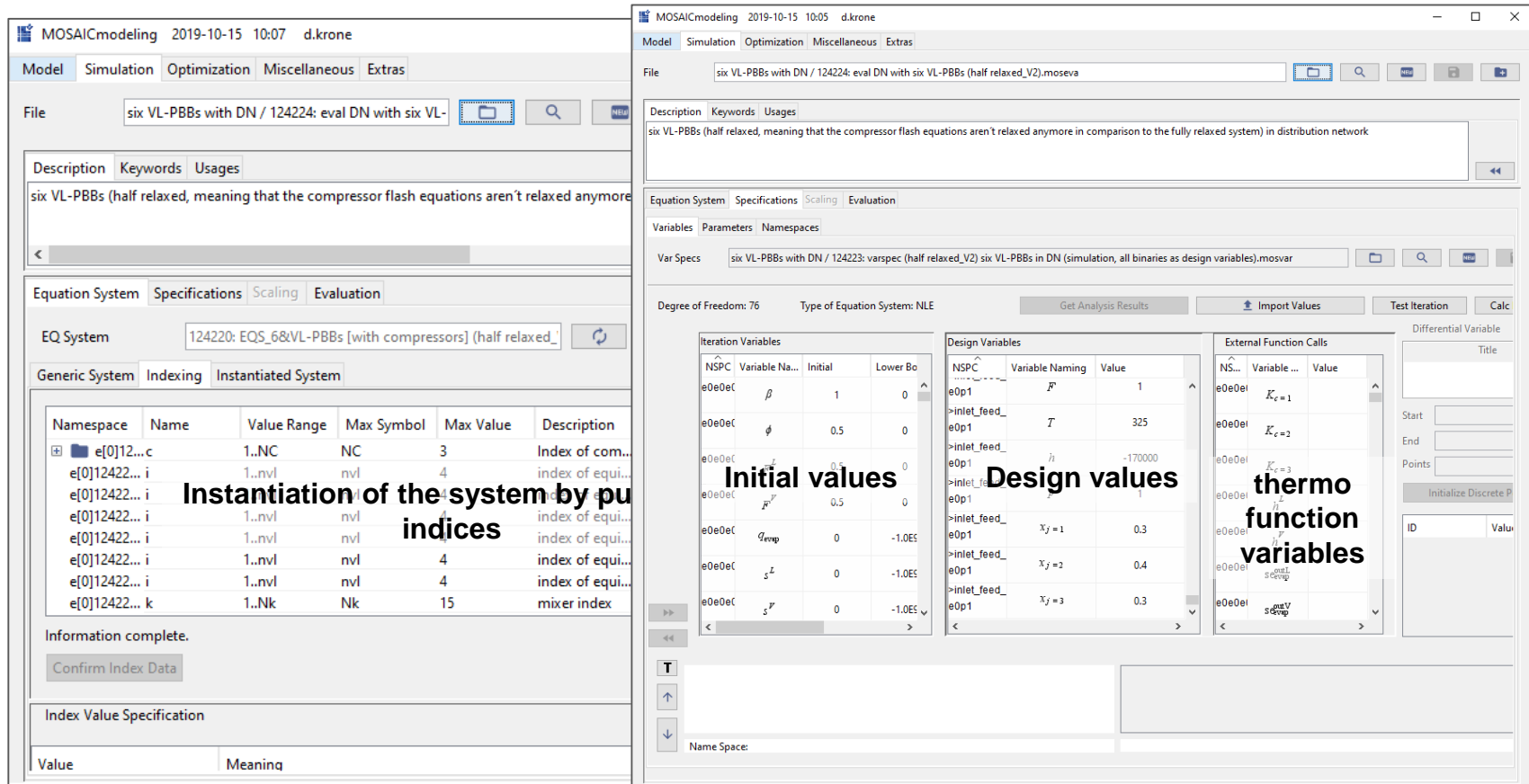
Bottom draw:

- $F = 0,6236$ kmol/s
- Composition =
{0.019, 0.345, **0.636**}



II. Optimization Workflow

1. Model Development – Instantiation and Initialisation



The screenshot displays the MOSAICmodeling software interface, showing the process of model development and instantiation. The interface is divided into several panes:

- File:** six VL-PBBs with DN / 124224: eval DN with six VL-
- Description:** six VL-PBBs (half relaxed, meaning that the compressor flash equations aren't relaxed anymore in comparison to the fully relaxed system) in distribution network
- Equation System:** 124220: EQS_6&VL-PBBs [with compressors] (half relaxed_)
- Generic System:** Indexing, Instantiated System
- Table:** A table showing the instantiation of the system by public indices. The table has columns: Namespace, Name, Value Range, Max Symbol, Max Value, and Description.
- Iteration Variables:** A table showing initial values for variables like β , ϕ , γ , γ^* , g_{evap} , δ^L , and δ^* .
- Design Variables:** A table showing design values for variables like F^* , T , η , $x_y = 1$, $x_y = 2$, and $x_y = 3$.
- External Function Calls:** A table showing thermo function variables like $K_c = 1$, $K_c = 2$, and $K_c = 3$.

Instantiation of the system by public indices

Namespace	Name	Value Range	Max Symbol	Max Value	Description
e[0]12...	c	1..NC	NC	3	Index of com...
e[0]12422...	i	1..nvl	nvl	4	index of equi...
e[0]12422...	i	1..nvl	nvl	4	index of equi...
e[0]12422...	i	1..nvl	nvl	4	index of equi...
e[0]12422...	i	1..nvl	nvl	4	index of equi...
e[0]12422...	i	1..nvl	nvl	4	index of equi...
e[0]12422...	k	1..Nk	Nk	15	mixer index

Iteration Variables

Variable Na...	Initial	Lower Bo
β	1	0
ϕ	0.5	0
γ	0.5	0
γ^*	0.5	0
g_{evap}	0	-1.0E5
δ^L	0	-1.0E5
δ^*	0	-1.0E5

Design Variables

Variable Naming	Value
F^*	1
T	325
η	-170000
$x_y = 1$	0.3
$x_y = 2$	0.4
$x_y = 3$	0.3

External Function Calls

Variable ...	Value
$K_c = 1$	
$K_c = 2$	
$K_c = 3$	

22 Mixed-Integer Optimization in GAMS using CO Thermodynamics via MOSAICmodeling and COBIA for Conceptual Design

D. Krone | CAPE-OPEN 2019 Annual Meeting | 22.10.2019

I. Process synthesis approach

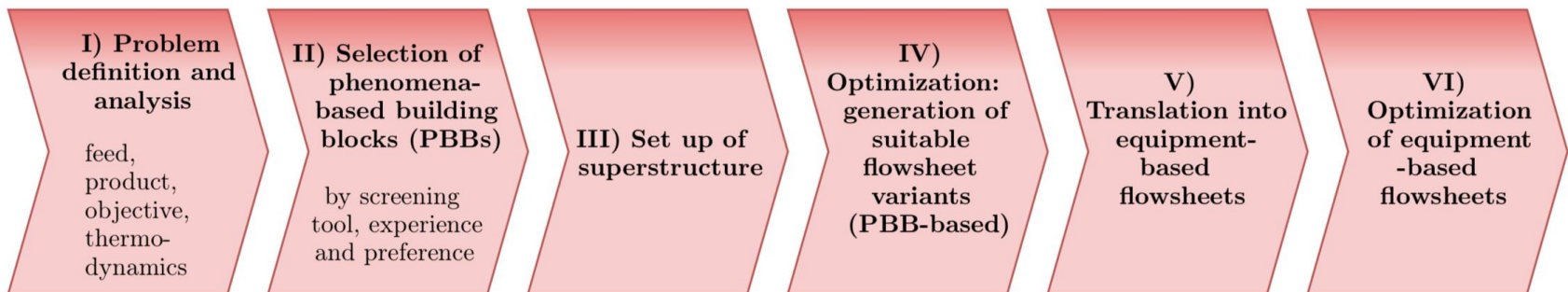


Fig. 1: Process synthesis approach based on the framework by Kuhlmann and Skiborowski¹

¹ H. Kuhlmann, M. Skiborowski, Ind. Eng. Chem. Res. 2017, 56 (45), 13461 - 13481