HiDiC in AspenPlus

Gregor Fernholz

Senior Consultant

Process Systems Enterprise

Michel Pons

Chief Technology Officer

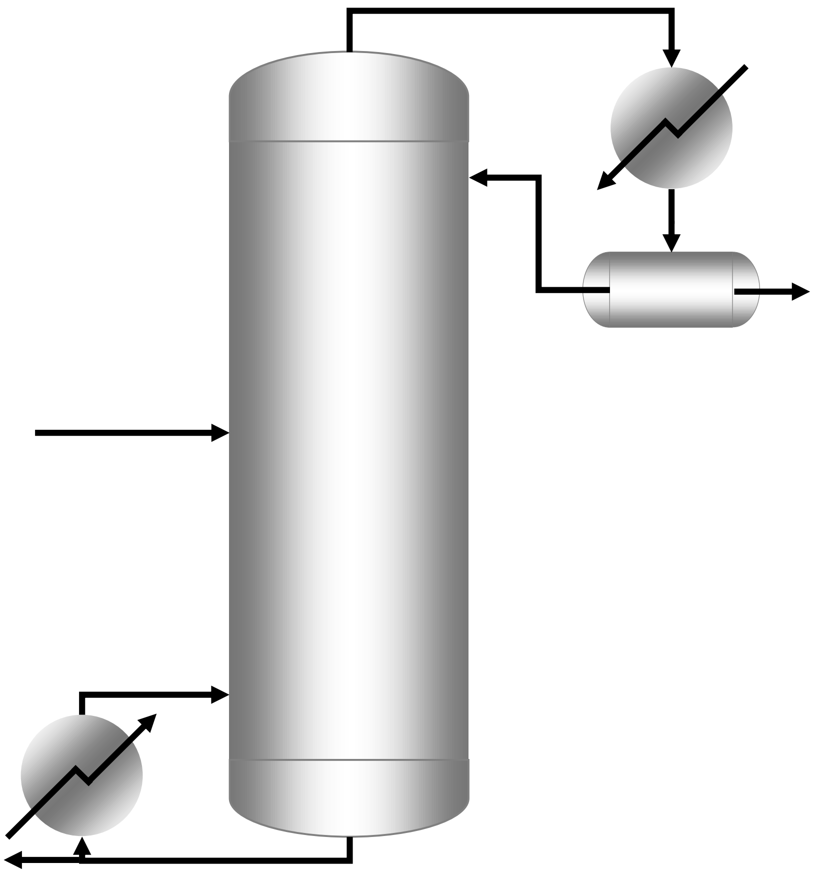
CAPE-OPEN Laboratories Network

Overview

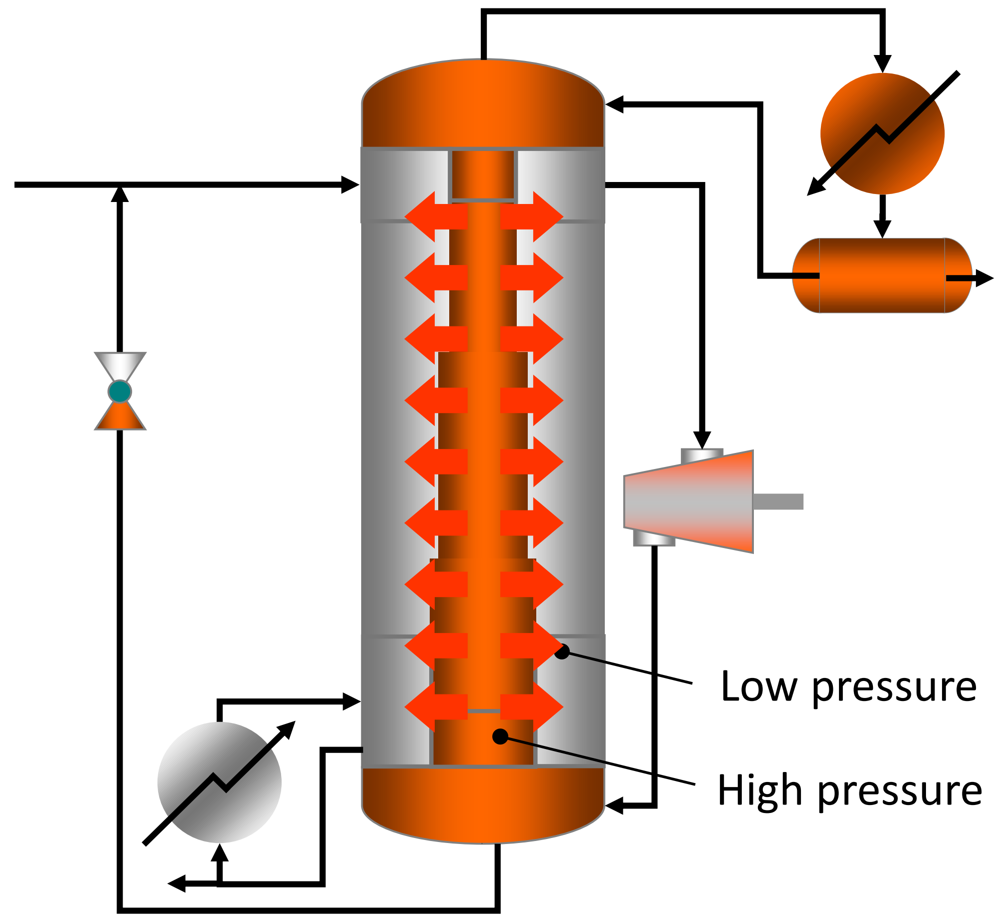
- Introduction: Heat integrated distillation columns (HiDiC)
- Using an gPROMS implementation of a HiDiC model as a gO:CapeOpenUnit in AspenPlus
- Modelling of a heat integrated distillation column (HiDiC) using the Gas-to-Liquid (GLC) library
- Export of a gPROMS model to a gO:CapeOpenUnit

Introduction: Heat integrated distillation columns

Conventional distillation column



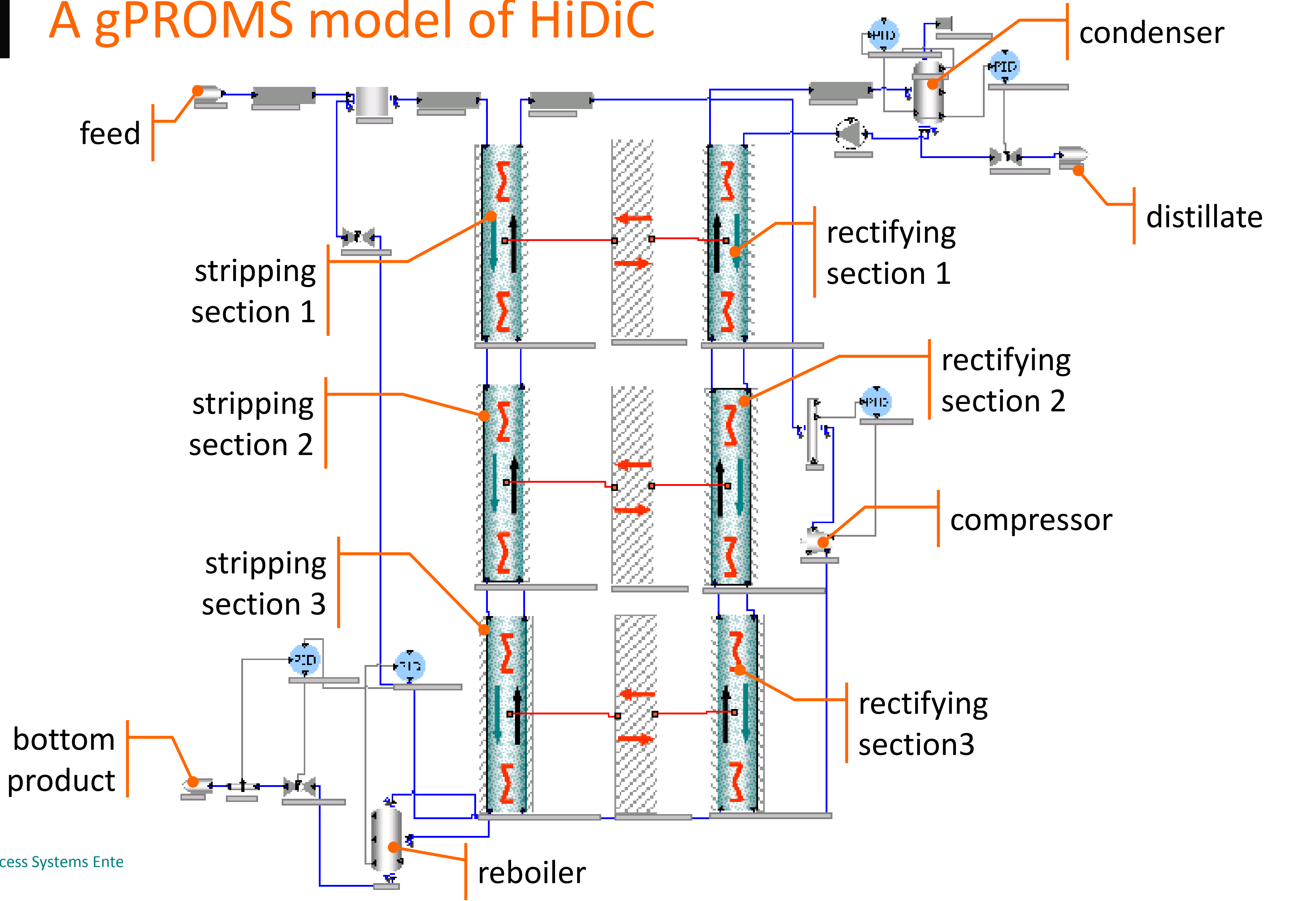
Heat-Integrated Distillation Column



Why HiDiC? – a BTX separation case study

Separation equipment	Total energy input (MJ/h)	Condenser duty (MJ/h)
Conventional column	136.8	132.7
HiDiC – concentric columns	76.6	56.8
HiDiC – compact exchanger	59.7	57.5

A gPROMS model of HiDiC



Using the HiDiC model in AspenPlus

demo

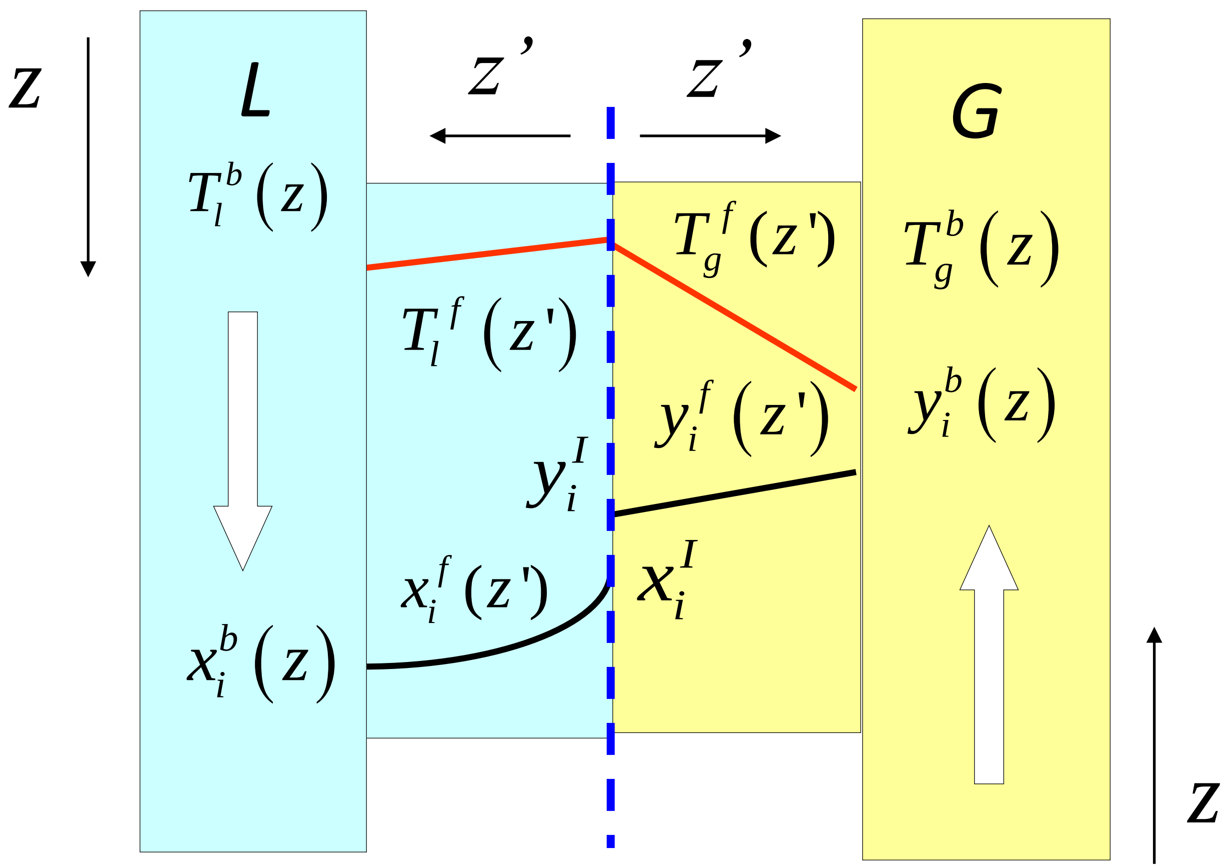
Modelling of a HiDiC column using the GLC library

- Gas-to-liquid (GLC) library scope:
  - Rate based modelling of equipment for gas and liquid phases
  - Applicable to many unit operations (distillation, absorption,…)
- Advantages of the rate-based approach:
  - much closer to physical reality
  - potentially much more accurate
- Challenges in rate-based approaches:
  - more complex to implement
  - there is no consensus on what is the best approach for solving the model equations
  - very limited availability in commercial simulators
  - development “in-house” models is time consuming and it is difficult to assure re-usability for various equipments/unit operations

GLC library key features

- Rate based approach
- Mass/heat transfer limitations accounted for on both sides of gas-liquid interface
- Maxwell-Stefan formulation used throughout models
- Characterisation of the equipment via dual flow hydrodynamics in its geometry
- Applicability not limited to cylindrical packing columns
- Can model equipment as complex as compact heat exchangers
- Single-sized and multiple stage equipment
- Equipment specific correlations for liquid hold-up, pressure drop and mass/heat transfer coefficients are easy to be introduced using templates
- Models fully dynamic
- Multiple operation modes
  - continuous, batch, semi-batch
- Handling non-condensibles

Core elements of the GLC library – the GLC section



- Dynamic mass and energy balances in fluid bulks
- Mass and heat transfer in the films
- Energy balance and V/L equilibrium at the interface

Core elements of the GLC library – the fluid film

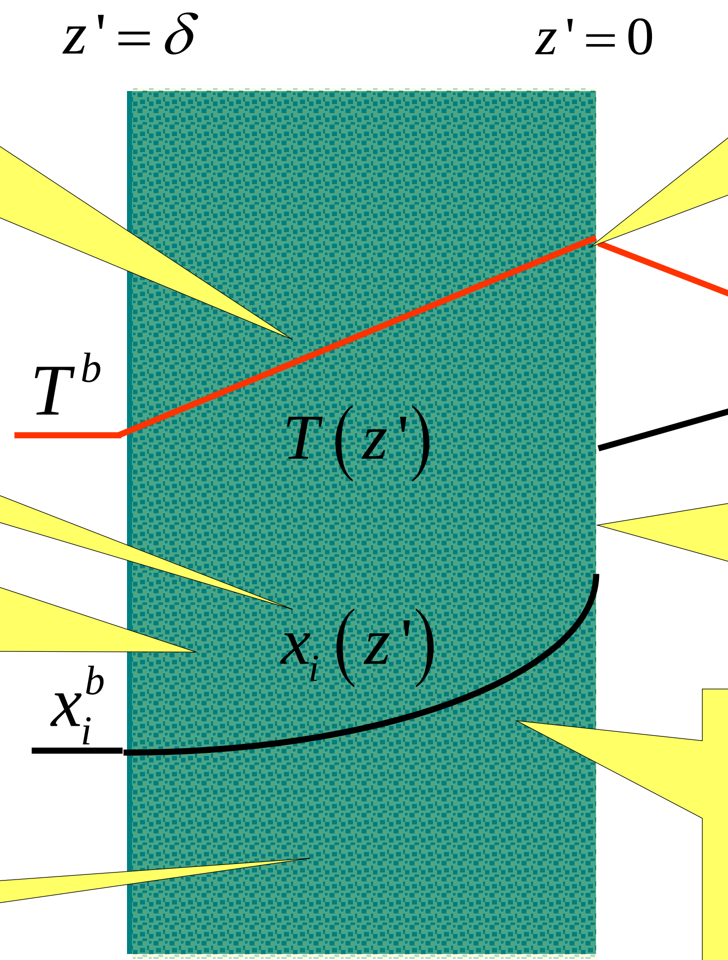
$$\frac{\partial}{\partial z'}\left(\lambda \frac{\partial T}{\partial z'}\right) = \frac{\partial}{\partial z'}\left(\sum_{i=1}^{n_l} N_i H_i\right)$$

$$\frac{\partial N_i}{\partial z'} = 0 \quad i = 1,\ldots,n_l$$

$$\frac{dx_i}{dz'} = \sum_{\substack{k=1\\k\neq i}}^{n_l} \frac{x_i N_k - x_k N_i}{c_t D_{ik}}$$

$$i = 1,\ldots,(n_l - 1)$$

$$\sum_{i=1}^{n_l} x_i = 1$$



$$T_l^I = T_g^I$$

$$-q_g^I = q_l^I + \sum_{i=1}^{n_{VLE}} N_i^I \lambda_i$$

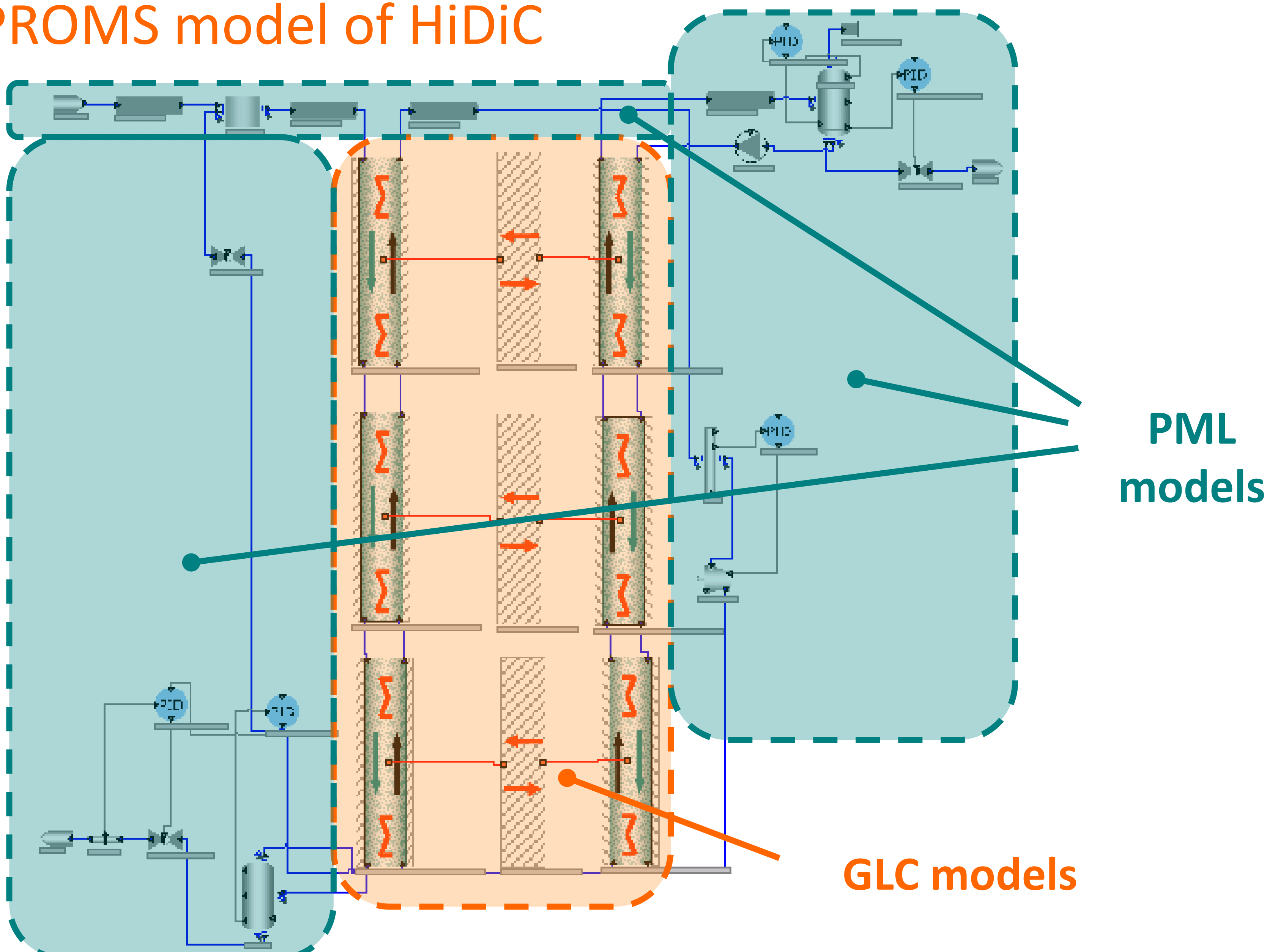
$$\varphi_i^l x_i = \varphi_i^g y_i$$

$$N_i^I\big|_l = -N_i^I\big|_g$$

$$i = 1,\ldots,n_{VLE}$$

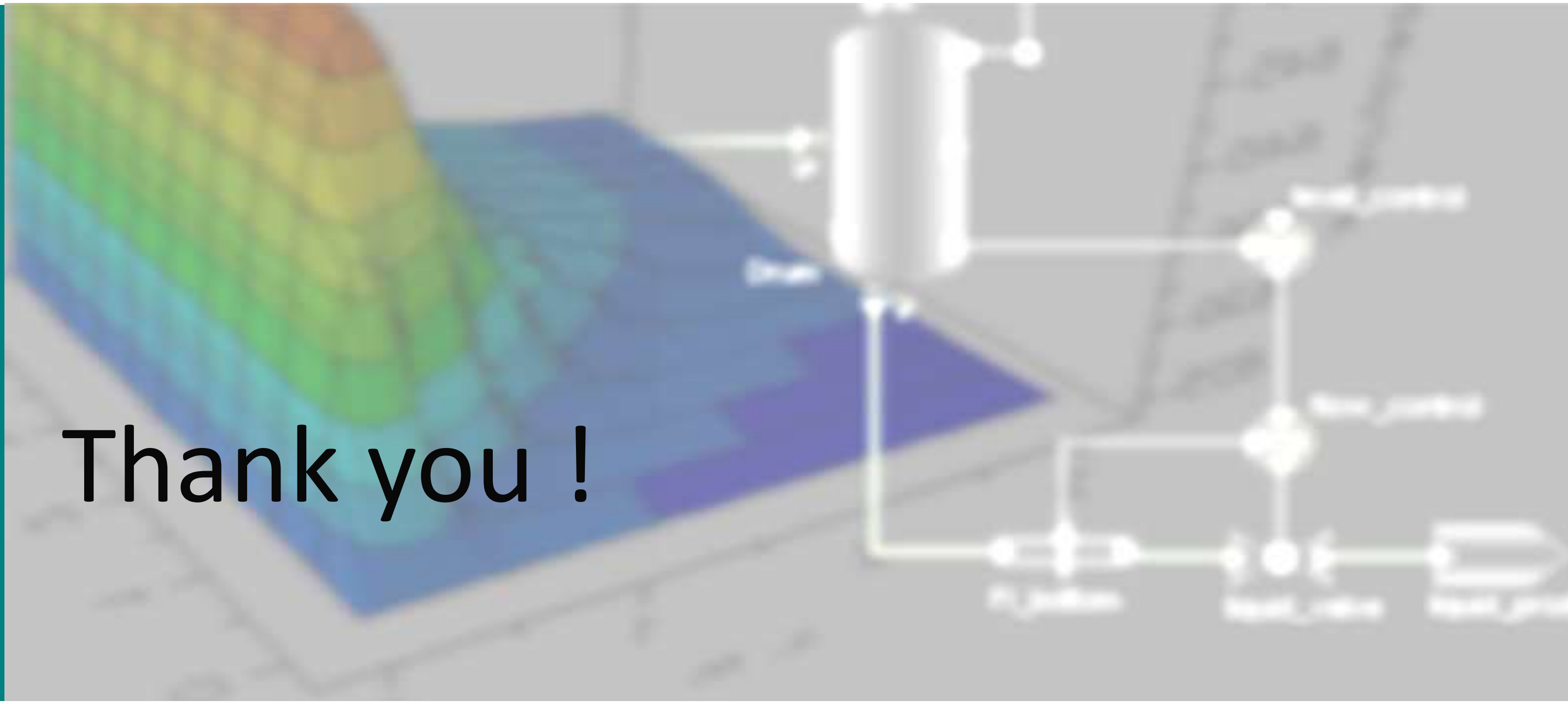
Dual flow hydrodynamics:
- *liquid holdup*
- *film thickness*
- *packing wetting ratio*
- *diffusivity coeff.*

A gPROMS model of HiDiC



Export of a gPROMS model to a gO:CapeOpenUnit

demo



Thank you !

www.psenterprise.com