



HiDiC in AspenPlus

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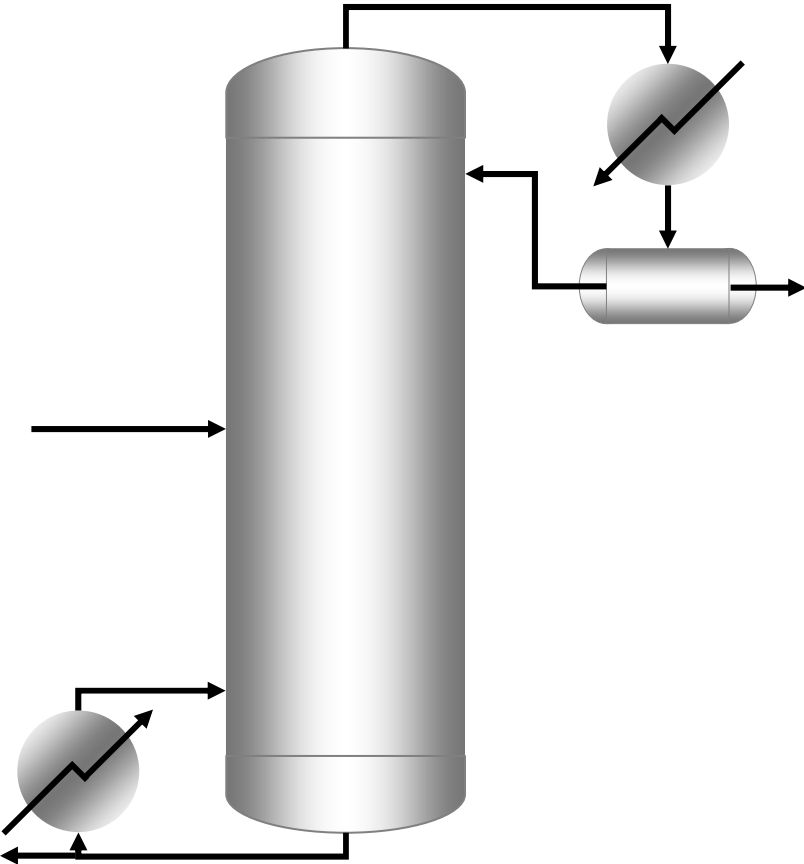
CAPE-OPEN Laboratories Network

Overview

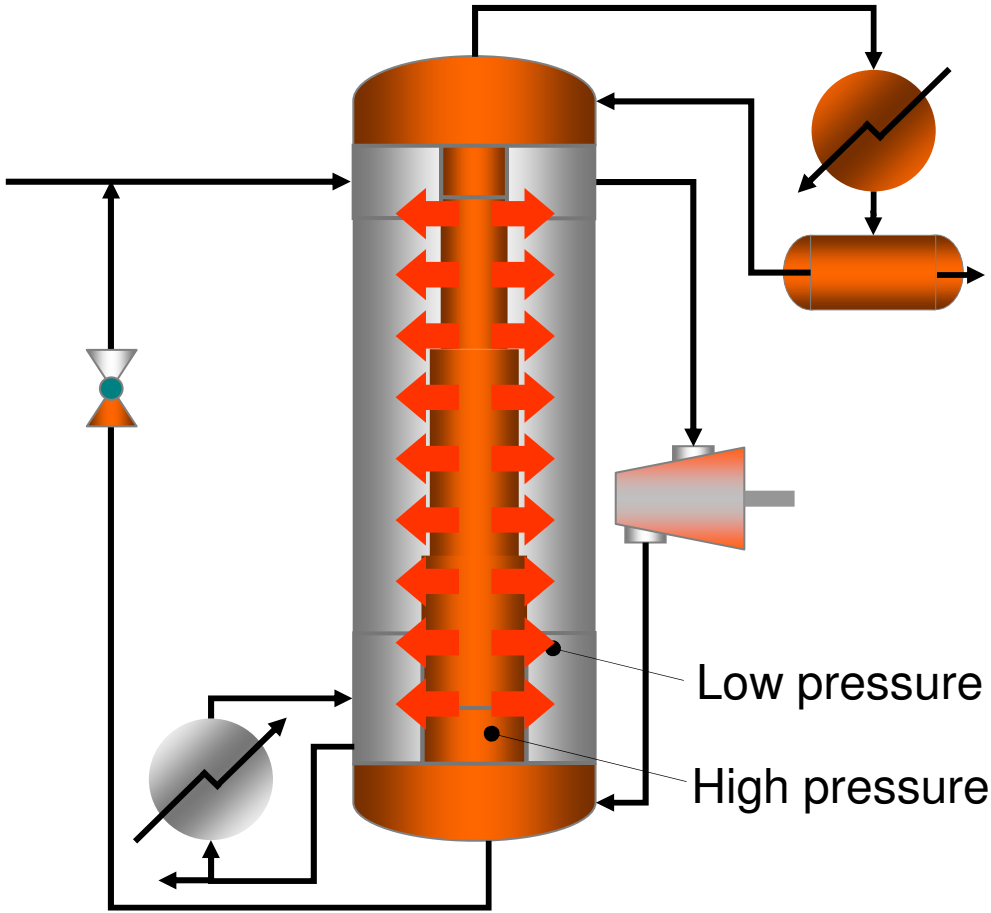
- Introduction: Heat integrated distillation columns (HiDiC)
- Using an gPROMS implementation of a HiDiC model as a gO:CapeOpenUnit in AspenPlus
- Modelling of a heat integrated distillation column (HiDiC) using the Gas-to-Liquid (GLC) library
- Export of a gPROMS model to a gO:CapeOpenUnit

Introduction: Heat integrated distillation columns

Conventional distillation column



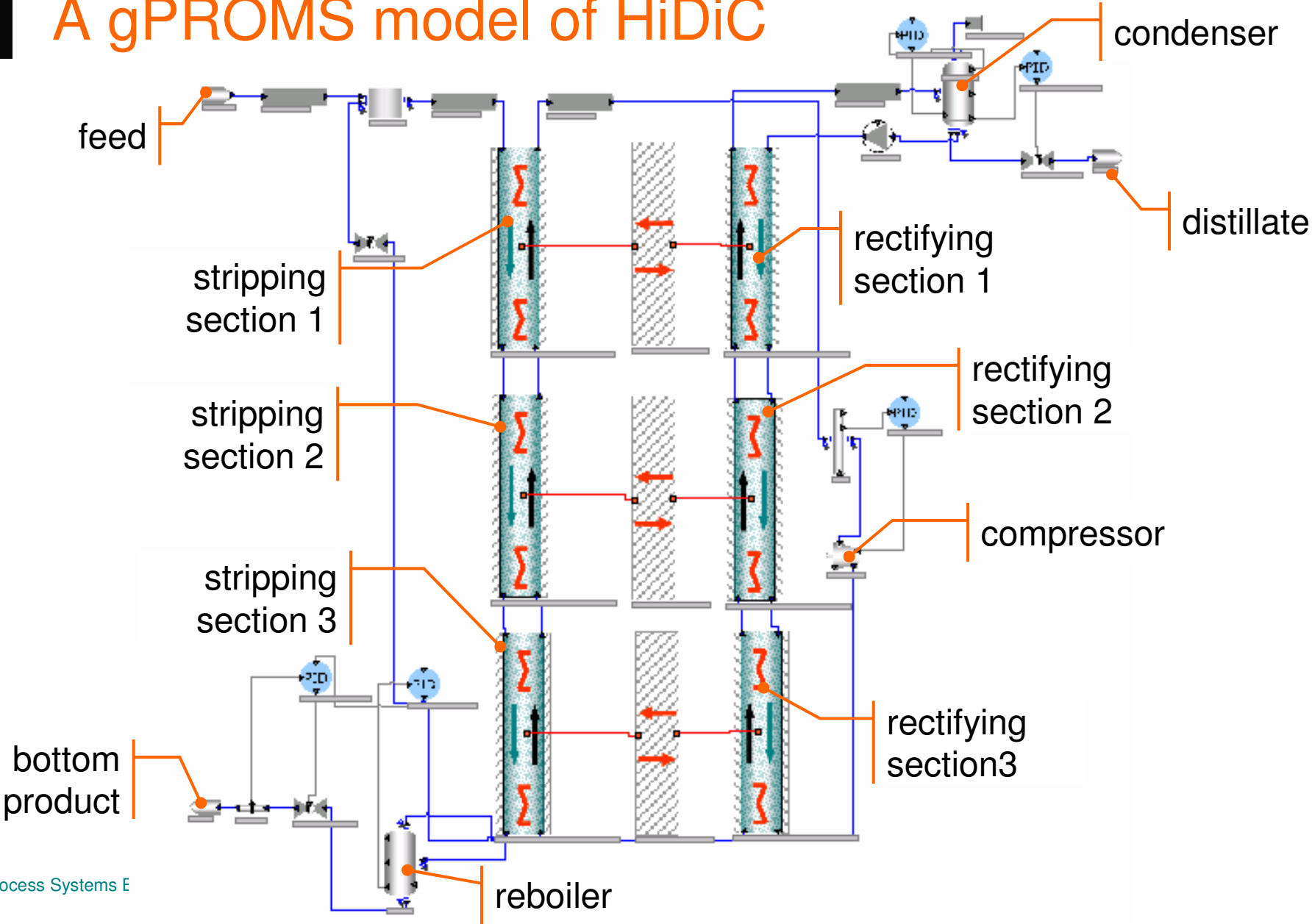
Heat-Integrated Distillation Column



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

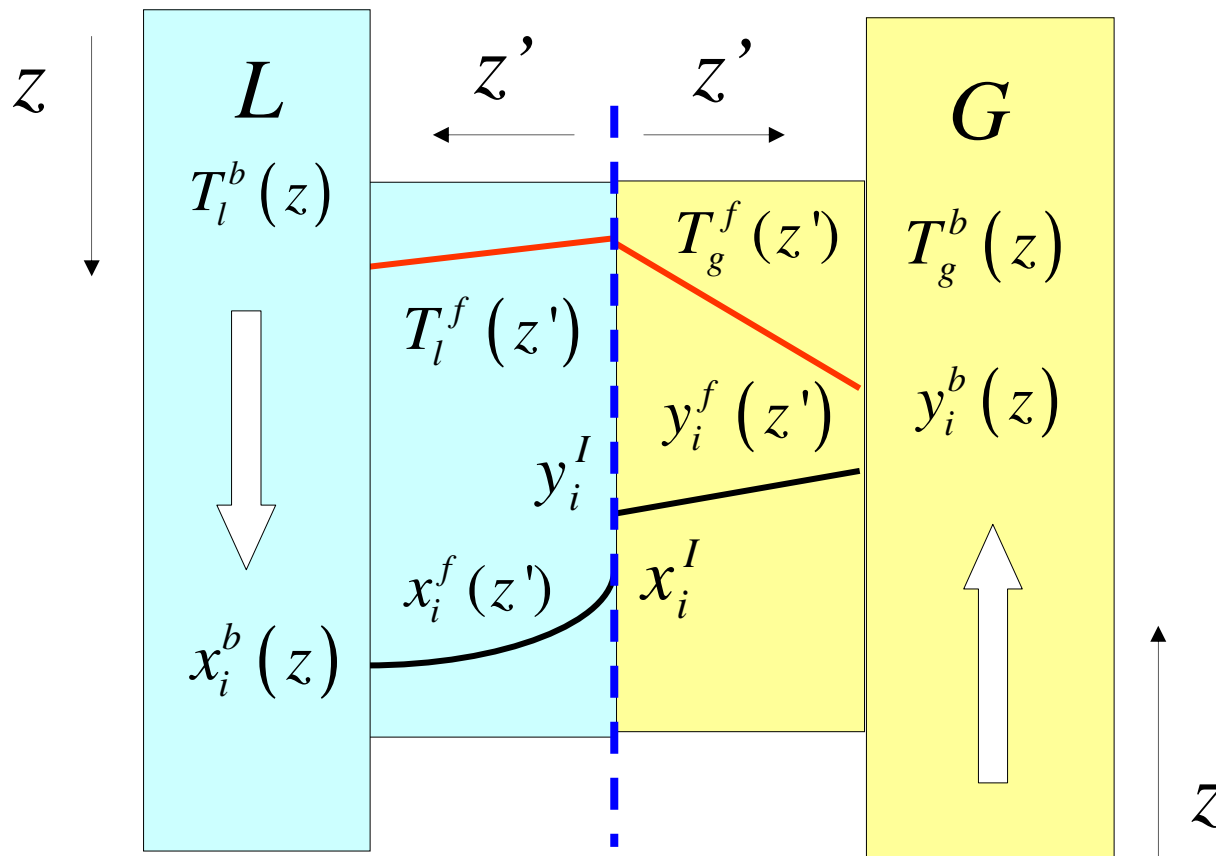
Modelling of a HiDiC column using the GLC library

- 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

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

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

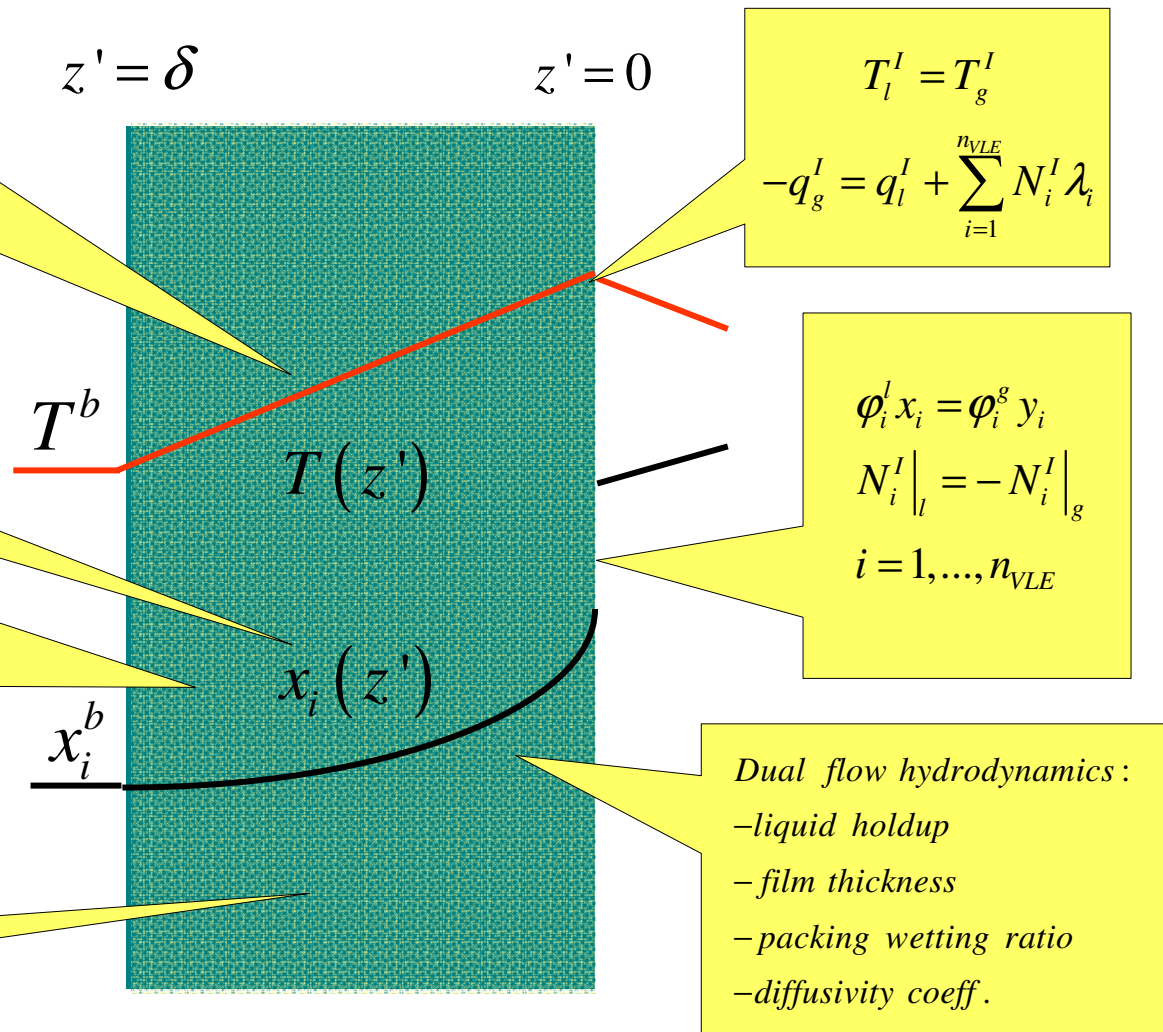
$$\frac{dx_i}{dz'} = \sum_{\substack{k=1 \\ k \neq i}}^{n_l} \frac{x_i N_k - x_k N_i}{c_t D_{ik}}$$

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

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

$z' = \delta$

$z' = 0$



$$T_l^I = T_g^I$$

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

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

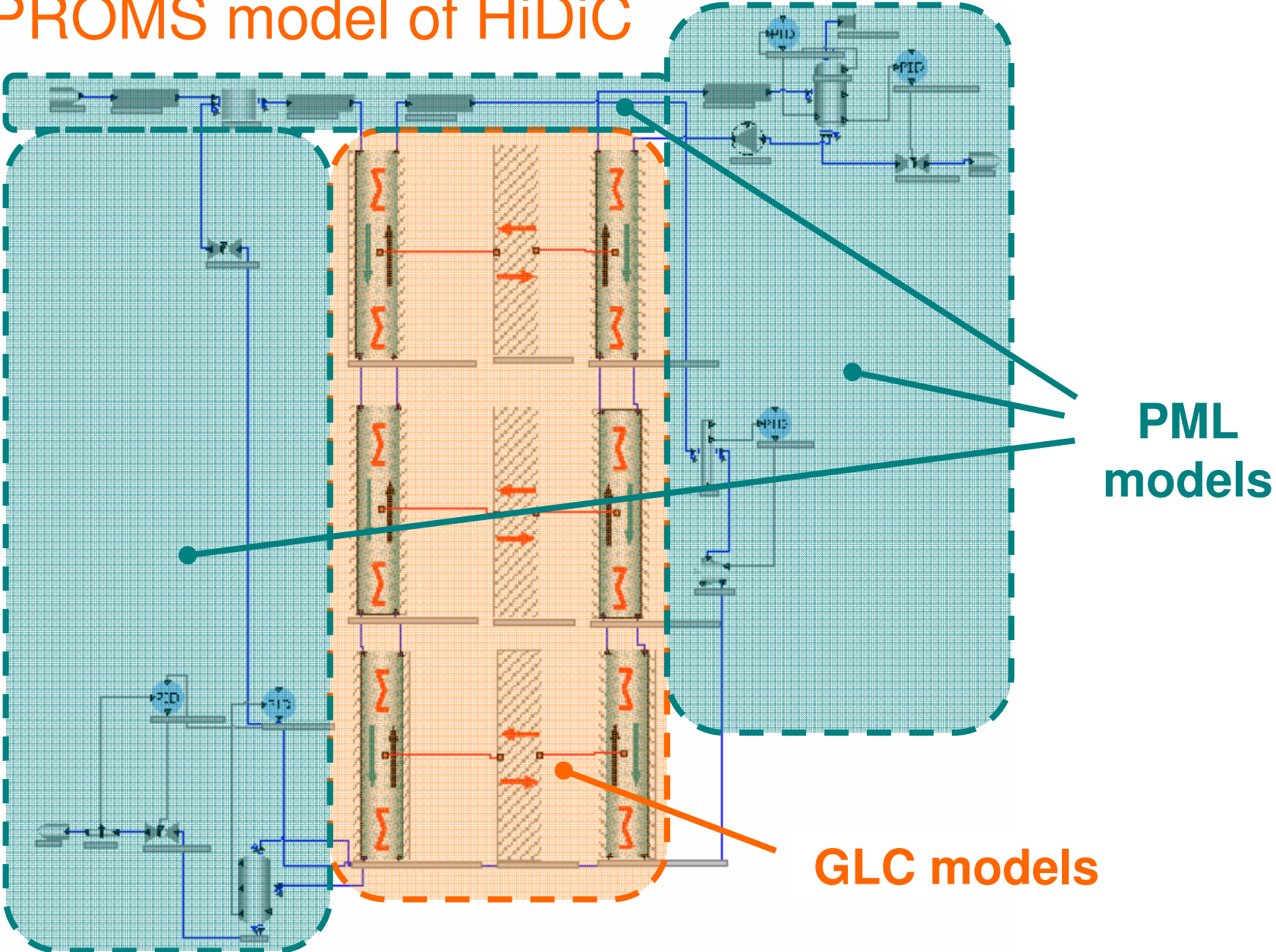
$$N_i^I|_l = -N_i^I|_g$$

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

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 !