ADVANCED PROCESS MODELLING FORUM 2017
London 25–26 April

gPROMS ProcessBuilder 1.2

New capabilities for modelling of catalytic reactors

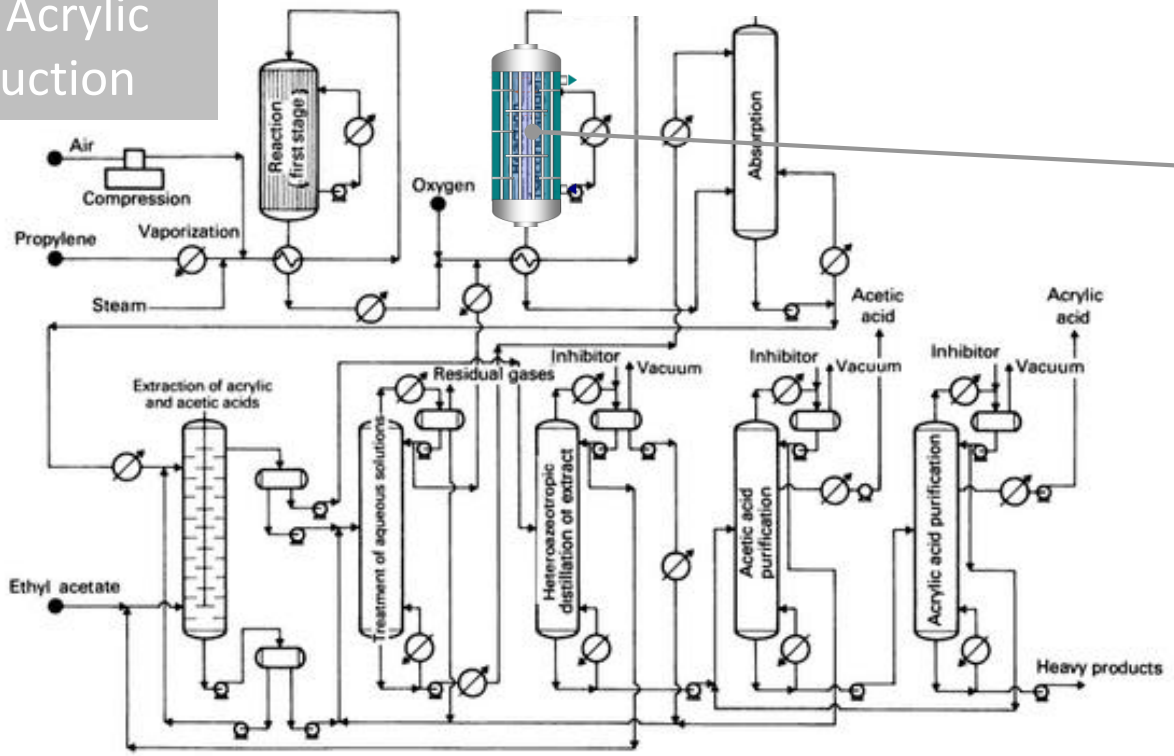
Vasco Manaças – Consultant Engineer

Multitubular reactors

Why are they important?

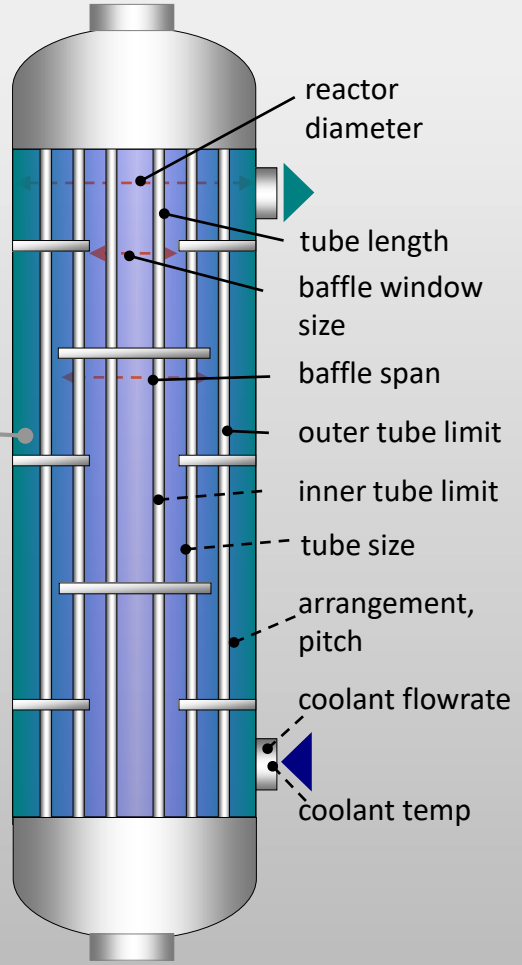
- Often at the heart of the process
- Complex multitubular reactor (MTR)
  - 10,000-20,000 catalyst-filled tubes
  - Many internal design decisions

Example: Acrylic acid production



Multitubular reactor

Key design variables



Ref: Petrochemical Processes – *Alain Chauvel, Gilles Lefebvre*

The multi-scale challenge

Reactor units

10s of m

Radial heat transport within a tube

cm/in

Reaction and mass transport within a catalyst pellet

mm - µm

What happens at micron-scale affects plant-scale!

Catalytic reactors and PSE

Reactions / products

Acrylic Acid/Acrolein

Fluid Catalytic Cracking

Propane Dehydrogenation

Dimethyl sulphide

Reforming

Propylene Oxide

Methanol

Hydrocracking

p-diiodobenzene

Vinyl Acetate Monomer

Styrene monomer

Fischer-Tropsch

Maleic anhydride

Terephthaldehyde

Phthalic anhydride

Customers

Arkema (FR)

SK Chemicals (KR)

LG Chem (KR)

REPSOL YPF (ES)

Clariant (Süd-Chemie) (DE)

Samsung-BP Chemicals (KR)

Shell (NL)

BP Chemicals (US)

IDESA (MX)

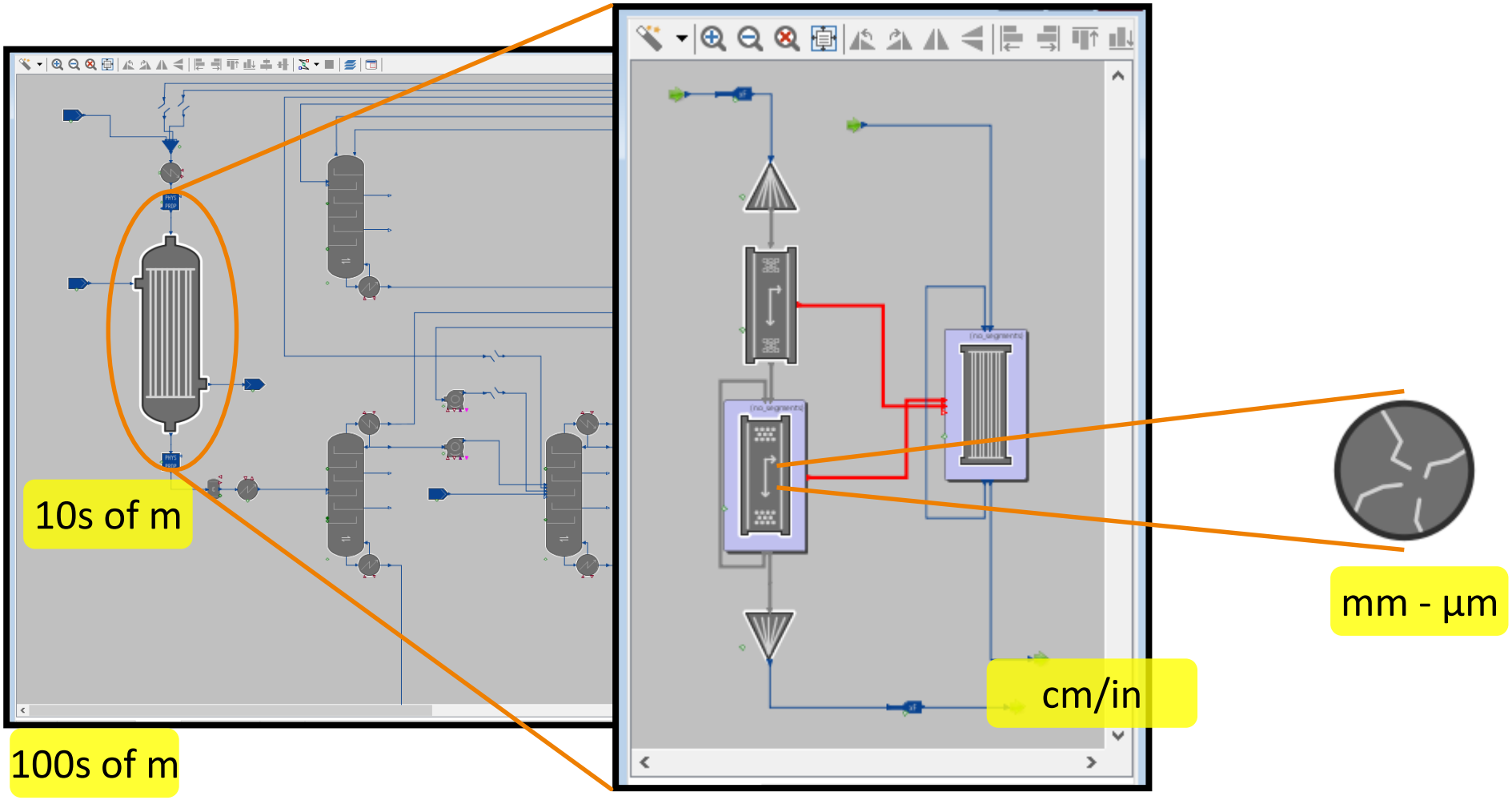
BP (UK)

SCG Chemicals (T)

SABIC (SA)

Hunt Refining (US)

The solution in gPROMS ProcessBuilder 1.2.0



Detailed reactors in a ProcessBuilder flowsheet

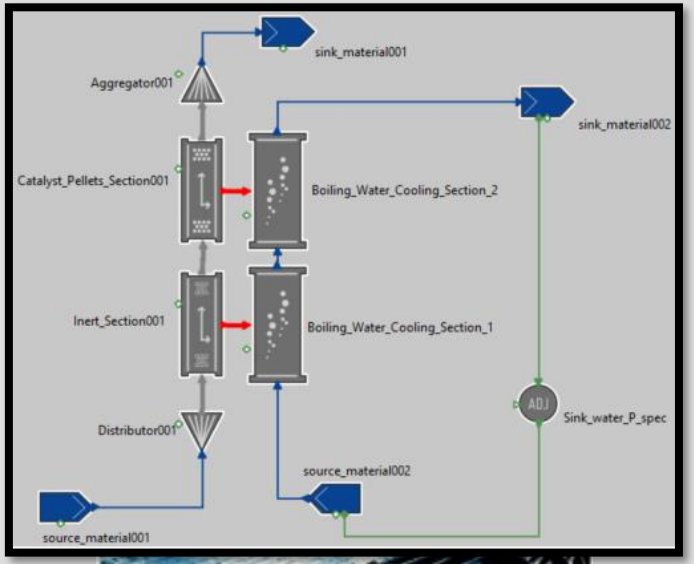
gPROMS ProcessBuilder 1.2.0

Product formulation

- Key features
  - Comprehensive set of model libraries
    - gML Process
    - gML Olefins (NEW in gPROMS ProcessBuilder 1.2.0)
    - gML Water (NEW in gPROMS ProcessBuilder 1.2.0)
    - gML Utilities (NEW in gPROMS ProcessBuilder 1.2.0)
    - AML:FBCR (UPGRADED in gPROMS ProcessBuilder 1.2.0)
    - AML:TBR (NEW in gPROMS ProcessBuilder 1.2.0)
    - AML:GLC (NEW in gPROMS ProcessBuilder 1.2.0)
    - gML Oilfield (Upcoming in ProcessBuilder 1.3.0)
    - gML Power (Upcoming in ProcessBuilder 1.3.0)
  - Built on gPROMS platform 5.0.0
  - Materials modelling
    - Multiflash + DIPPR
    - gSAFT
  - online help, reference examples, workflow guides, training videos, training courses

AML:FBCR – an overview

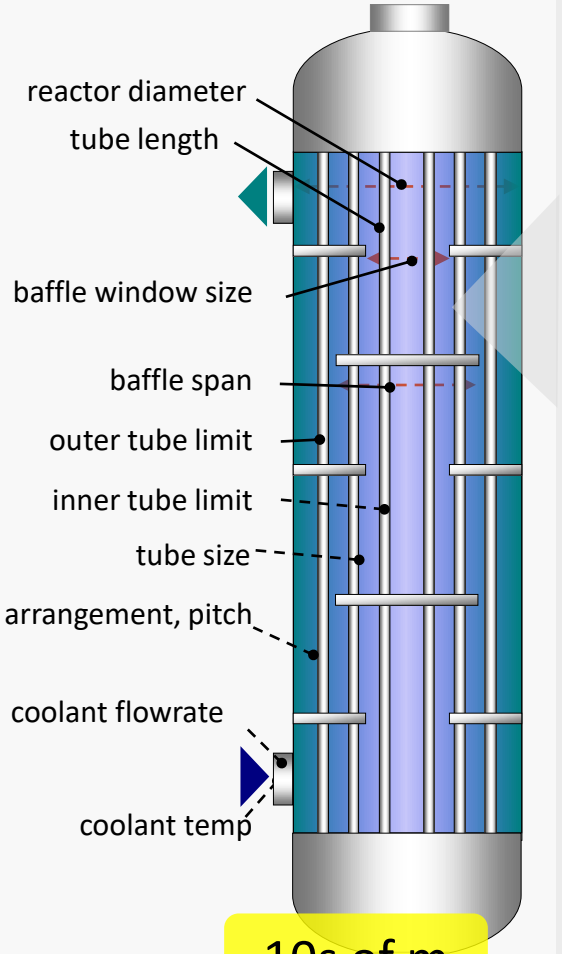
- High fidelity models for
  - Fixed bed catalytic reactors
  - Single phase systems
- Applications
  - Gas or liquid phase reactions
    - Styrene, Methanol, Reforming, …
- Key improvements
  - Liquid phase (NEW in gPROMS ProcessBuilder 1.2.0)
- Modular library
  - Configure model with preferred complexity and detail
  - Multiple configurations available



The Advanced Model Library approach

Reactor unit

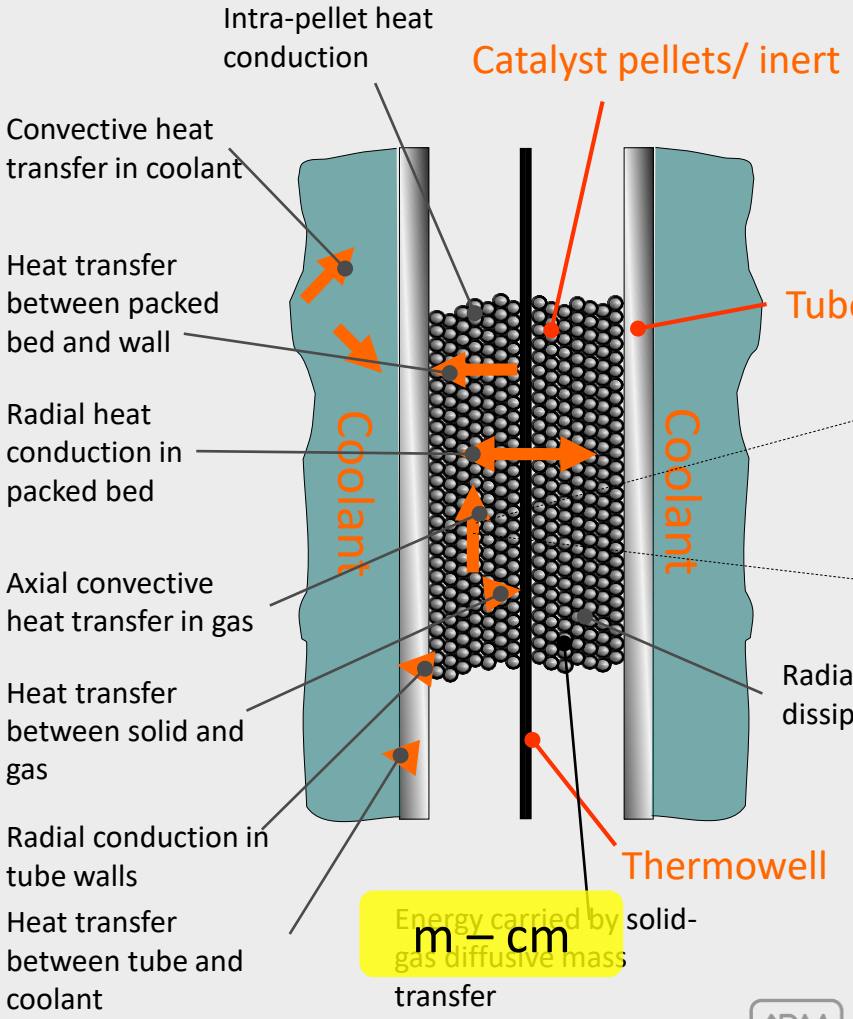
Design variables



10s of m

Tube

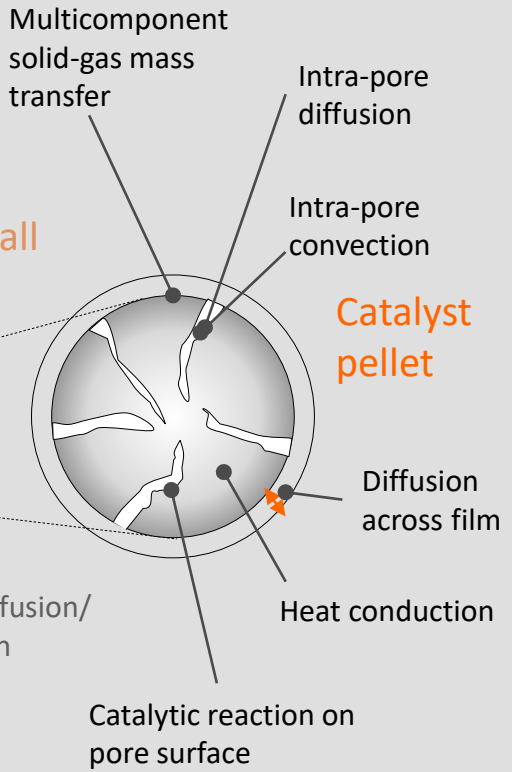
Bed heat and mass transfer phenomena



m – cm

Catalyst pellet

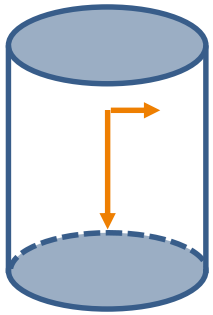
Heat and mass transfer phenomena



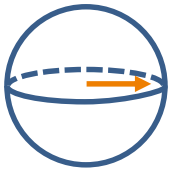
µm

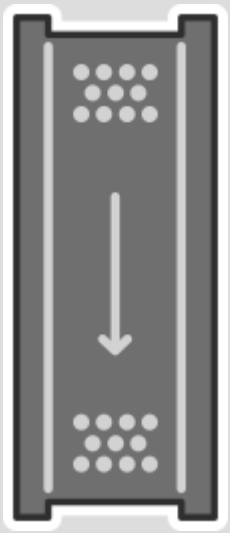
Contents: Axial flow

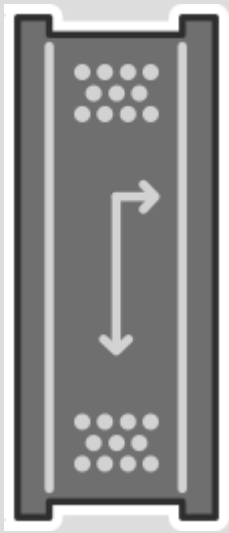
- Detail in packed bed
  - 1D: Axial
  - 2D: Axial and radial



- Detail in pellet
  - Lumped (effectiveness factor)
  - Distributed (intra-particle)

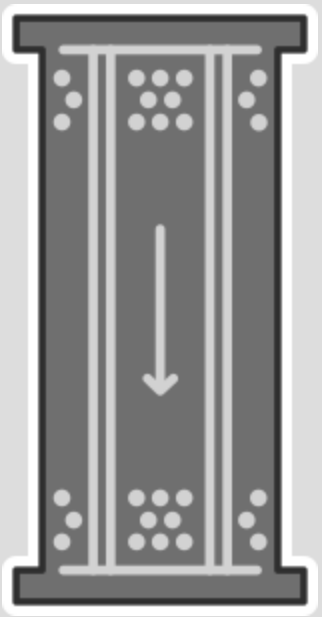






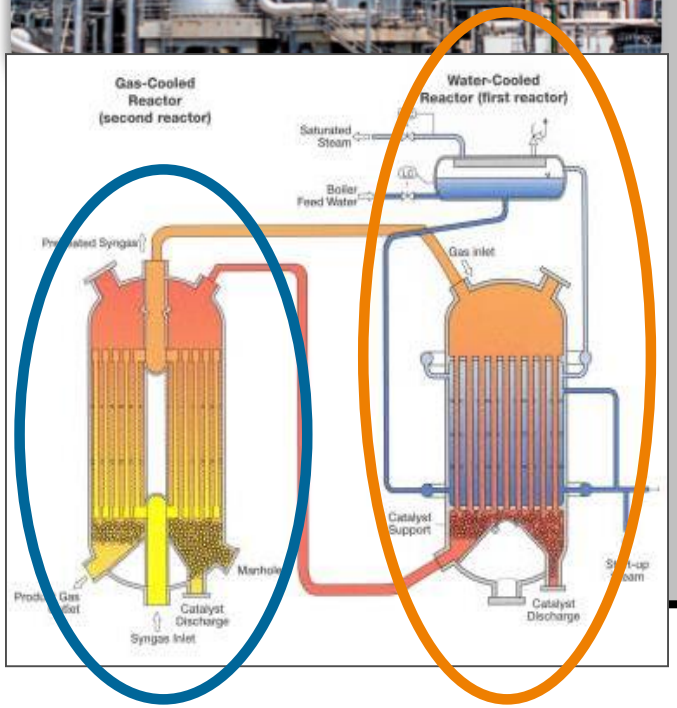
Contents: Axial flow – Gas cooled bed

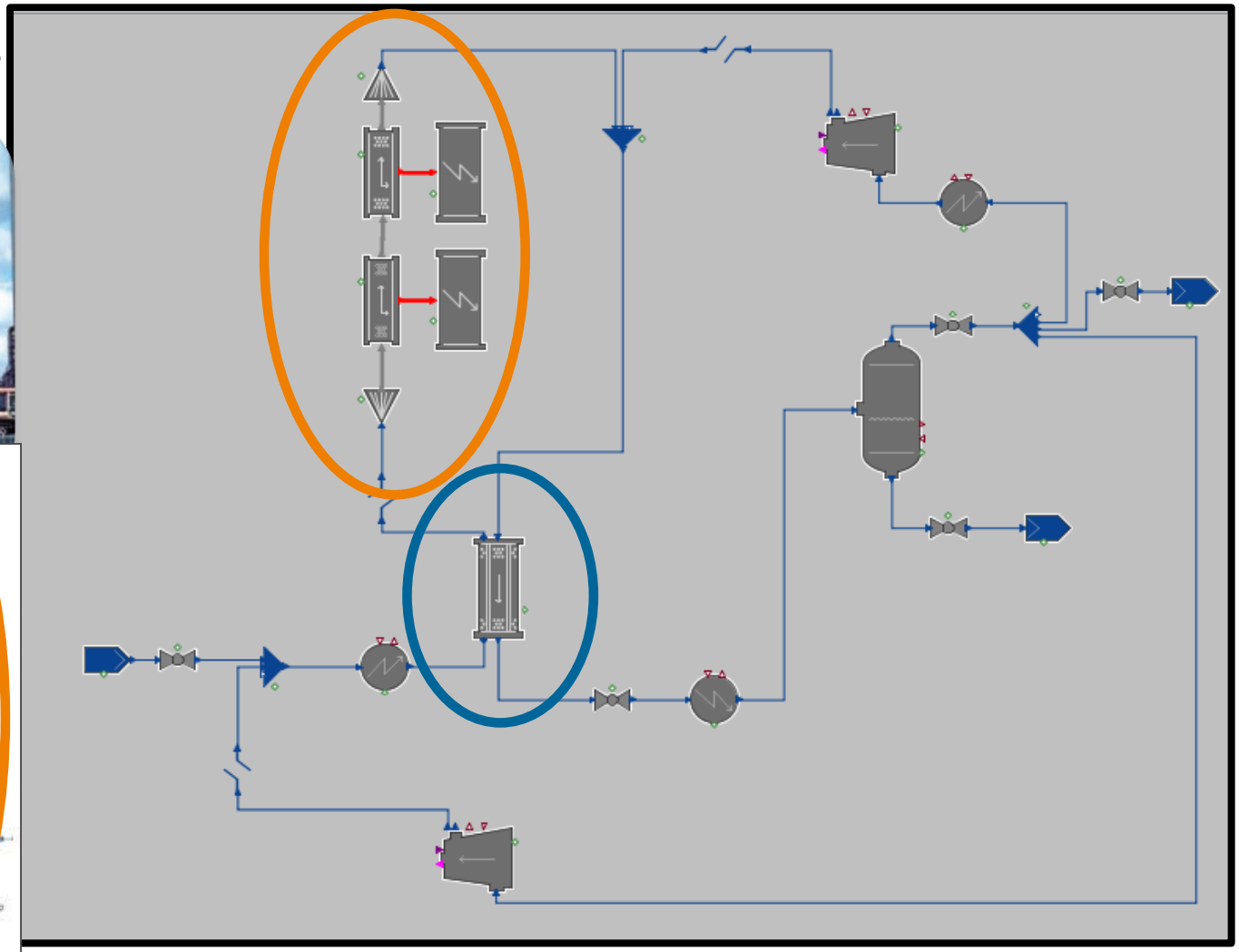
- Detail in packed bed
  - 1D: Axial
- Detail in pellet
  - Lumped (effectiveness factor)
  - Distributed (intra-particle)
- Different configuration
  - Catalyst on shell side
  - Coolant on tube side



Axial flow example: Methanol production

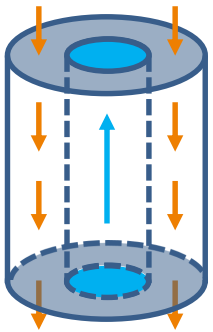
Lurgi MegaMethanol®

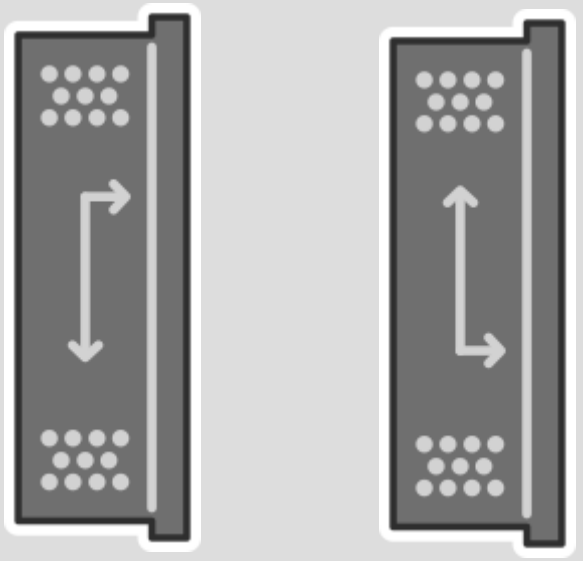




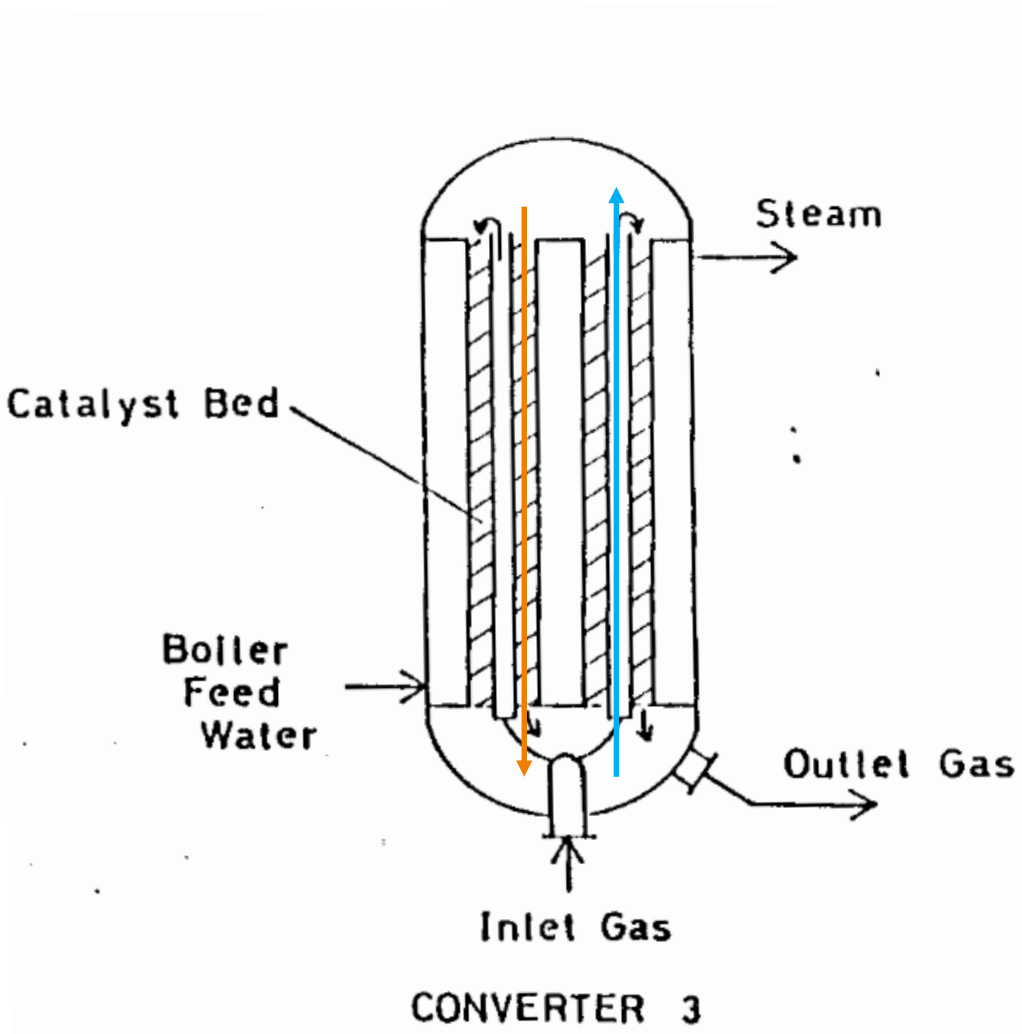
Contents: Axial annular flow

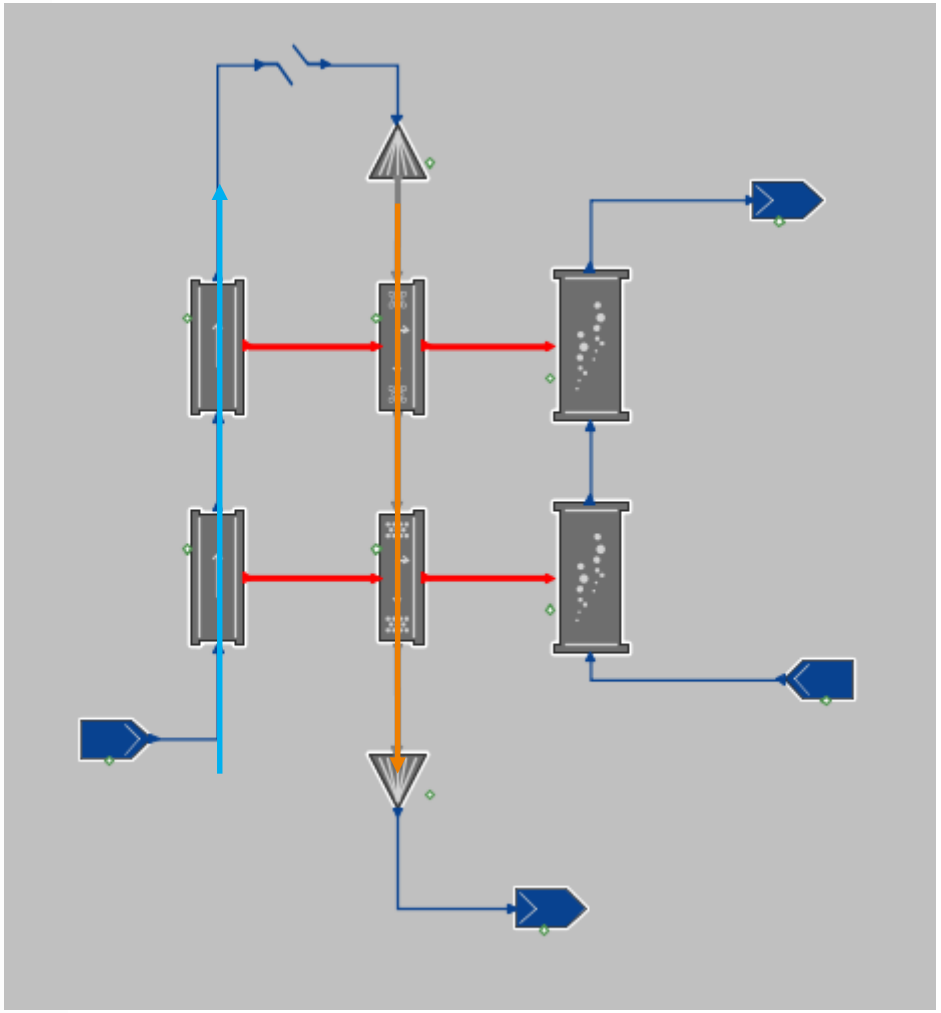
- Detail in packed bed
  - 2D: Axial and radial
  - Different flow directions
- Detail in pellet
  - Lumped (effectiveness factor)
  - Distributed (intra-particle)





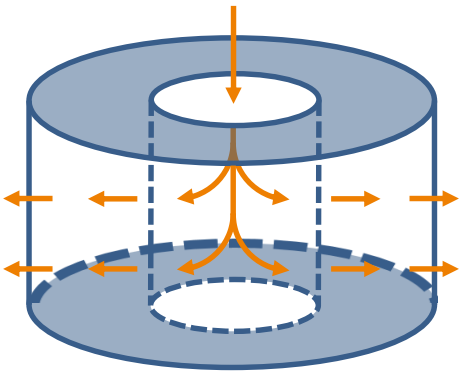
Radial flow example: Methanol SuperConverter

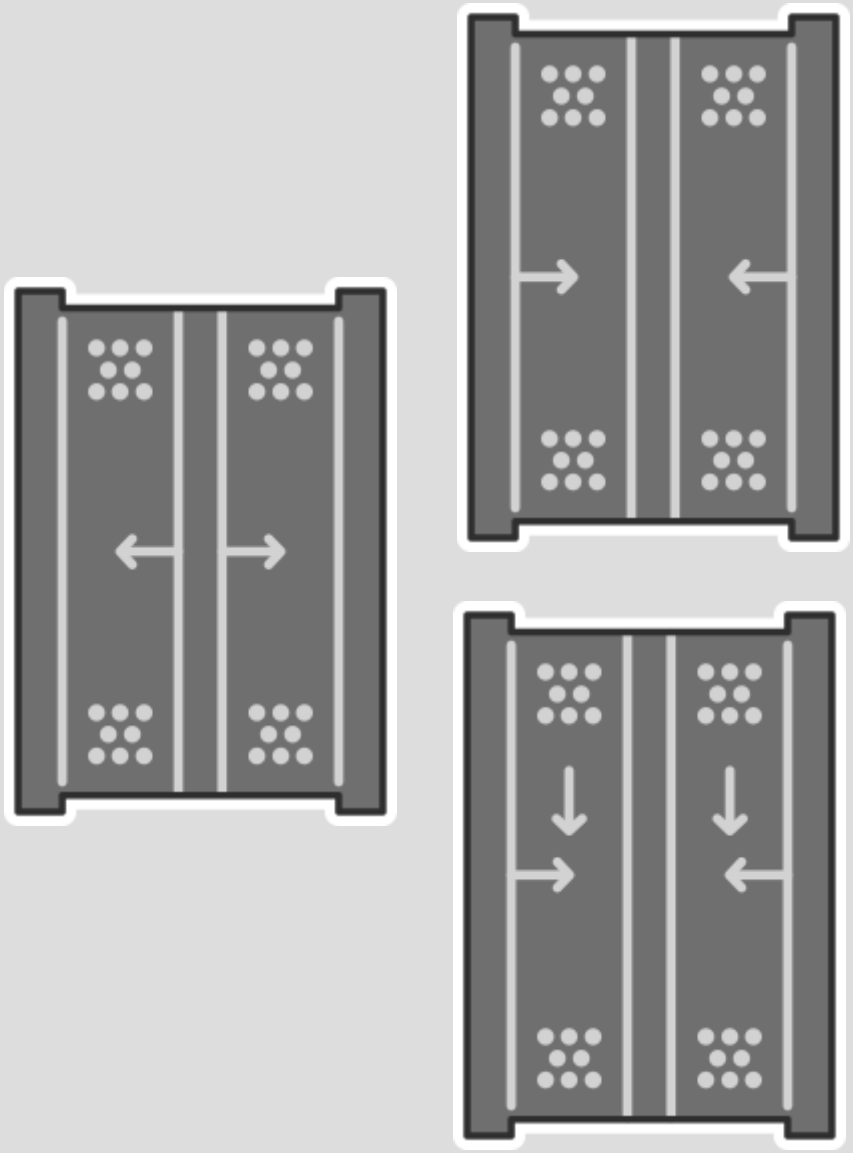




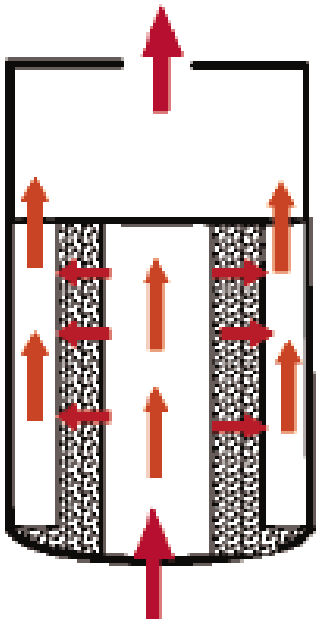
Contents: Radial flow reactor

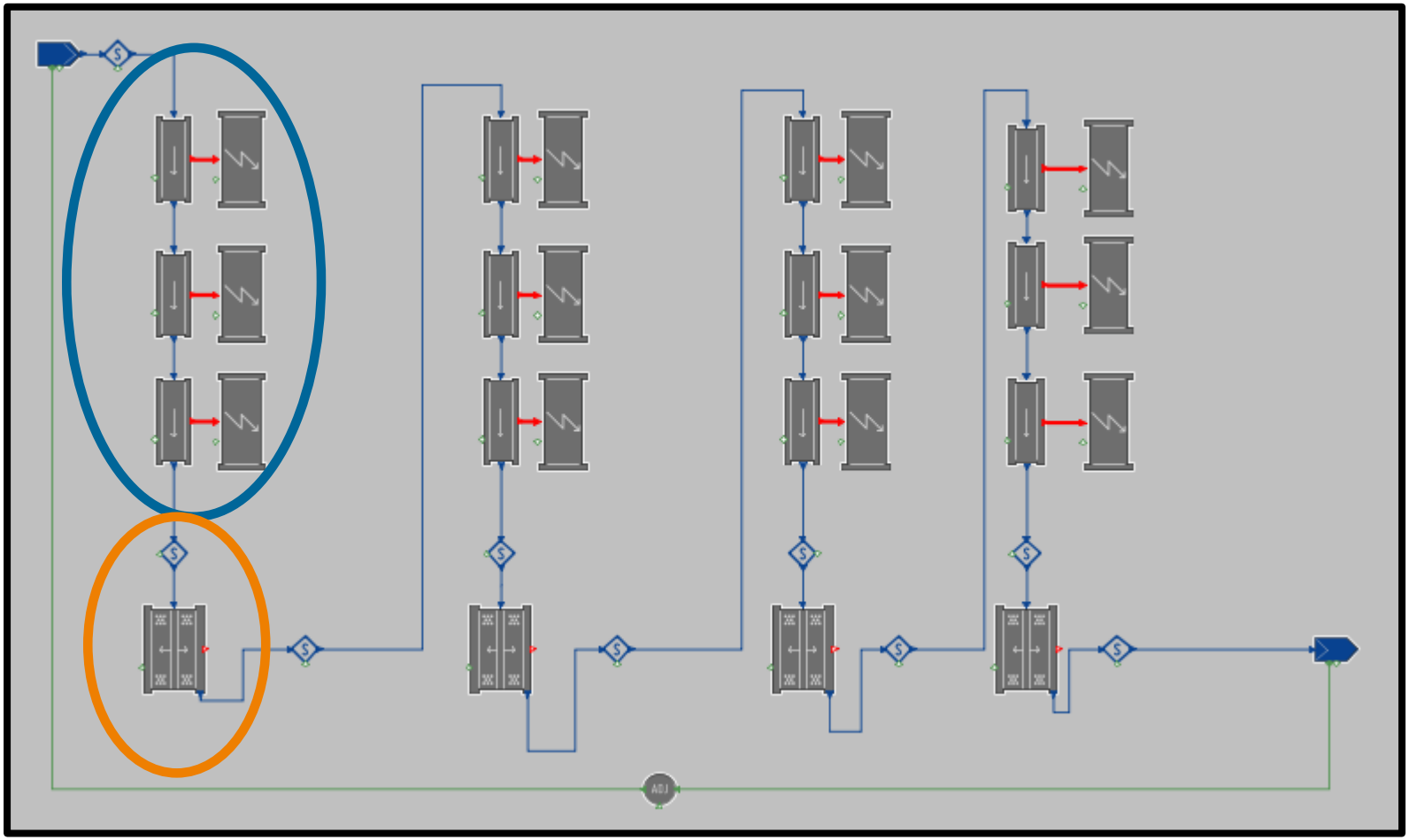
- Detail in packed bed
  - 2D: Radial and axial
  - Different flow directions
- Detail in pellet
  - Lumped (effectiveness factor)
  - Distributed (intra-particle)





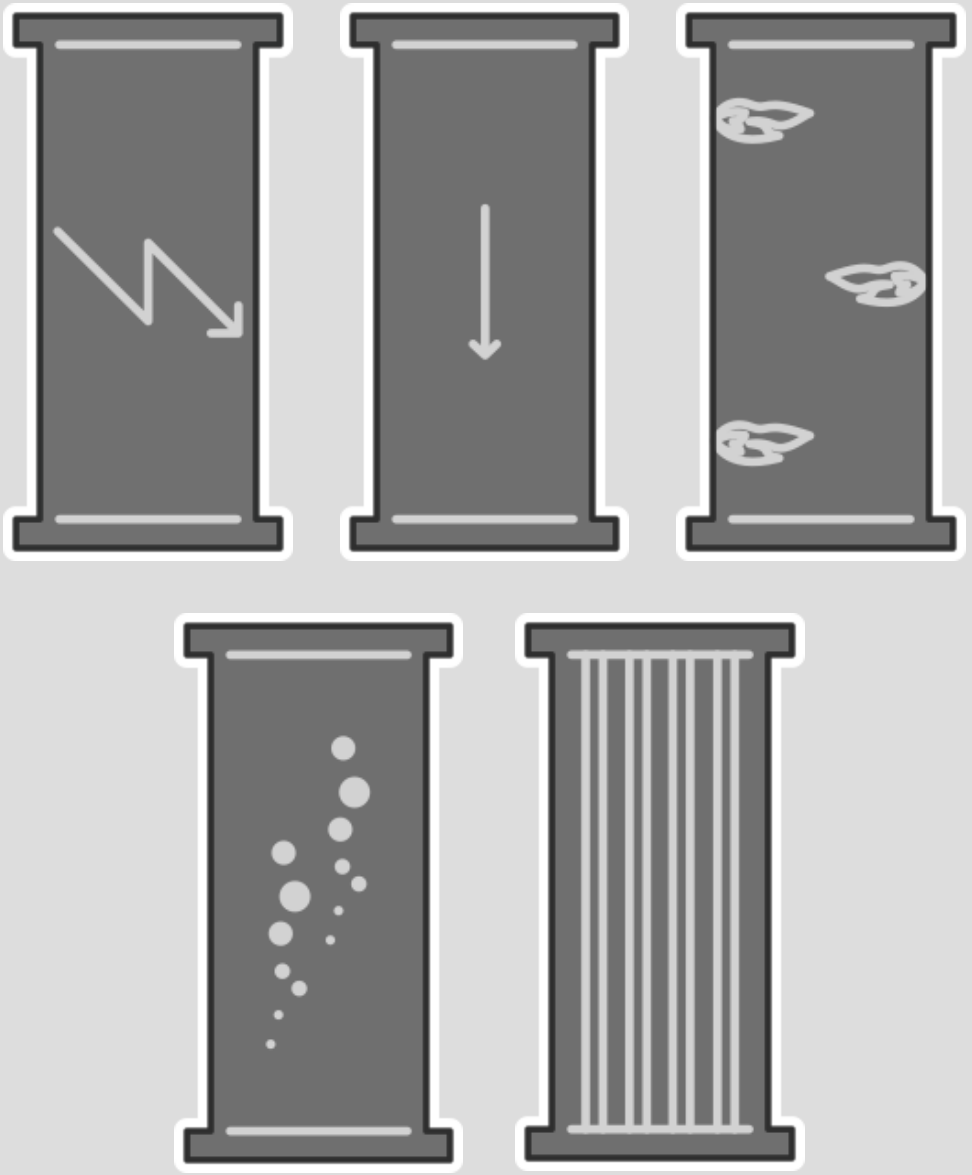
Radial flow example: Propane Dehydrogenation





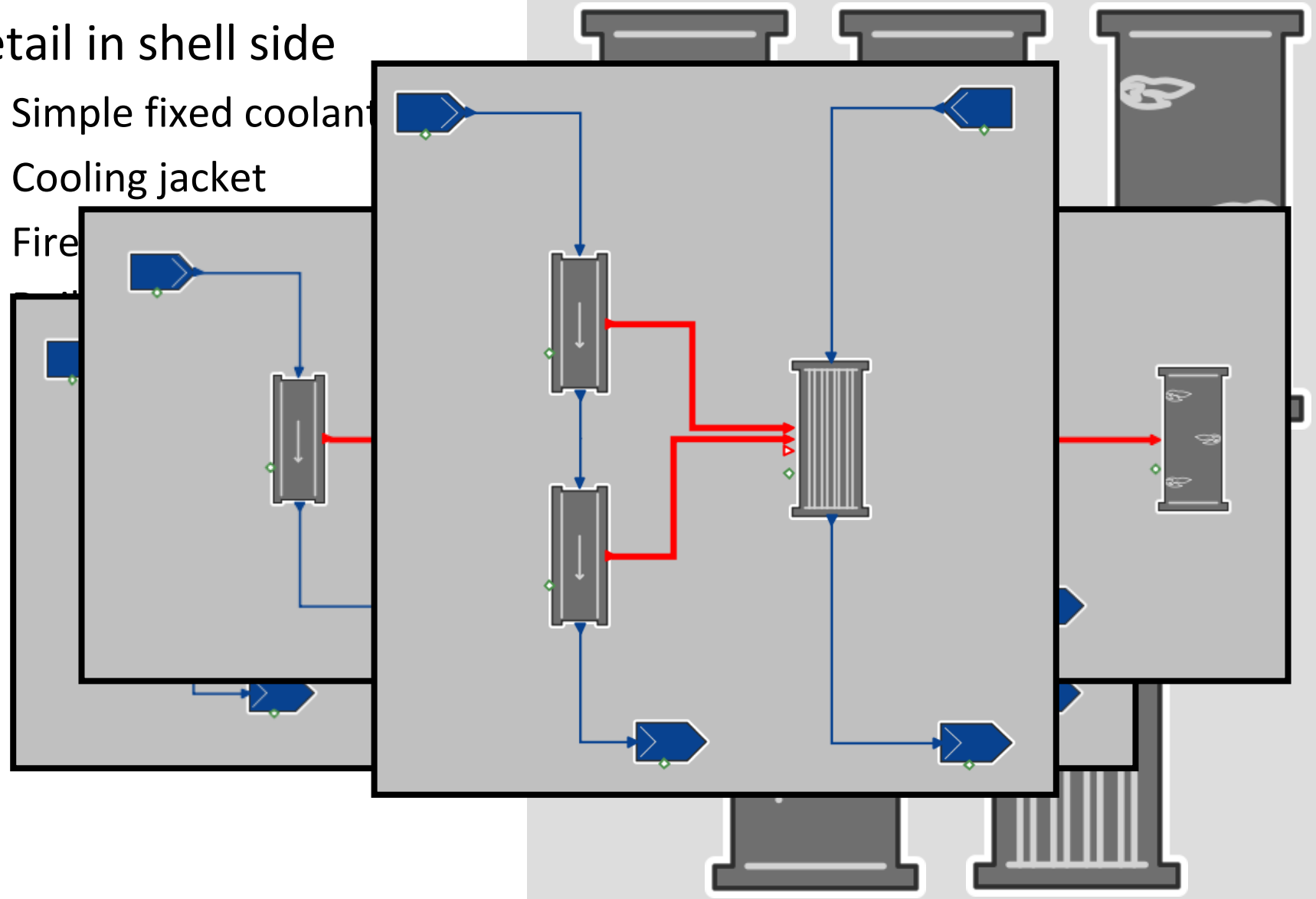
Contents: Cooling system

- Detail in shell side
  - Simple fixed coolant
  - Cooling jacket
  - Fired heater
  - Boiling water
  - Multitubular cooling compartment



Contents: Cooling system

- Detail in shell side
  - Simple fixed coolant
  - Cooling jacket
  - Fire
  -
  -



gPROMS ProcessBuilder 1.2.0

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  - Built on gPROMS platform 5.0.0
  - Materials modelling
    - Multiflash + DIPPR
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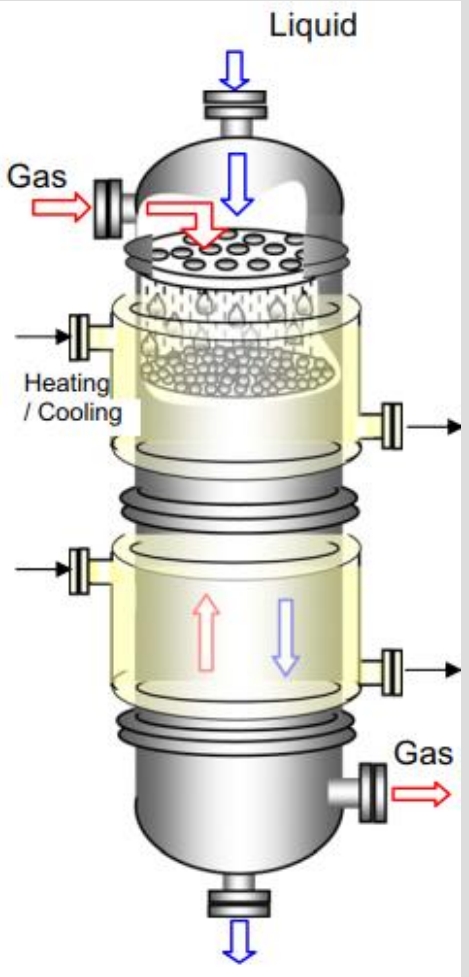
  - online help, reference examples, workflow guides, training videos, training courses

Trickle Bed Reactors

- Gas – Liquid – Solid contactors
  - Fixed bed of catalyst pellets
  - Gas-Liquid flow

- Challenges
  - Vapour liquid equilibrium
  - Hydrodynamics
  - Liquid holdup
  - Pressure drop
  - Mass and heat transfer
  - Catalyst exposed to gas and liquid



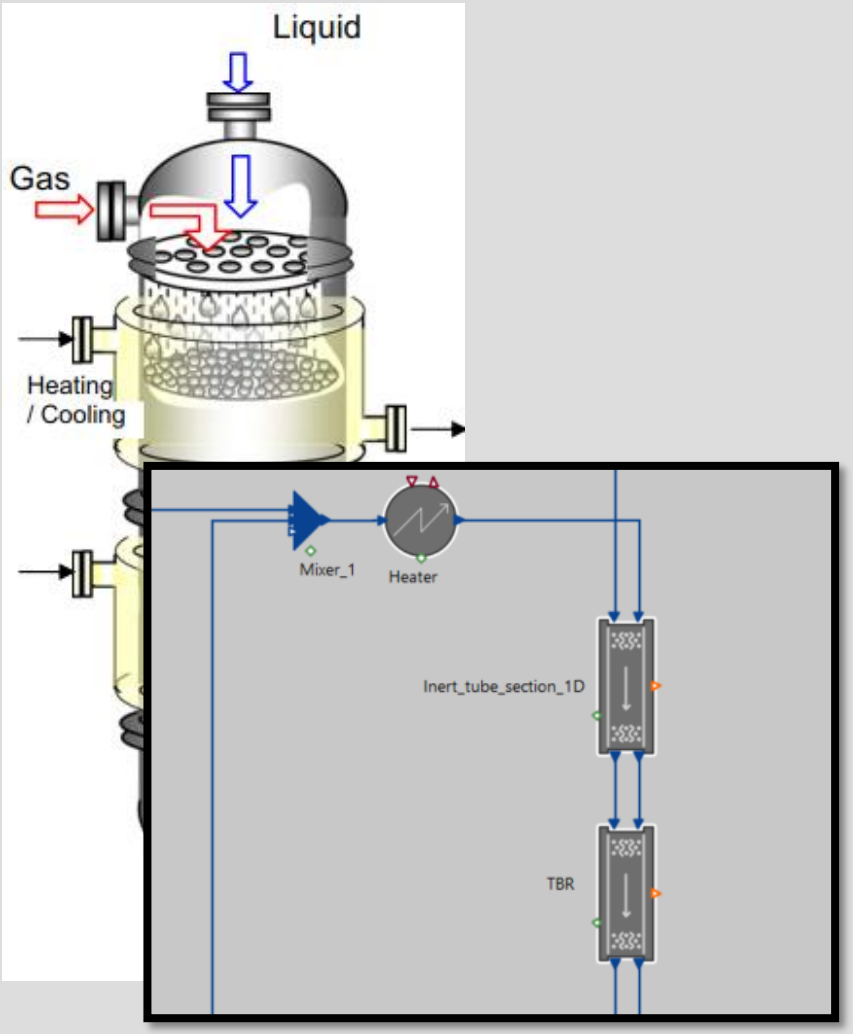
Jacketed TBR

(adapted from Ranade et al., Elsevier 2011)

gPROMS ProcessBuilder 1.2.0

AML:TBR (NEW in ProcessBuilder 1.2.0)

- High fidelity models for
  - Trickle bed catalytic reactors
- Applications
  - Refining
  - Petrochemicals
  - Fine chemicals
  - Biochemicals
- Processes
  - Hydrogenation
  - Oxidation
  - Fischer-Tropsch synthesis
- Modular library
  - Different reactor configurations
  - Different level of detail



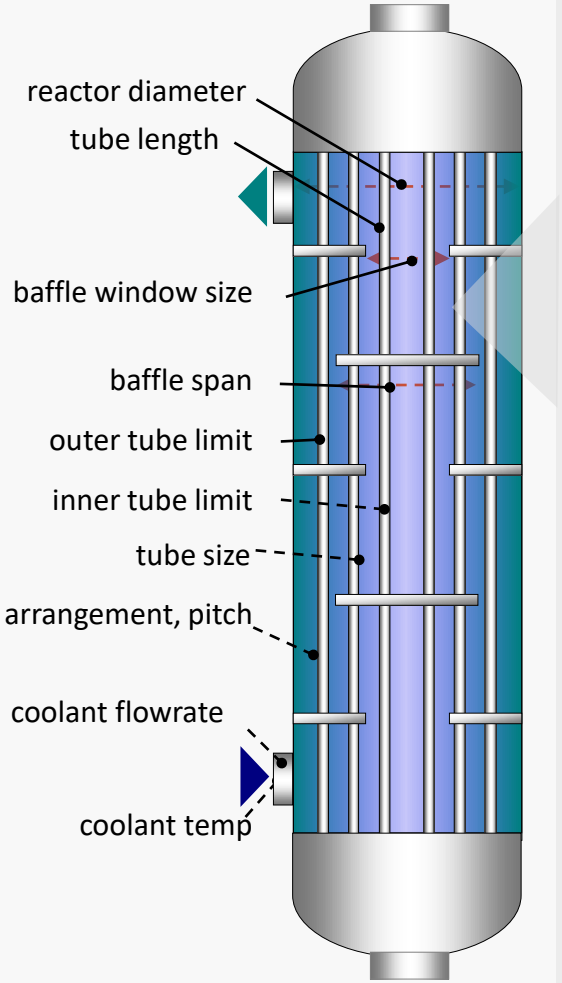
Jacketed TBR

(adapted from Ranade et al., Elsevier 2011)

The Advanced Model Library approach

Reactor unit

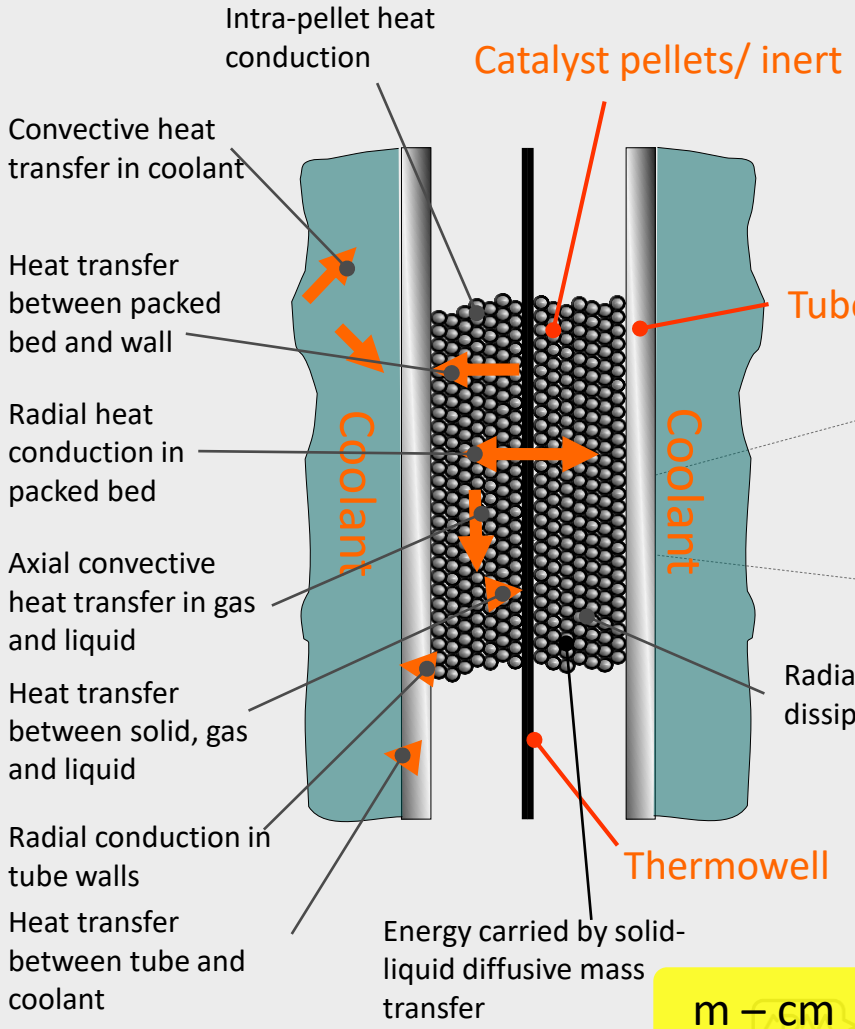
Design variables



10s of m

Tube

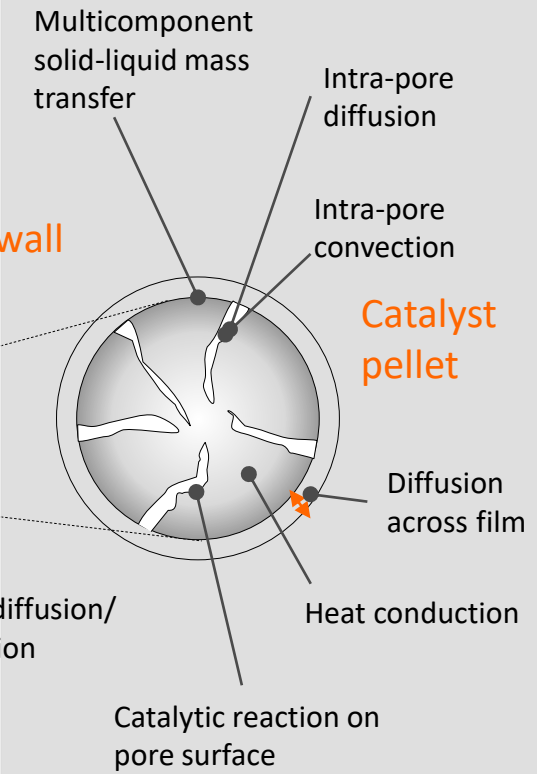
Bed heat and mass transfer phenomena



m – cm

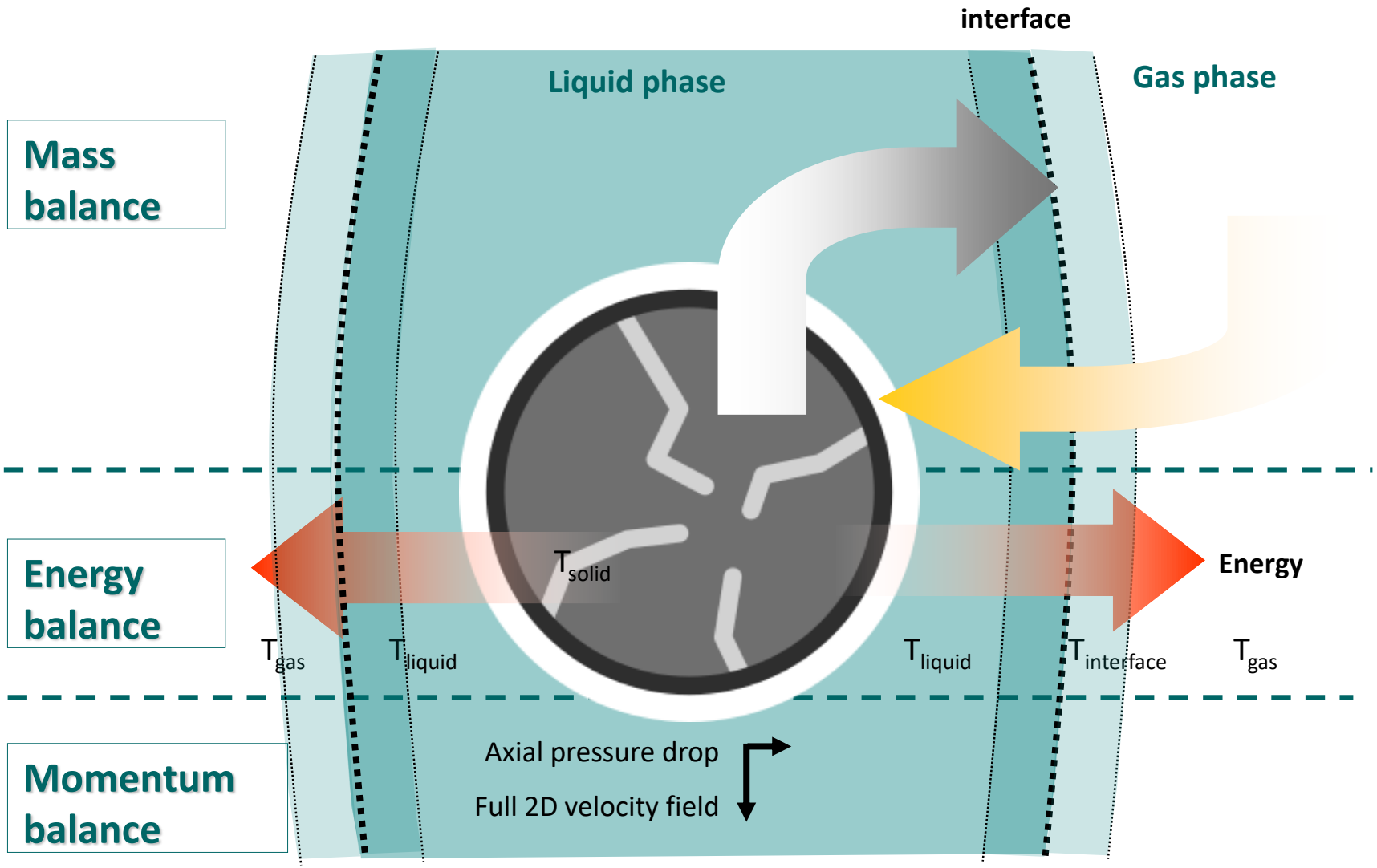
Catalyst pellet

Heat and mass transfer phenomena

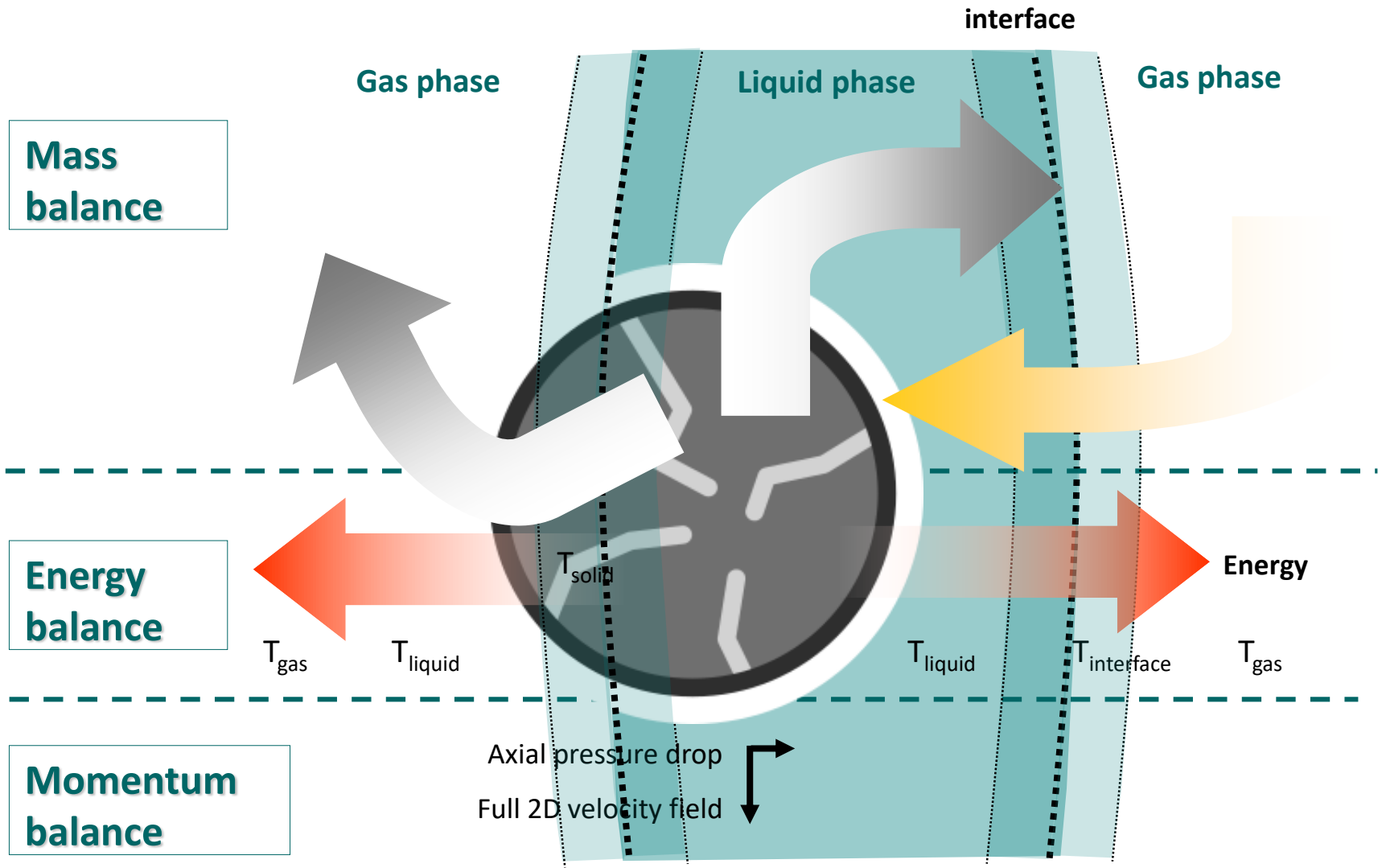


µm

AML:TBR – Transport phenomena between phases

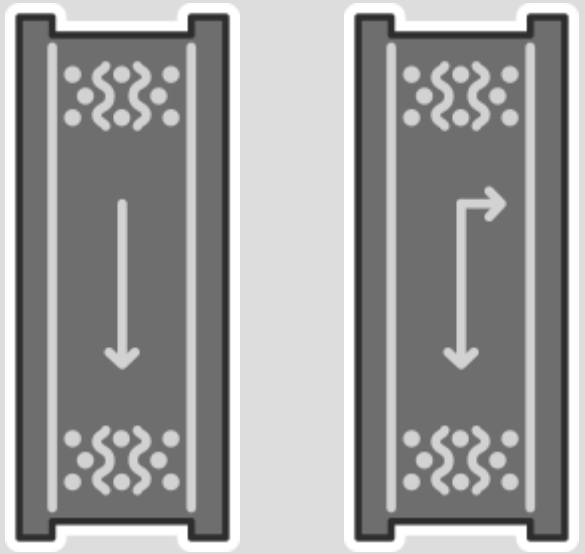


AML:TBR – Transport phenomena between phases



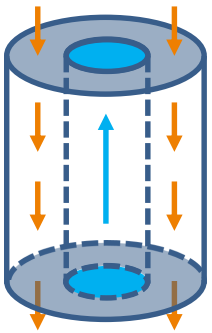
Contents: Axial flow

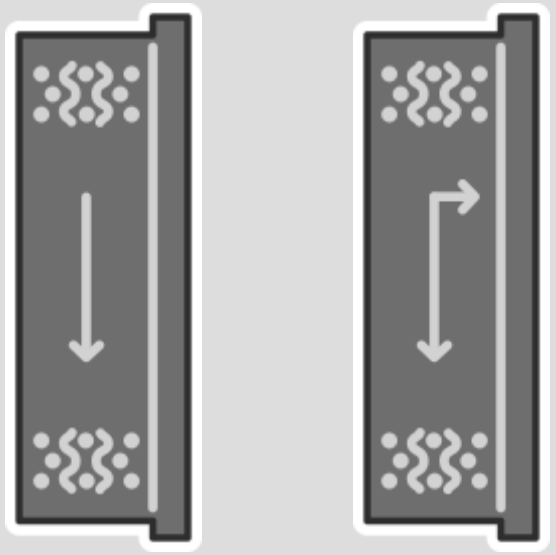
- Detail in pellet
  - Lumped (effectiveness factor)
  - Distributed (intra-particle)
- Detail in packed bed
  - 1D: Axial
  - 2D: Axial and radial



Contents: Axial annular flow

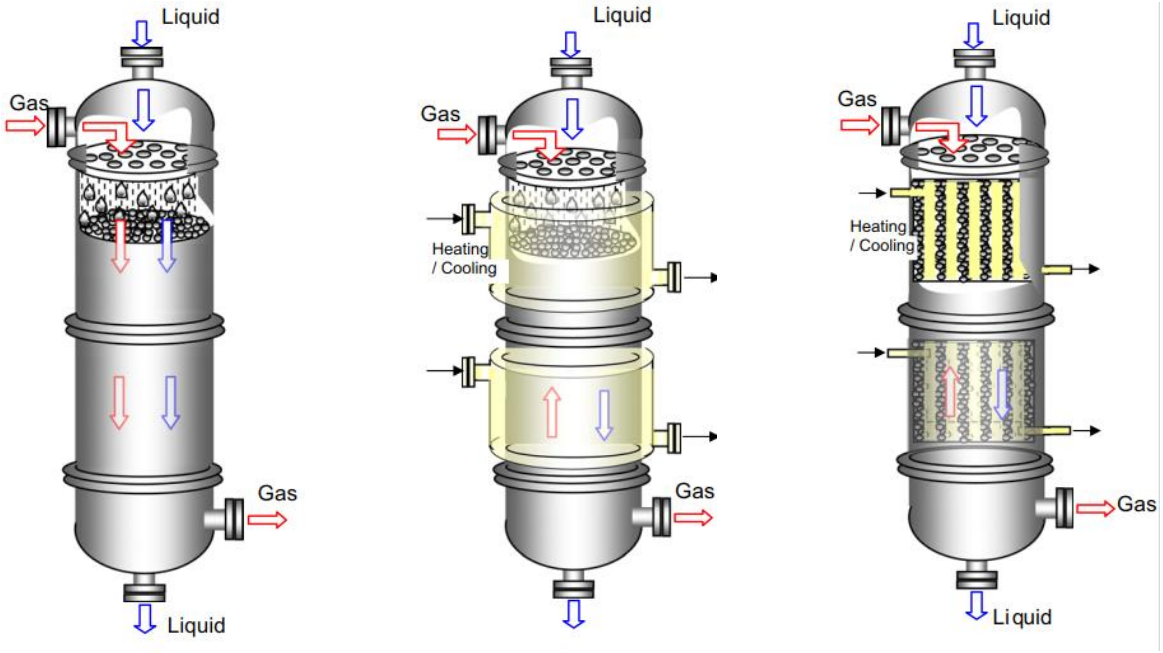
- Detail in pellet
  - Lumped (effectiveness factor)
  - Distributed (intra-particle)
- Detail in packed bed
  - 1D: Axial
  - 2D: Axial and radial
  - Different flow directions





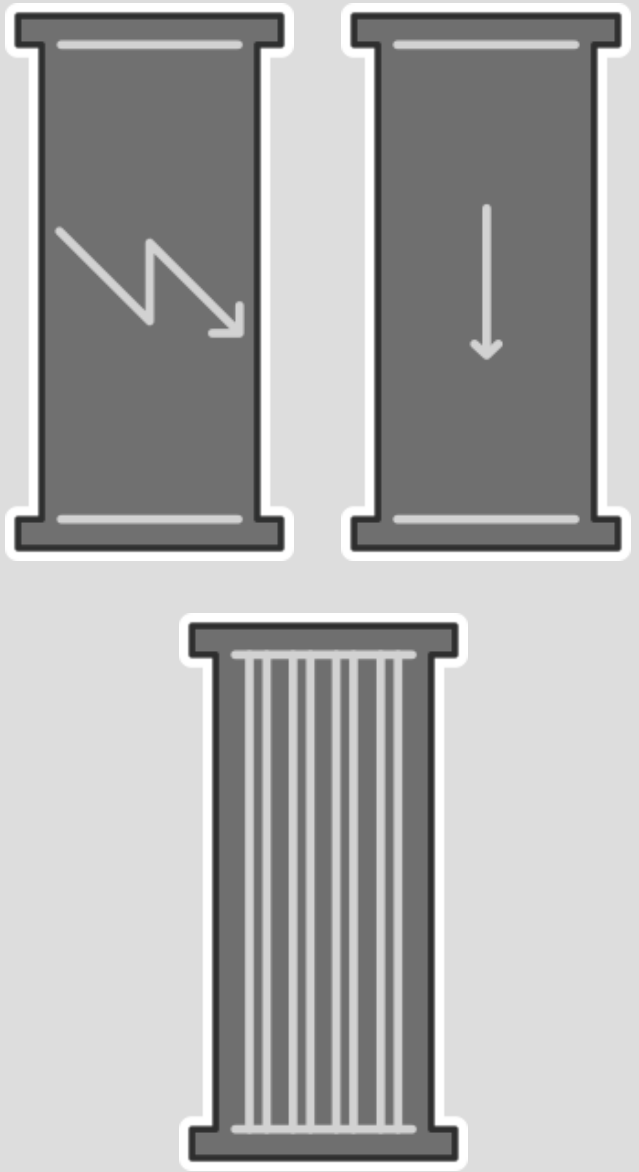
Contents: Heat Exchange

- Detail in shell side
  - Simple fixed coolant
  - Cooling jacket
  - Multitubular cooling compartment



Adiabatic / Jacketed / Internally cooled TBR

(adapted from Ranade et al., Elsevier 2011)



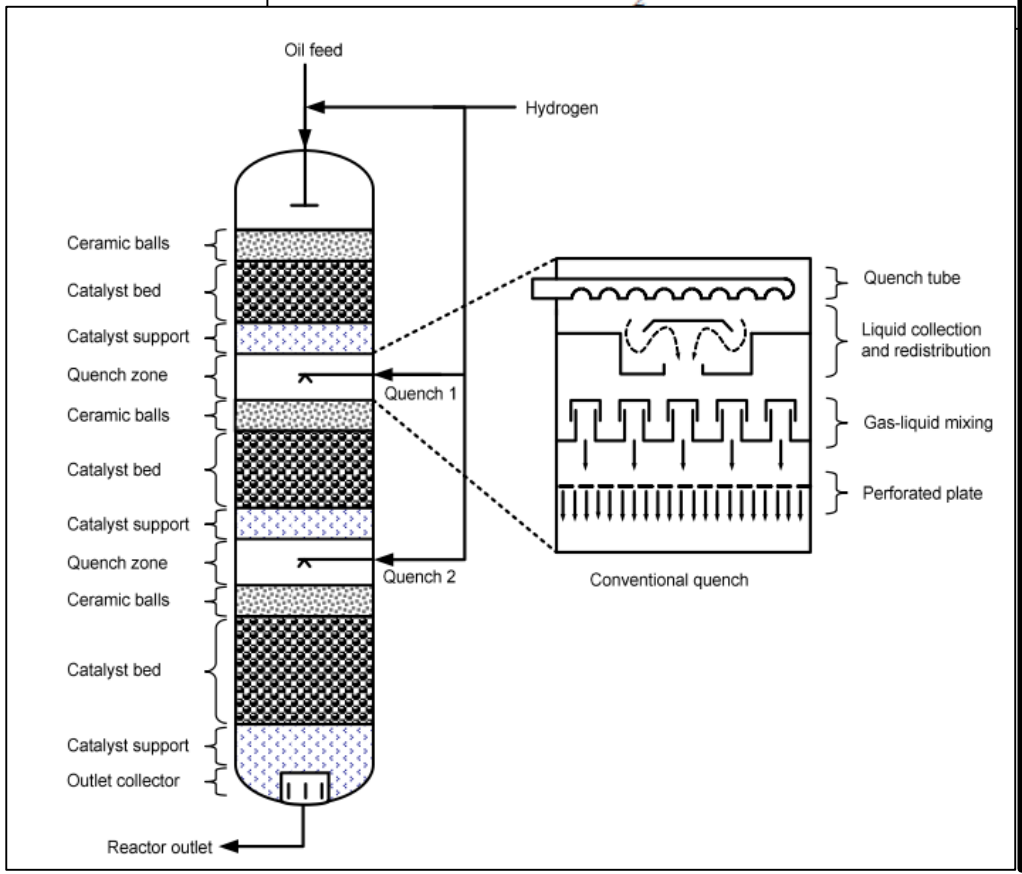
AML:TBR Example: Hydrotreating of oil fractions

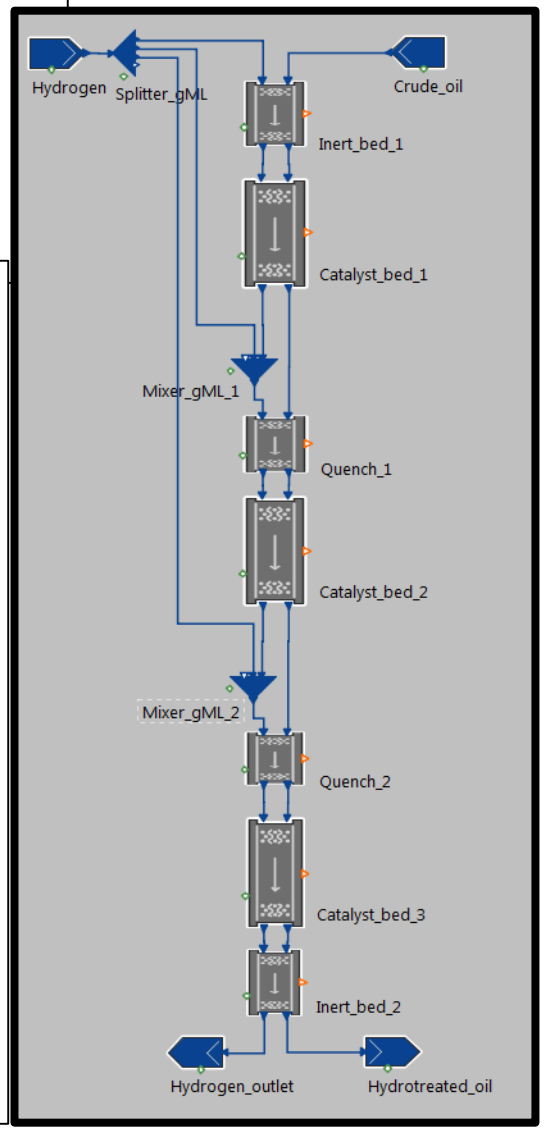
- Hydrodesulfurization (HDS)
- Hydrodenitrification (HDN)
- Hydrodemetallization (HDM)

HDS: $R-S+H_2 \rightarrow R+H_2S$

HDN: $R-NH_2+H_2 \rightarrow RH+NH_3$

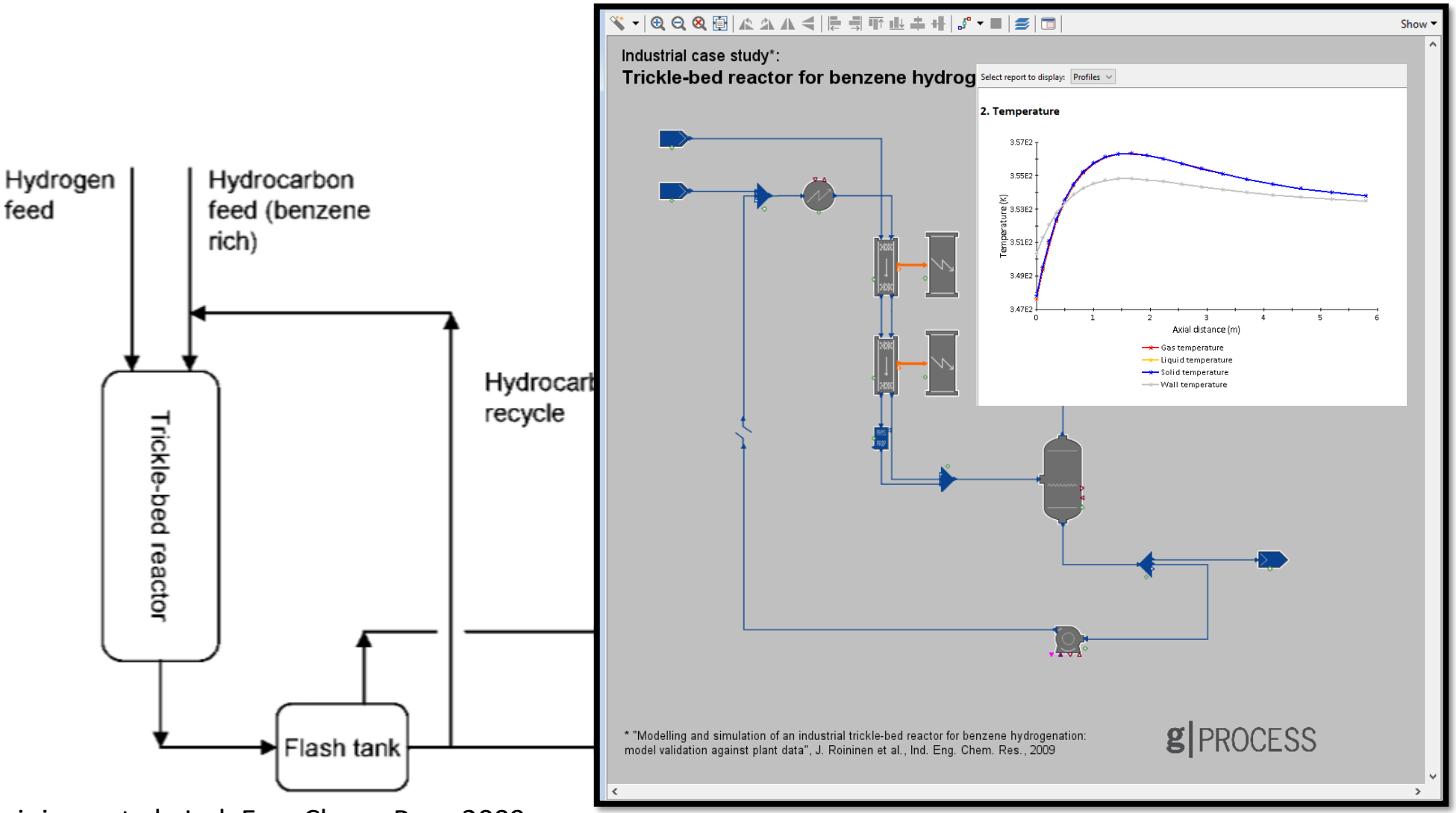
HDM: $R-M+H_2 \rightarrow RH+M$





TBR with multicatalytic bed and quench technology
(*A.T.Jarullah, PhD thesis, University of Bradford, 2011*)

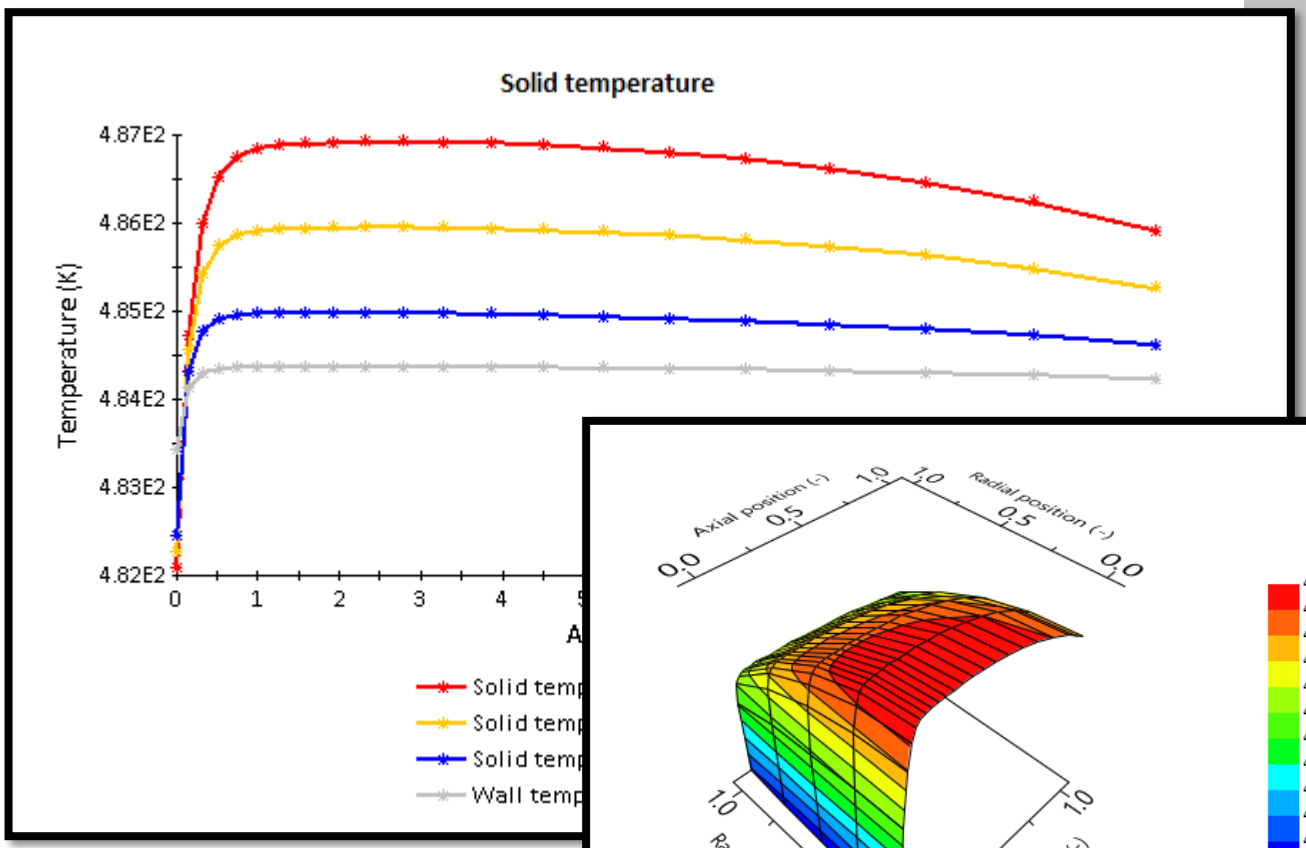
AML:TBR Example: Benzene hydrogenation

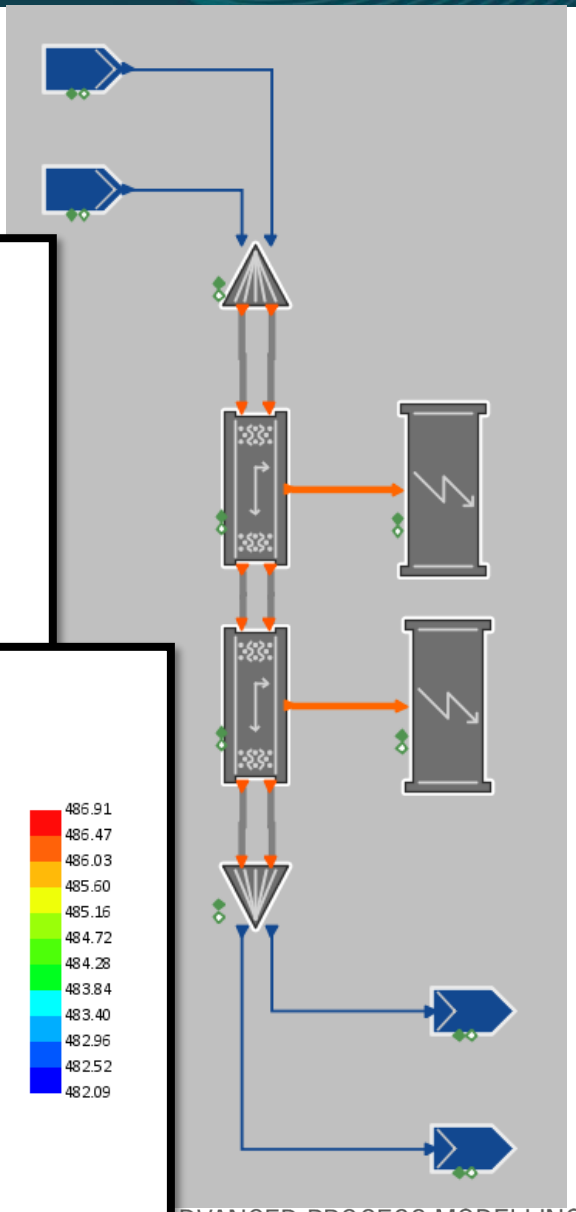


J. Roininen et al., Ind. Eng. Chem. Res., 2009

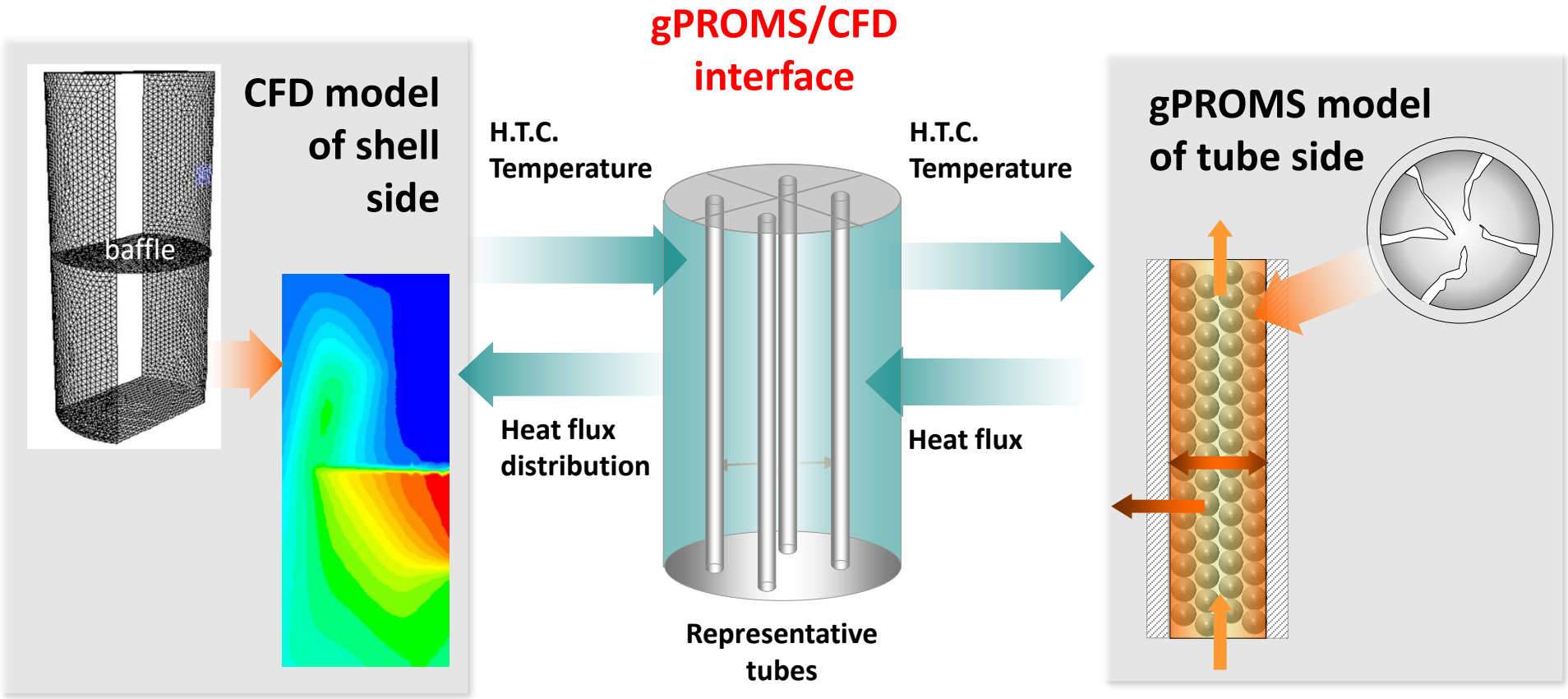
Example: Fischer Tropsch

$$(2n+1)H_2 + nCO \rightarrow C_nH_{2n+2} + nH_2O$$





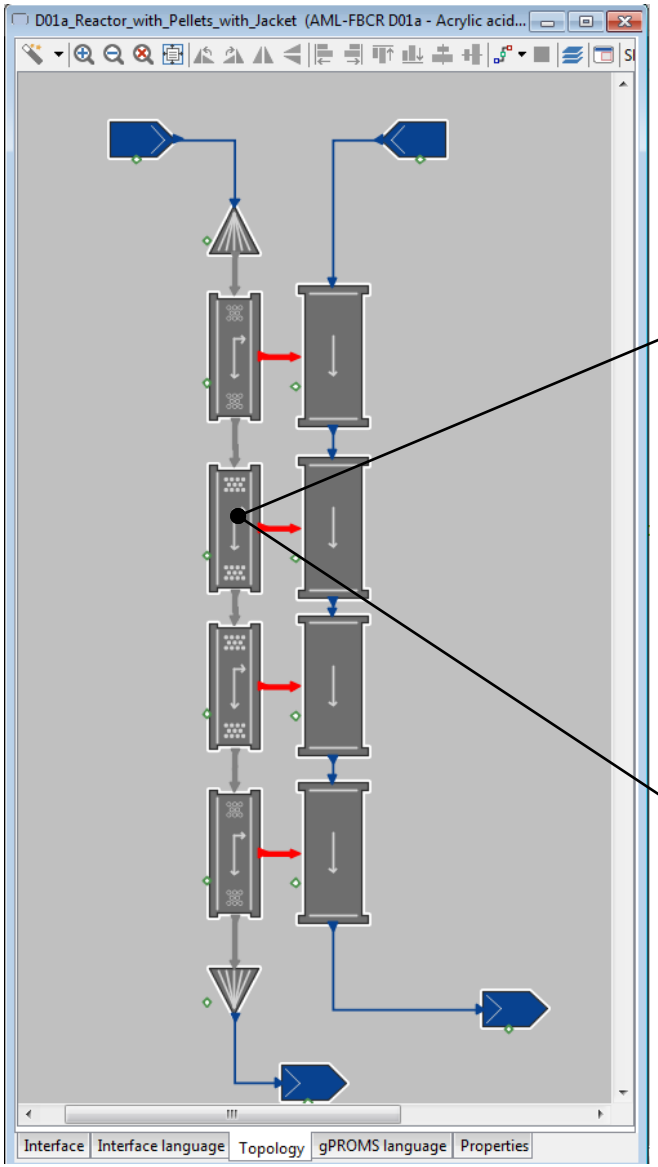
Multitubular gPROMS/CFD interface

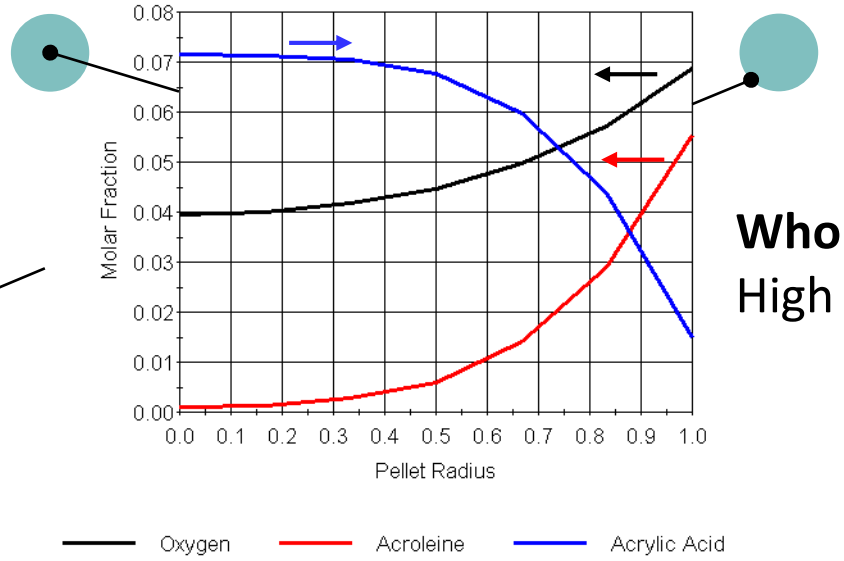


→ Highest-accuracy predictive model on both tube-and shell sides

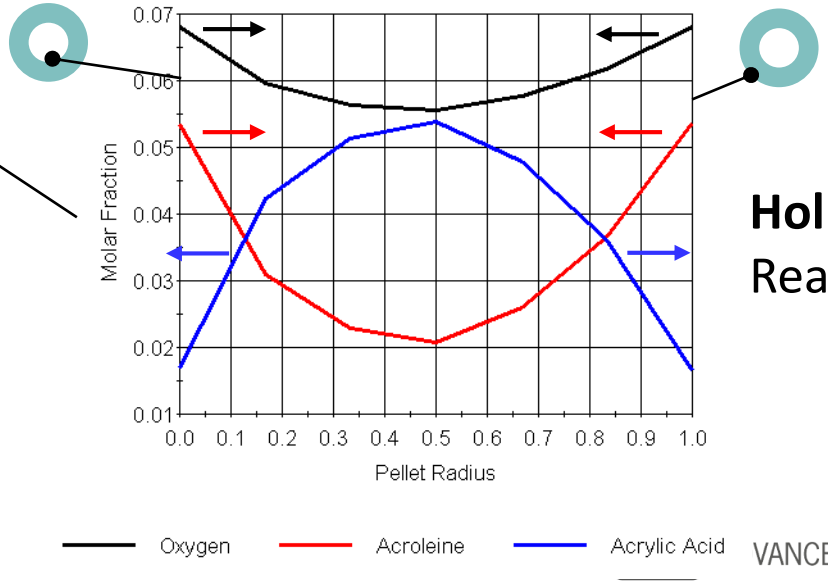
Available for both AML:FBCR and AML:TBR

AML:FBCR and AML:TBR – One final example





Whole cylinder:
High selectivity to CO, CO2



Hollow cylinder:
Reactor prone to runaway

PSE reactor libraries not yet in gPROMS ProcessBuilder…

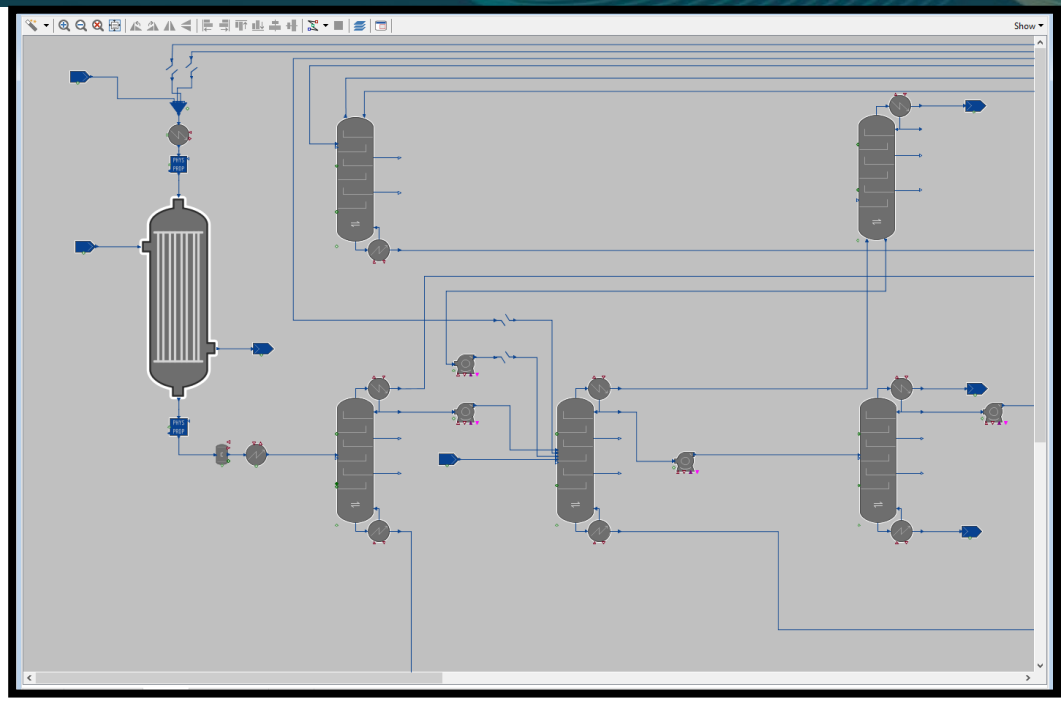
- Slurry Reactors
- Bubble Column Reactors
- Fluidised Bed Reactors

Reactor AMLs in gPROMS ProcessBuilder
Key advantages

- Combine
  - high fidelity multi-scale reactor model
  - detailed separation section
- Take into account *all* key interactions
  - reactor/separation trade-offs
  - recycles
  - heat integration

➔ Optimal process design

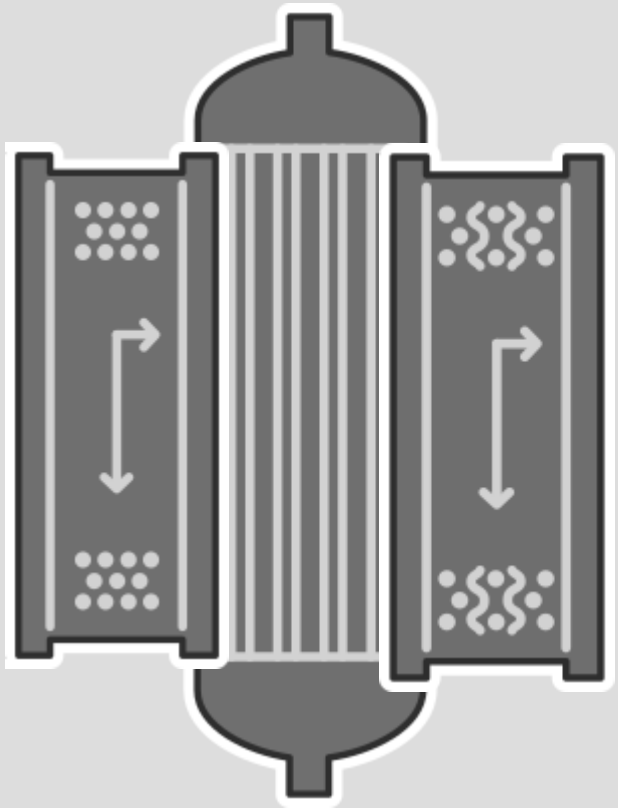
➔ Optimal plant operation



Take-away message

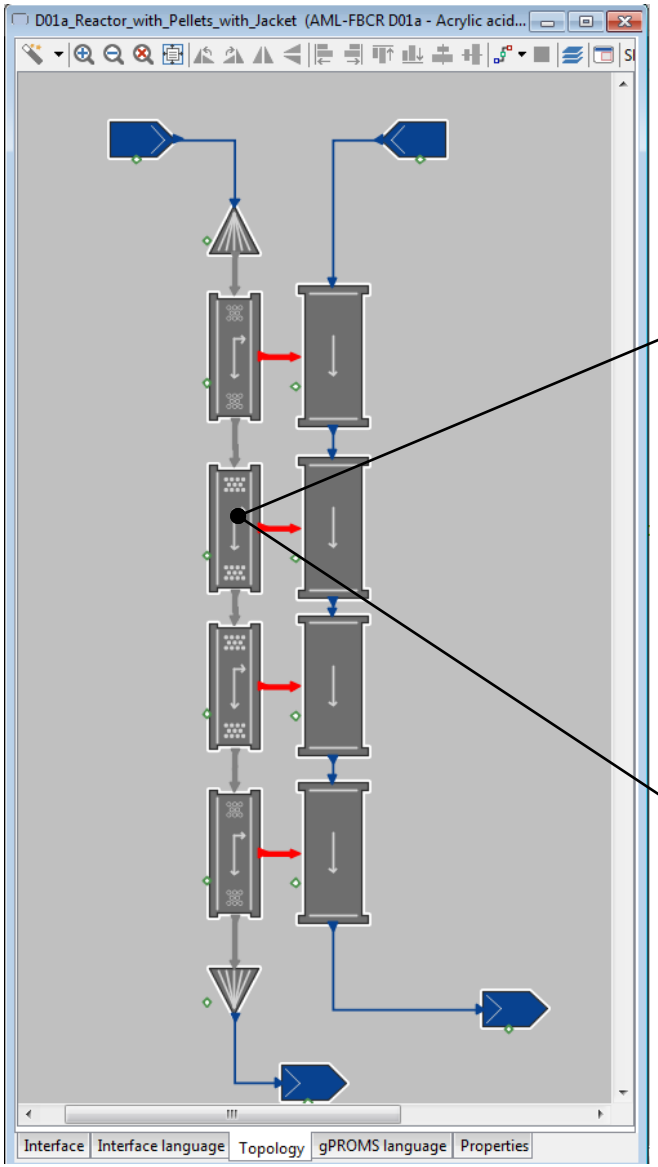
- Reactor modelling is a core focus for PSE
- High-fidelity predictive reactor models now in ProcessBuilder
  - AML:FBCR
  - AML:TBR

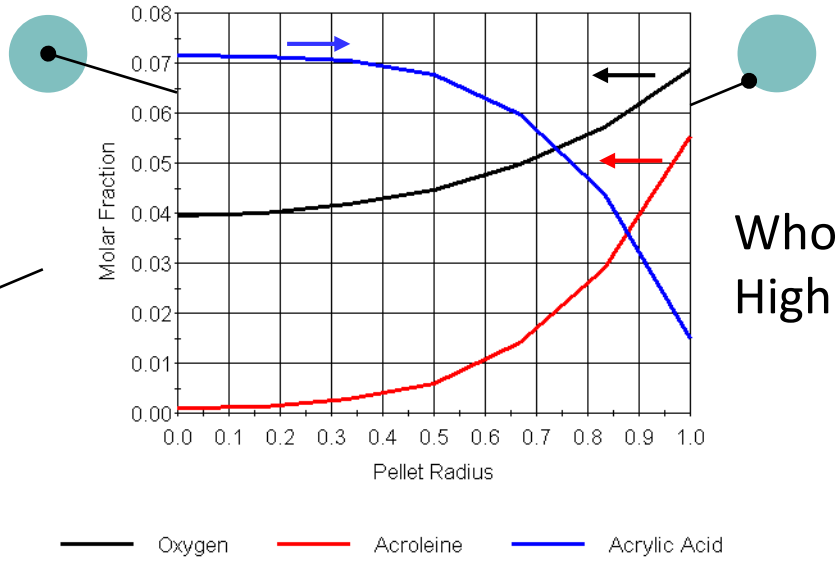
g|PROCESS



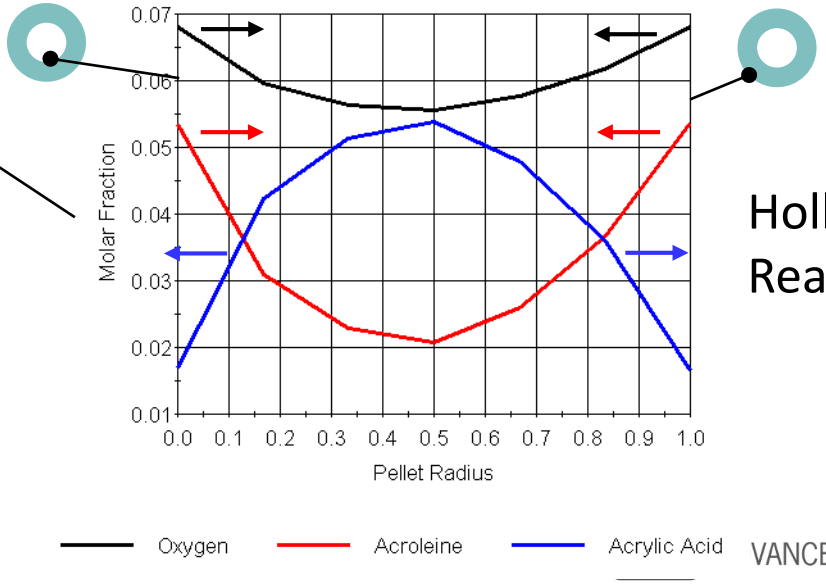
Thank you

Why modelling distributed pellet is important?





Whole cylinder:
High selectivity to CO, CO_2



Hollow cylinder:
Reactor prone to runaway