



Custom Process Unit Models in a Flowsheet Simulator

User Experiences

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Presentation Outline

- Generic Unit Operation Models
- Examples:
 - Membrane Unit
 - Trickle Bed Reactor
- Interfacing Generic (EO) Unit Operation Models in a SM Flowsheet:
 - Initialisation
 - Re-initialisation
 - Speed of convergence
- Conclusions



Generic Unit Operation Models (1)

- Flowsheet models are getting developed to a much more detailed level (large number of components, recycle loops closed, etc.) to meet process design requirements:
 - generating (optimized) M&E balances
 - generating detailed equipment design specifications
- Flowsheet libraries are limited in type and number of models:
 - “sub-flowsheets” (using library models) are frequently used to **mimic** M&E balances of a single unit operation
 - not straight-forward to use this type of model setup for (automated) equipment design specifications



Generic Unit Operation Models (2)

- We like to use generic custom (EO) unit operation models using e.g. ACM or gPROMS inside Aspen Plus for those unit operations not present in the Aspen Plus model libraries
 - re-use of custom models for different applications
 - increase usage by non ACM / gPROMS users
 - more accurate representation of the process physics & chemistry
 - (automated) generation of equipment design specifications

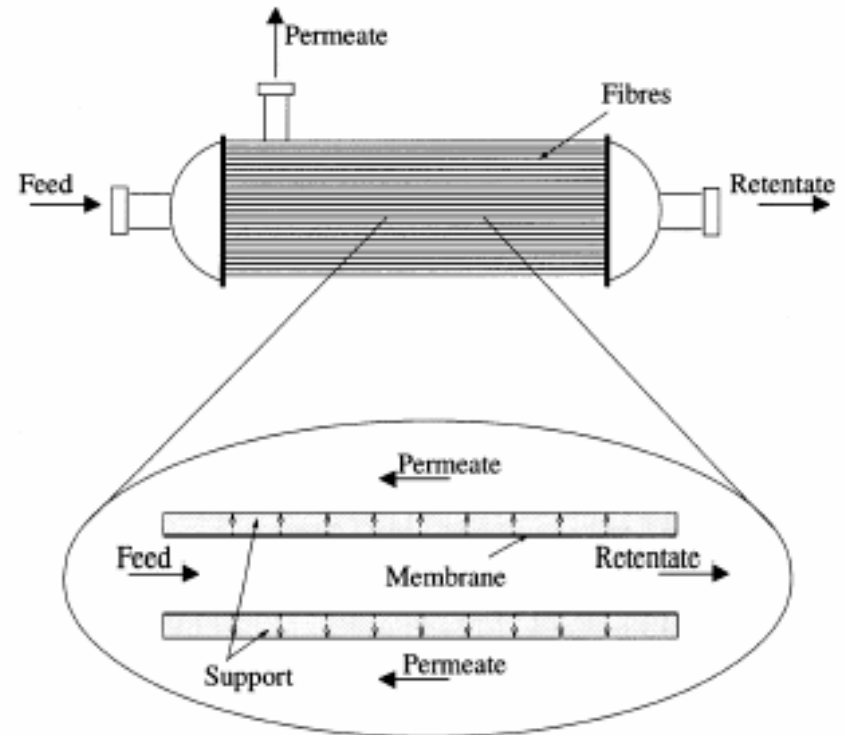


Generic Unit Operation Models (3)

- **Issue 1 : Initialisation of generic EO models**
 - can't use an initialisation data set from a previous application of the same model (different component set and operating conditions)
- **Issue 2 : Re-initialisation during flowsheet iterations (recycles)**
 - complex unit operation models can be hard to re-initialise when step changes are applied to the input variables (e.g. inlet stream composition, which can vary quite a bit during flowsheet iterations)

Example 1: Membrane Unit

- Model type
 - Rate-based
 - Distributed parameter system
- Various design specifications
 - Operation mode:
Co- / Counter-current
 - Feed location:
Shell / Fibre side
 - Membrane type:
Symmetric / Asymmetric



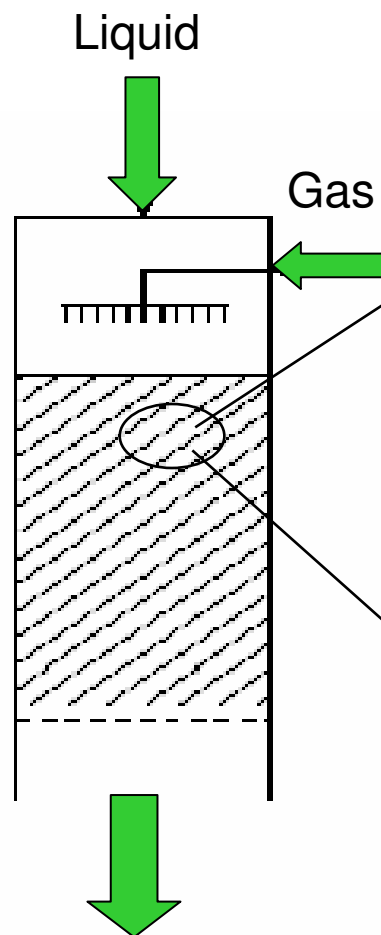


Example 1: Membrane Unit – Step Wise Initialisation

Init. Step No. #	Differential balance equations of flow through fibres and shell side	Transport of components through membrane	
		Symmetric membrane	Asymmetric membrane
1	No profiles in x, P, T along axial length Variables set equal to conditions in feed stream	No transport through membrane	No transport through membrane
2	Profile in x along axial length No profiles in P, T	Transport described by Permeability x Driving force	Transport described by Permeability x Driving force
3	Profiles in x and P along axial length No profile in T	Transport described by Permeability x Driving force	Driving force term is different for asymmetric membranes
4	Profiles in x, P, T along axial length	Transport described by Permeability x Driving force	Driving force term different for asymmetric membranes
5	Profiles in x, P, T along axial length	Permeability function of temperature	Permeability function of temperature

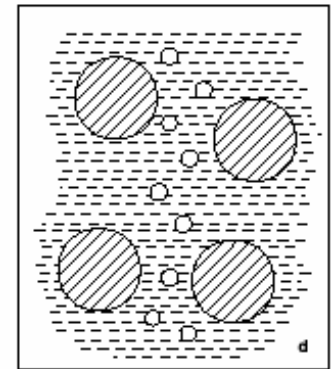
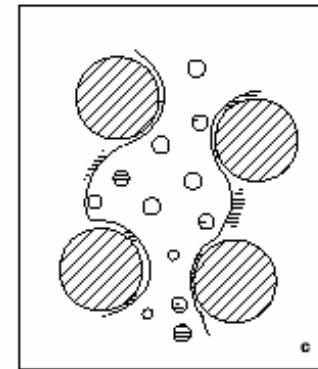
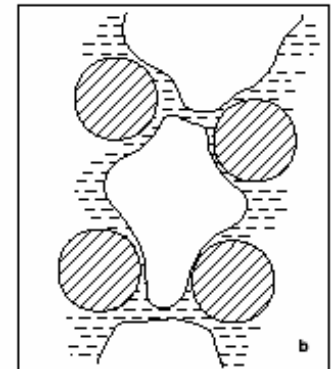
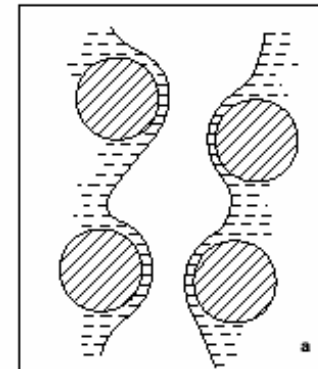
Example 2: Trickle Bed Reactor

- Process conditions
 - Flowrate
 - Concentrations
 - Temperature
 - Pressure
- Kinetic system
- Holdup
- Wetting efficiency
- Mass transfer
 - Liquid-Gas
 - Liquid-Particle
 - Gas-Particle
- Heat transfer
 - Liquid-Gas
 - Liquid-Particle
 - Gas-Particle



Trickle

Pulse



Spray

Bubble



Example 2: Trickle Bed Reactor – Step Wise Initialisation

Init. Step No. #	Concentration profile - gas phase	Mass transfer between phases
1	$\frac{\partial}{\partial z} u_{IG} = 0$	$N_i^{GL} a_{GL} = 0$
2	$\frac{\partial}{\partial t} (\epsilon_G C_{iG}) + \frac{\partial}{\partial z} (u_{IG} \epsilon_G C_{iG}) = 0$	$N_i^{GL} a_{GL} = 0$
3	$\frac{\partial}{\partial t} (\epsilon_G C_{iG}) + \frac{\partial}{\partial z} (u_{IG} \epsilon_G C_{iG}) = -N_i^{GL} a_{GL} - N_i^{GS} a_{GS}$	



Interfacing Generic (EO) Unit Operation Models in a SM flowsheet – Initialisation / Re-initialisation

- Number of variables and equations is equal for each initialisation step
- Initialisation structure automated in gPROMS (Tasks) and ACM (Visual Basic script)
- Export to Aspen Plus: gPROMS Tasks / ACM Visual Basic scripts are NOT exported in current interface definitions
 - Automated model initialisation procedure fails in when custom model is incorporated in Aspen Plus
 - Automated model re-initialisation procedure (going from previous initial condition to next one during flowsheet iteration) can't be used



Interfacing Generic (EO) Unit Operation Models in a SM flowsheet – Speed of Convergence

“Balancing Act”

- Aspen Plus Flowsheet
 - large number of (trace) components to increase accuracy of mass and energy balance
- Custom Unit Operation Model
 - large number of equations to increase accuracy of physical and chemical representation
- Issue: incorporation of such a Custom Model in an Aspen Plus flowsheet simulation can result in very large, impractical situations



Conclusions

- We start to built confidence in the ability to create our own custom unit operation model libraries for use in Aspen Plus using CAPE-OPEN
- Need to further develop initialisation & re-initialisation strategies for robust and computational performance. Automated transport of tasks (gPROMS) and Visual Basic Scripts (ACM) is required
- Performance of custom models inside Aspen Plus is an issue which needs further attention when remaining interface issues have been addressed : balance model complexity and size vs. model performance (CPU)



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