MEMSIC 2.0

MEMBRANE GAS SEPARATION SIMULATOR

Presentation and CO development:
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Theory and numerical development:
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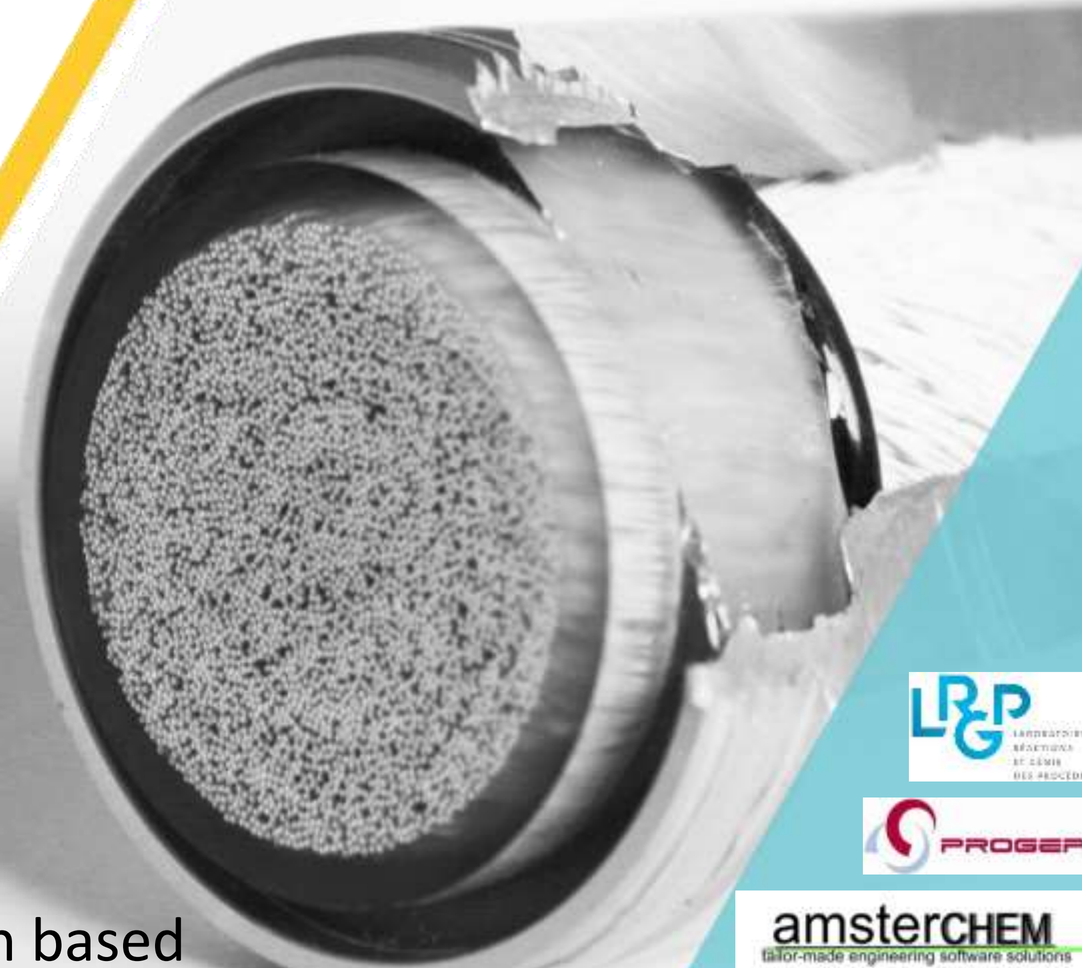


MEMSIC

A CAPE-OPEN unit operation based on dedicated multicomponent membrane gas separation software

LRGP

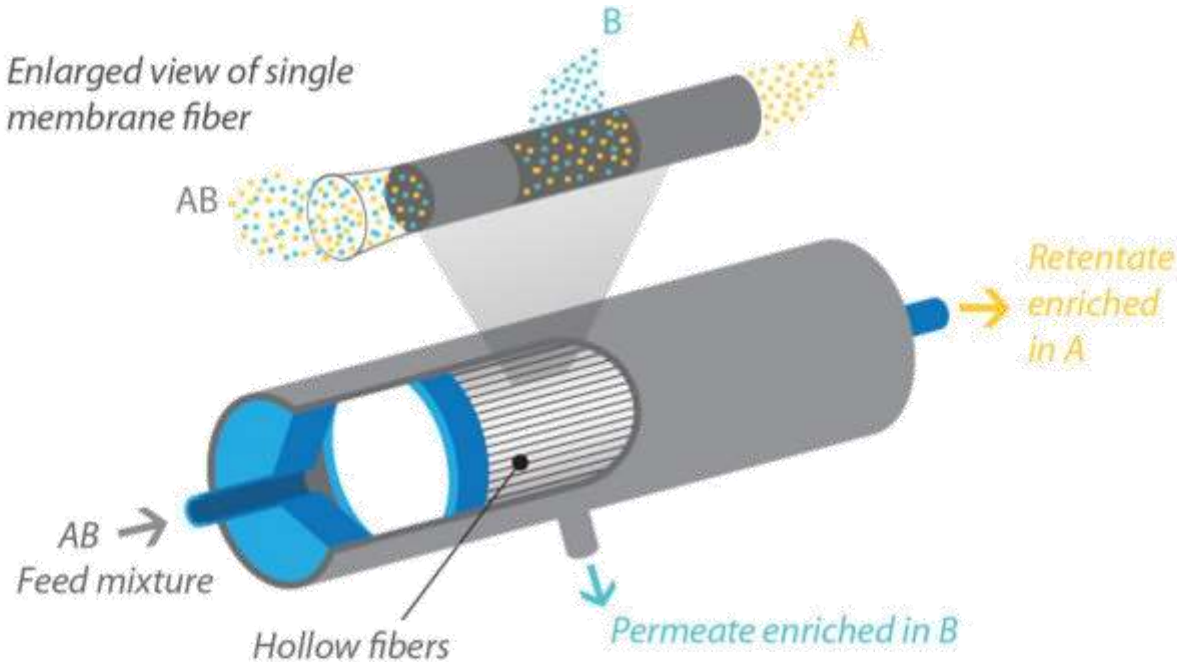
PROGEPI

amsterCHEM
tailor-made engineering software solutions

Membrane separation technology offers an attractive solution for bringing environmental sustainability to the chemical industries.

Advantages of membrane technology

- ❑ Simplicity, plug-and-play process with no regeneration steps
- ❑ Energy efficiency, involves no phase change
- ❑ Environmentally friendly, no chemical reactions or solvents are used
- ❑ Compactness, based on intensified separation process



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MEMBRANE GAS SEPARATION SIMULATOR

Market applications

- ❑ Air separation
- ❑ Hydrogen purification
- ❑ Natural gas treatment
- ❑ Volatile Organic Compounds recovery
- ❑ Natural gas drying
- ❑ CO_2 sequestration

Our main clients

SAIPEM

Technip

LIEBHERR

ZODIAC AEROSPACE

ARKEMA

جامعة الملك عبدالله للعلوم والتقنية

King Abdullah University of Science and Technology

Our main competitors

(1) Almeesoft

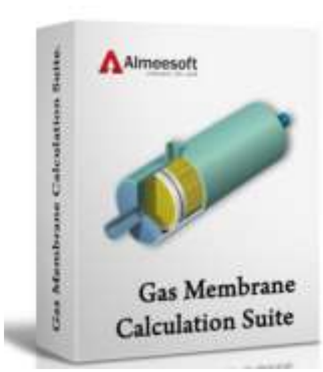
- Stand alone and compatible with Aspen HYSYS®
- Pressure drop for complex geometries
- Thermal effects for 2 equations of state
- Sweep gas and 3 module cascade with recycle
- Data fitting

Services

- Online test
- Academic and industrial licences

(for stand-alone 1000 – 2000 US$/year/pc)

- http://almeesoft.com



(2) PMEs

Aspen Plus® & PRO/II®

- Isothermal crossflow with constant permeability

ProSimPlus®

- Isothermal counter-current separation module with theoretical prediction of permeability

(3) MemCal

Options

- Standalone
- Specifically CO2 from NG
- Data of several commercial membrane modules
- No technical support
- http://sales.gastechnology.org/950197.html

MEMSIC 2.0

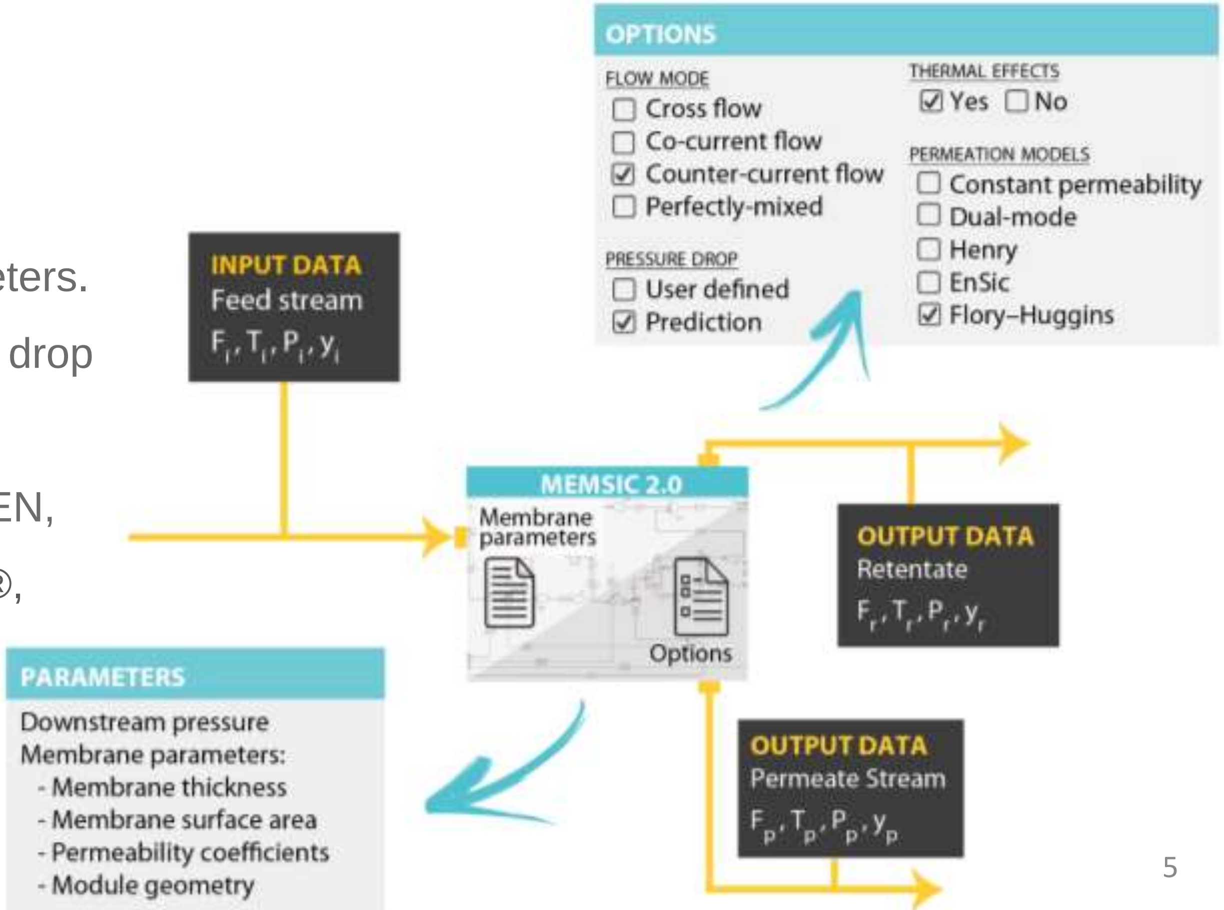
MEMBRANE GAS SEPARATION SIMULATOR

MEMSIC:

- multicomponent membrane gas separation software
- available as CAPE-OPEN Unit

Key advantages of MEMSIC 2.0

- ❑ A User-friendly interface
- ❑ A Robust and powerful tool
- ❑ A database of more than 5000 compound - membrane parameters.
- ❑ Possibility to estimate pressure drop and Joule-Thomson effects
- ❑ Compatible through CAPE-OPEN, with ProsimPlus®, Aspen Plus®, Aspen HYSYS®, PRO/II®, ...



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MEMBRANE GAS SEPARATION SIMULATOR

Model Assumptions

Thermodynamics:

1. Stand-alone: internal Redlich-Kwong EoS model
2. When running as CAPE-OPEN unit: from PME

Flow assumptions:

2. Steady state
3. Plug flow, no axial dispersion and uniform flow distribution
4. Laminar flow (i.e. $Re_{internal} < 2000$ and $Re_{external} < 100$)

Model Assumptions

Transfer phenomena:

5. In the direction perpendicular to the membrane, there are no concentration gradients (the dense skin membrane layer is the only mass transfer resistance)
6. No phase-change
7. Rapid heat-transfer in gas phases (no heat transfer resistance)
8. Influence of pressure variation on fluid enthalpy is neglected
9. Hydrodynamics are decoupled from mass and heat transfer.
10. For laminar flow and HFMM (Hollow Fibre Membrane Module), the pressure drop of parallel flow using Poiseuille formulations
11. No flux coupling (each compound permeates through the membrane according to its own driving force)

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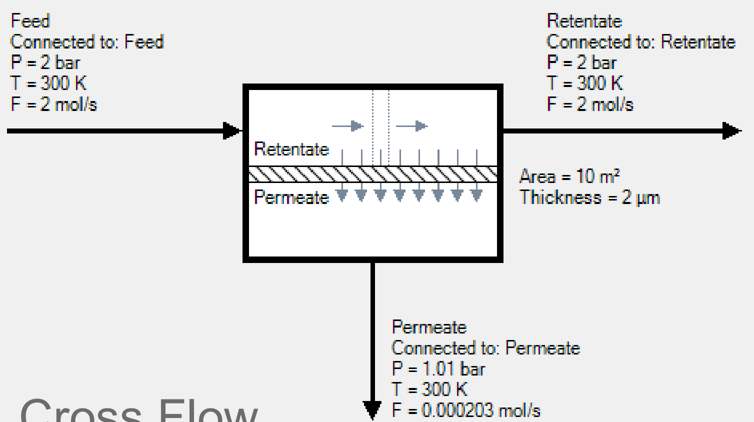
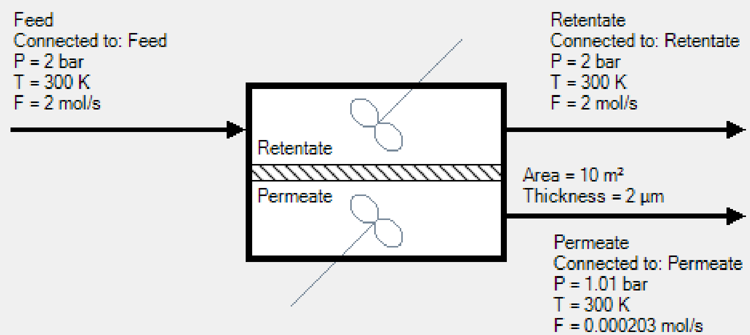
MEMBRANE GAS SEPARATION SIMULATOR

Membrane Modelling Options
(using CAPE-OPEN parameters or ICapeUtilities::Edit)

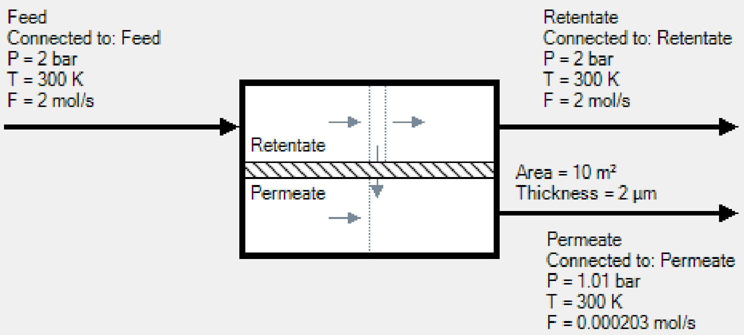
Flow mode:



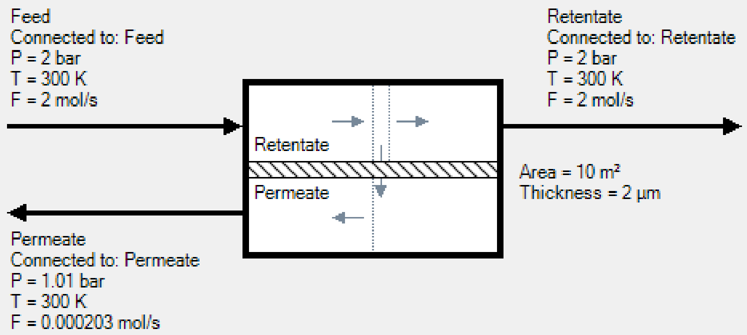
Cross Flow



Perfectly Mixed



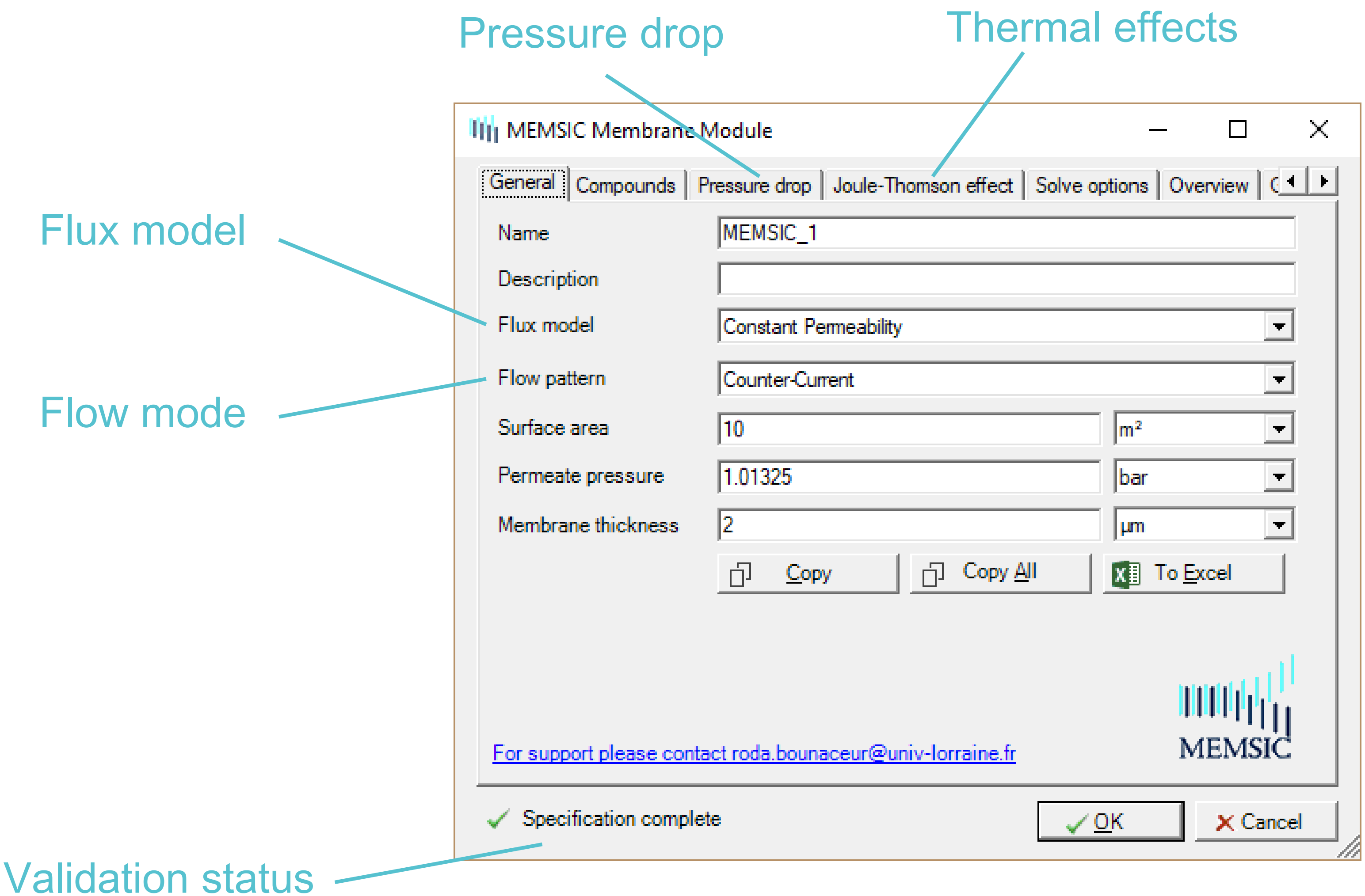
Co-Current



Counter-Current

Membrane Modelling Options

(using CAPE-OPEN parameters or ICapeUtilities::Edit)



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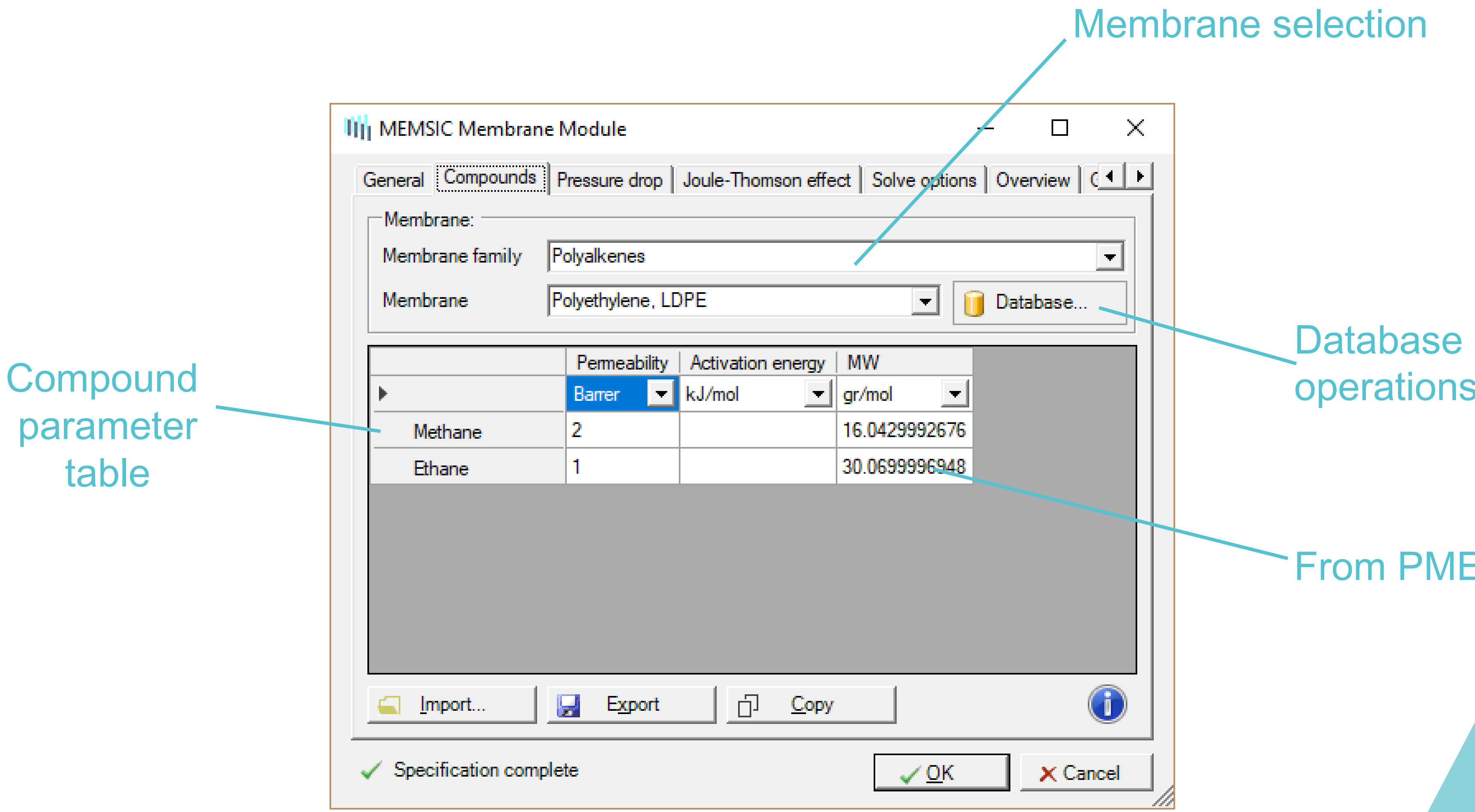
MEMBRANE GAS SEPARATION SIMULATOR

Membrane Modelling Options

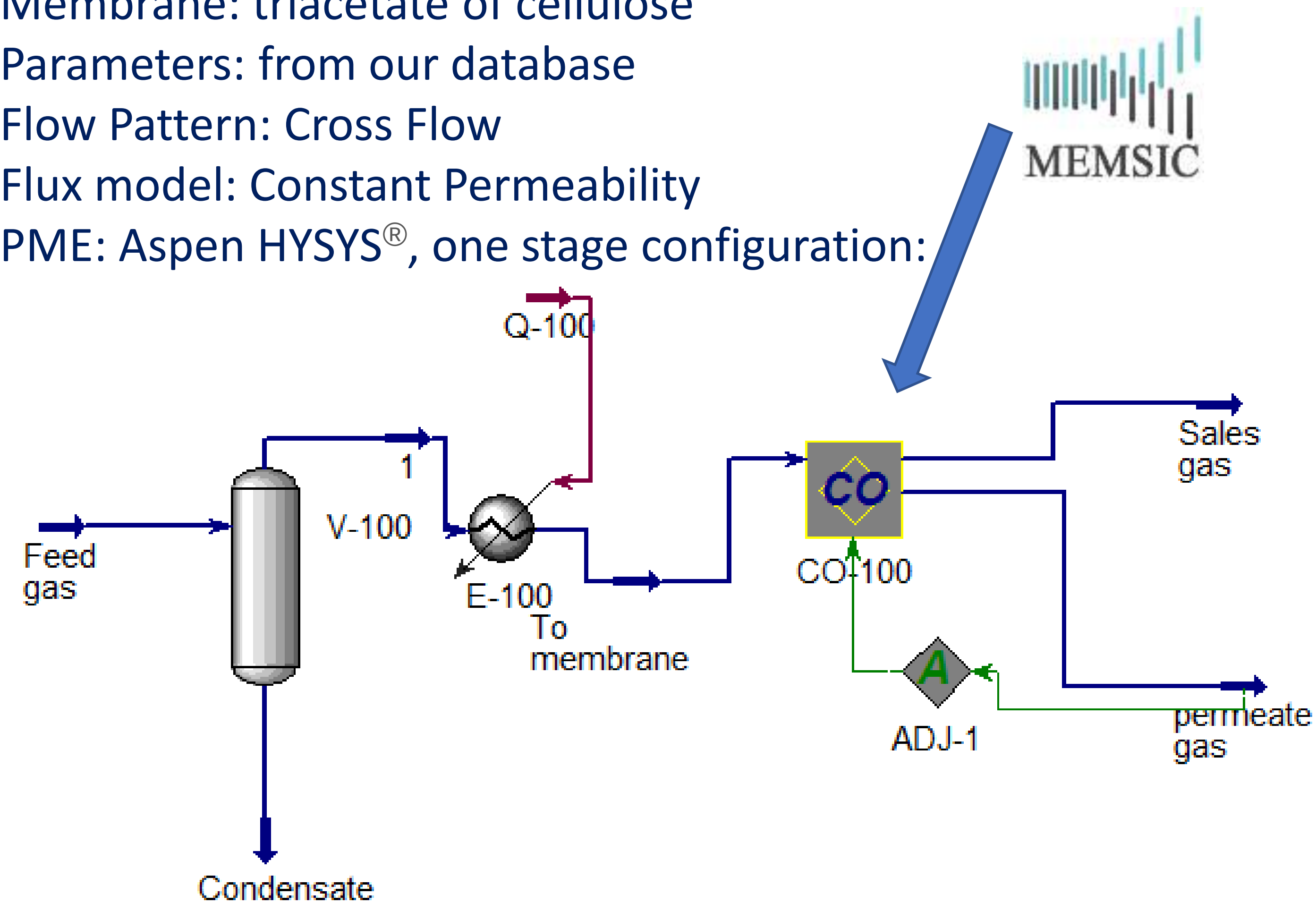
(using CAPE-OPEN parameters or ICapeUtilities::Edit)



A case study

Comparison between Memsic Simulation and data from a supplier

- Results from a confidential study
- Membrane: triacetate of cellulose
- Parameters: from our database
- Flow Pattern: Cross Flow
- Flux model: Constant Permeability
- PME: Aspen HYSYS®, one stage configuration:



DATA PROVIDED BY SUPPLIER

DATA PROVIDED BY SUPPLIER			
	Feed gas	Sales gas	permeate gas
Temperature [C]	40	55	55
Pressure [bar]	100	98	2.0
Molar Flow [kgmole/h]	13178	11240	1938
Composition %mol			
Comp Mole Frac (Methane)	84.07	84.4	82.0
Comp Mole Frac (Ethane)	6.64	7.40	2.10
Comp Mole Frac (Propane)	2.580	3.000	0.300
Comp Mole Frac (n-Butane)	2.99	3.50	0.30
Comp Mole Frac (Nitrogen)	0.67	0.60	0.80
Comp Mole Frac (CO2)	2.93	1.10	13.70
Comp Mole Frac (H2S)	0.02	<50ppm	0.10
Comp Mole Frac (Helium)	0.01	0	0.1
Comp Mole Frac (H2O)	0.1	<30ppm	0.7

Results from Memsic simulation:

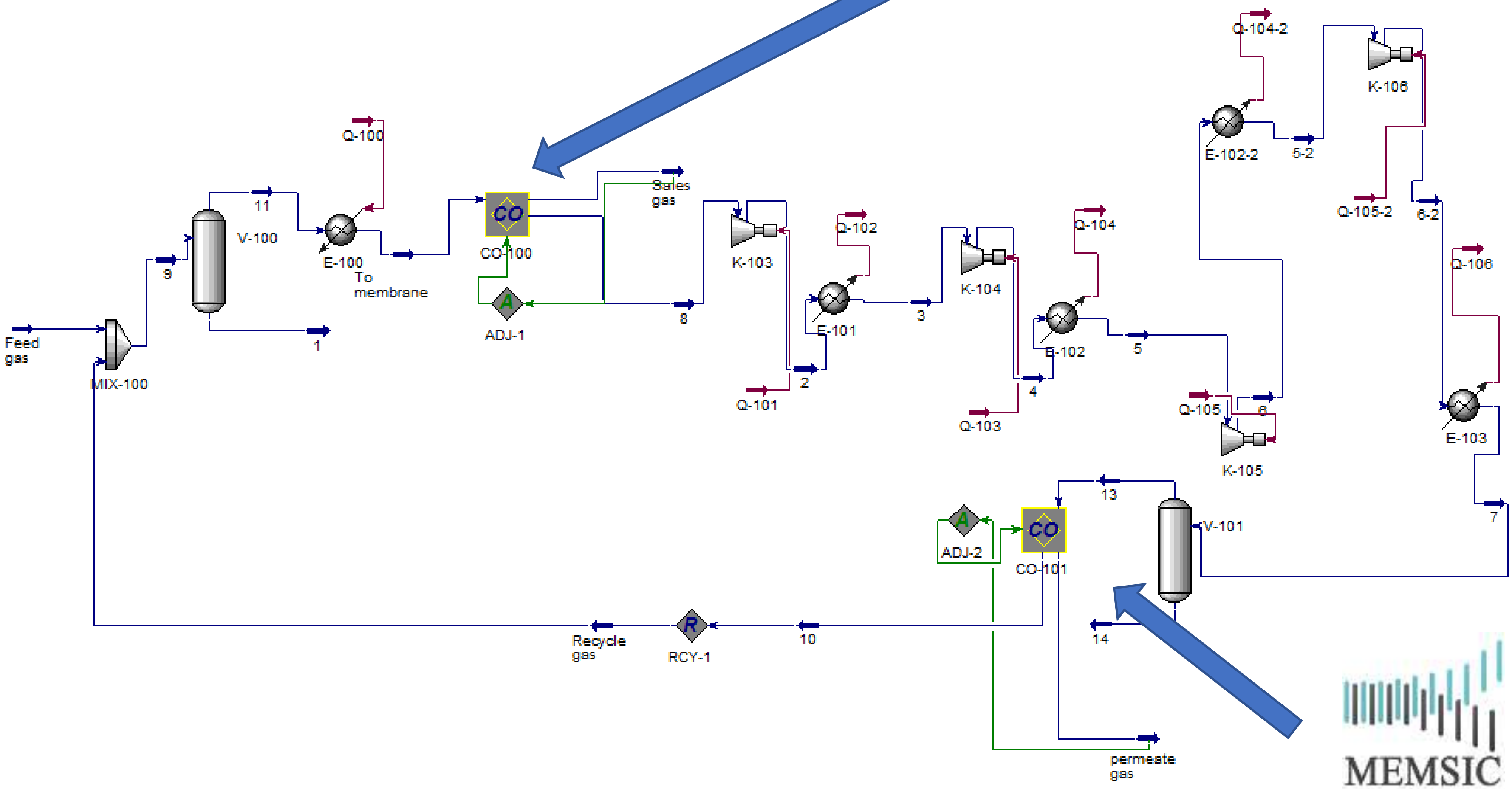
SIMULATION HYSYS			
	Feed gas	Sales gas	permeate gas
Temperature [C]	40	55	55
Pressure [bar]	100	100	2
Molar Flow [kgmole/h]	13178	11240	1938
Composition %mol			
Comp Mole Frac (Methane)	84.06	84.98	78.74
Comp Mole Frac (Ethane)	6.64	7.21	3.33
Comp Mole Frac (Propane)	2.58	2.97	0.33
Comp Mole Frac (n-Butane)	2.99	3.44	0.30
Comp Mole Frac (Nitrogen)	0.67	0.65	0.78
Comp Mole Frac (CO2)	2.93	0.75	15.57
Comp Mole Frac (H2S)	0.02	50 ppm	0.11
Comp Mole Frac (Helium)	0.01	0.00	0.10
Comp Mole Frac (H2O)	0.10	1 ppm	0.68

Membrane Area (m²)	**19874**
Membrane thickness (µm)	0.1
permeability (barrer)	
Methane	0.782
Ethane	0.4
Propane	0.1
n-Butane	0.1
Nitrogen	1
CO2	9.8
H2S	10
Helium	30
H2O	4000

Component	**Sales gas (%error)**	**Permeate gas (%error)**
CH4	0.7%	4%
H2S	OK	10%
H2O	OK	3%

Good agreement

- Flow Pattern: RPC
- Flux model: constant permeability
- PME: Aspen HYSYS®, two-stage configuration:



DATA PROVIDED BY SUPPLIER

DATA PROVIDED BY SUPPLIER			
	Feed gas	Sales gas	permeate gas
Temperature [C]	40	55	55
Pressure [bar]	100	98	2
Molar Flow [kgmole/h]	13178	12730	442
Composition %mol			
Comp Mole Frac (Methane)	84.07	85.6	42.1
Comp Mole Frac (Ethane)	6.64	6.90	0.50
Comp Mole Frac (Propane)	2.580	2.700	0.00
Comp Mole Frac (n-Butane)	2.99	3.10	0.00
Comp Mole Frac (Nitrogen)	0.67	0.70	0.40
Comp Mole Frac (CO2)	2.93	1.10	55.70
Comp Mole Frac (H2S)	0.02	<50 ppm	0.30
Comp Mole Frac (Helium)	0.01	0	0.3
Comp Mole Frac (H2O)	0.1	<30 ppm	0.5

Results from Memsic simulation:

Dans la configuration à deux étages :			
SIMULATION ASPEN HYSYS®			
	Feed gas	Sales gas (1st membrane)	permeate gas (2nd membrane)
Temperature [C]	40	55	55
Pressure [bar]	100	98	2
Molar Flow [kgmole/h]	13178.00	12730.00	442.00
Composition %mol			
Comp Mole Frac (Methane)	84.06	85.84	34.33
Comp Mole Frac (Ethane)	6.64	6.85	0.71
Comp Mole Frac (Propane)	2.58	2.67	0.02
Comp Mole Frac (n-Butane)	2.99	3.10	0.02
Comp Mole Frac (Nitrogen)	0.67	0.68	0.44
Comp Mole Frac (CO2)	2.93	0.86	62.32
Comp Mole Frac (H2S)	0.02	50 ppm	0.43
Comp Mole Frac (Helium)	0.01	0.00	0.29
Comp Mole Frac (H2O)	0.10	1 ppm	1.43

	1 étage	2 étages
Membrane Area (m^2)	24000	1979
Membrane thickness (µm)	0.1	0.1
permeability (barrer)		
Methane	0.782	0.782
Ethane	0.4	0.4
Propane	0.1	0.1
n-Butane	0.1	0.1
Nitrogen	1	1
CO2	9.8	9.8
H2S	10	10
helium	30	30
H2O	4000	4000

Component	**Sales gas (%error)**	**Permeate gas (%error)**
CH4	0.3%	18%
H2S	OK	40%
H2O	OK	186%

Relative good agreement except for water (initially its concentration is very low)

Gas separation of a gas from Pakistan

- Comparison of results coming from the supplier and from Memsic code
- 3 different configurations studied
- Simulation made with HYSYS
- Comparison of the total area obtained to reach objective

Total Area	**Case 1**	**Case 2**	**Case 3**
From Memsic / HYSYS (m^2)	33385	13745	32327
Provided by supplier(m^2)	33000	13200	31800
% error	1%	4%	2 %

Membrane: PEEK

Experiences with CAPE-OPEN

- Generally in good shape
- Problems with one particular simulator
  - Persistence does not work
  - Unexpected crashes
  - Unexpected problems with dynamic collection of parameters
  - List of compounds not available until first run
  - Parameter values frequently disappear
  - Little support from PME vendor

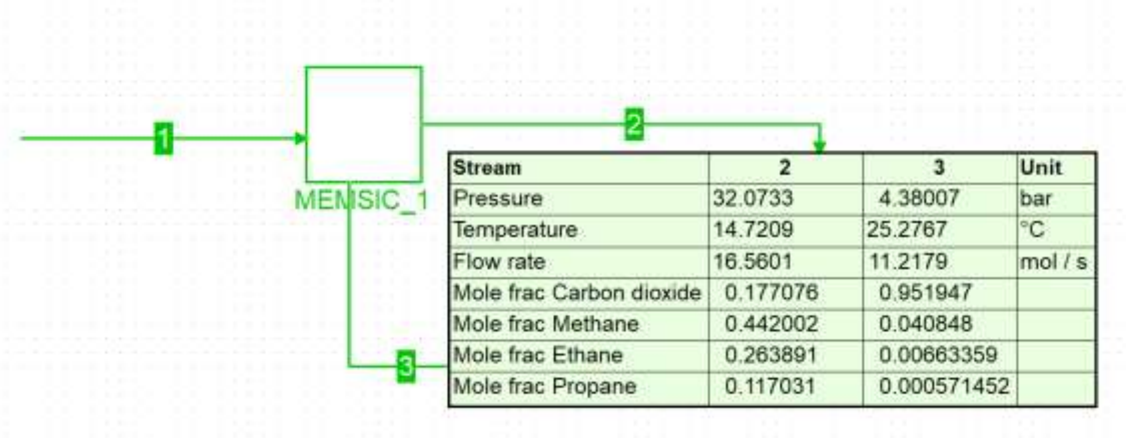
We eventually got it to work – many concessions were made and not very user friendly

We are willing to make software (without numerical back-end) available to PME vendor for debugging!

Experiences with CAPE-OPEN

- Code consists out of 3 parts
  - Numerics
  - GUI + Database
  - CAPE-OPEN layer
- We have control over the first two parts, which work fine
- Not having control over the (quality of the) other party's CAPE-OPEN layer can be frustrating
- PME vendor is kindly requested to put in best effort to make their socket work better

Demonstration



Stream	2	3	Unit
Pressure	32.0733	4.38007	bar
Temperature	14.7209	25.2767	°C
Flow rate	16.5601	11.2179	mol / s
Mole frac Carbon dioxide	0.177076	0.951947	
Mole frac Methane	0.442002	0.040848	
Mole frac Ethane	0.263891	0.00663359	
Mole frac Propane	0.117031	0.000571452	

SHOW THE CODE THROUGH AN EXAMPLE .....

Perspectives

- MEMSIC 1.0 (without pressure drop and thermal effect) is provided under license

- MEMSIC 2.0 (with pressure drop and thermal effect+database): the code is still under validation – expected to the end of 2017

- Under development, other unit operations to take into account separation of mixture in different phases:

    1. Liquid-Liquid
    2. Gas-Liquid
    3. Gas-Liquid with chemical reaction

MEMSIC

LICENCE PROVIDED BY PROGEPI

DEVELOPED BY LRGP & PROGEPI

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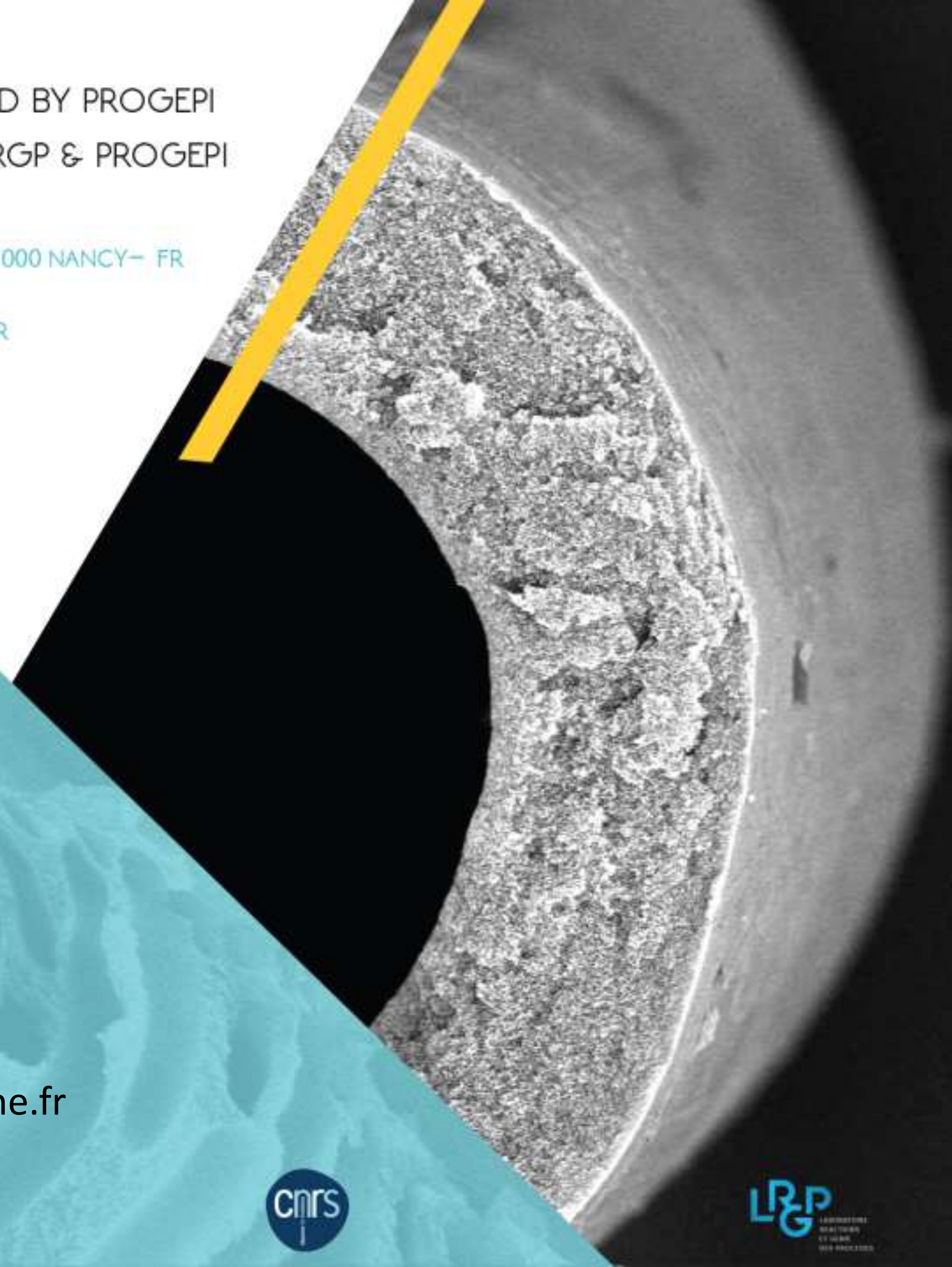


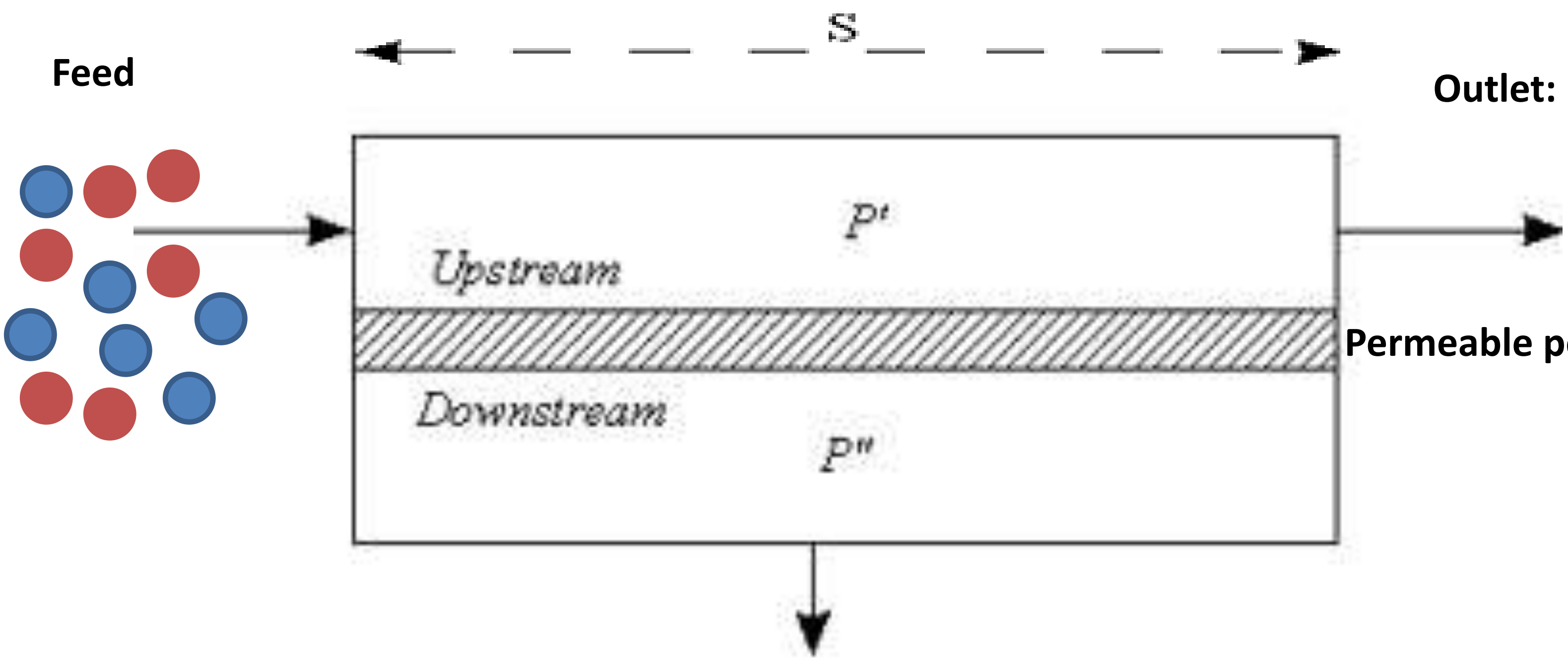
Contact: roda.bounaceur@univ-Lorraine.fr

PROGEPI   UNIVERSITÉ DE LORRAINE   CNRS   LRGP

How works a membrane

Feed

Outlet: Retentate



Permeable polymeric film

Outlet: Permeate

The efficiency of the separation depends on:

$$\Psi = P'' / P'$$

$$\theta = Q_p / Q_{in} = 1 - Q_{out} / Q_{in}$$

$$St = S \,.\, K_1 \,.\, P' / \delta \,.\, Q_{in}$$

$$R = \theta \cdot y_p / x_{in}$$

-the pressure ratio

- the flow rate

-the surface area

-the permeability coefficient of each compounds respect to the polymeric film