CCSI²
Carbon Capture Simulation for Industry Impact

MTR Pilot Support: Modeling Framework Capturing Non-Idealities in Membrane Module Performance

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AGENDA

- Motivation
- Ideal Module Performance
- Source of Non-idealities
- Identifying Non-ideal Performance

MEMBRANE SUCCESS STORIES

- Desalination
- Nitrogen production
- Solvent nano-filtration (oil dewaxing)
- Pervaporative dehydration (oil/lubricant dewatering)

Lipscomb and Giraud, Encyclopedia of Sustainable Technologies, 2017

MEMBRANE PROCESS EVOLUTION

NATIONAL ENERGY TECHNOLOGY LABORATORY

Material Development

Material science of transport and separation

Process Synthesis

Evaluation of operating conditions and economics

Membrane and Module Manufacture

Formation of hollow fiber or sheet membranes and assembly into modules

Pre/Post Treatment

Identification of needs for pre and post membrane treatment to increase lifetime and deliver desired product

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"Ideal" countercurrent assumption – same for hollow fiber and sheet

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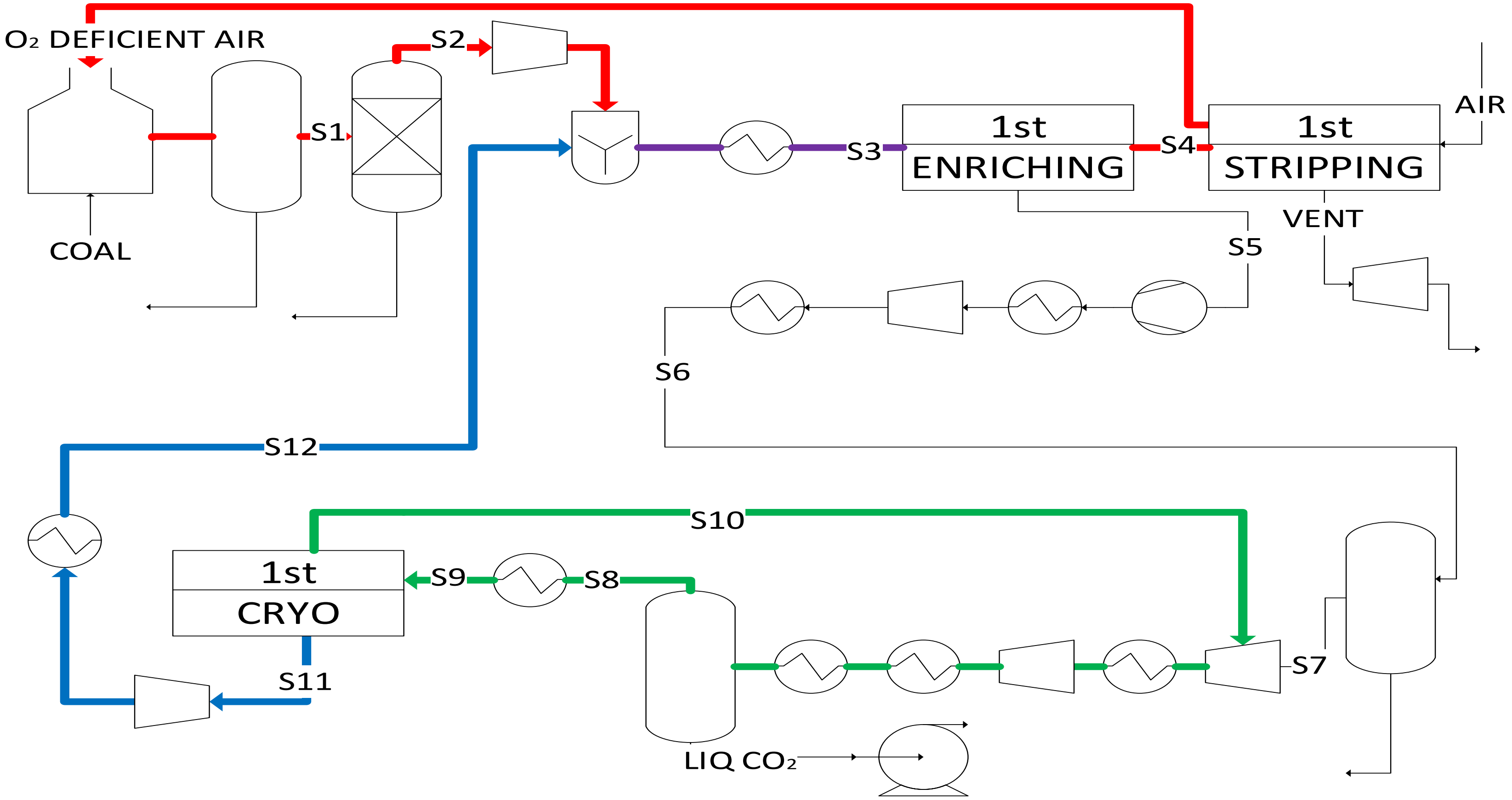
"Ideal" countercurrent assumption – same for hollow fiber and sheet

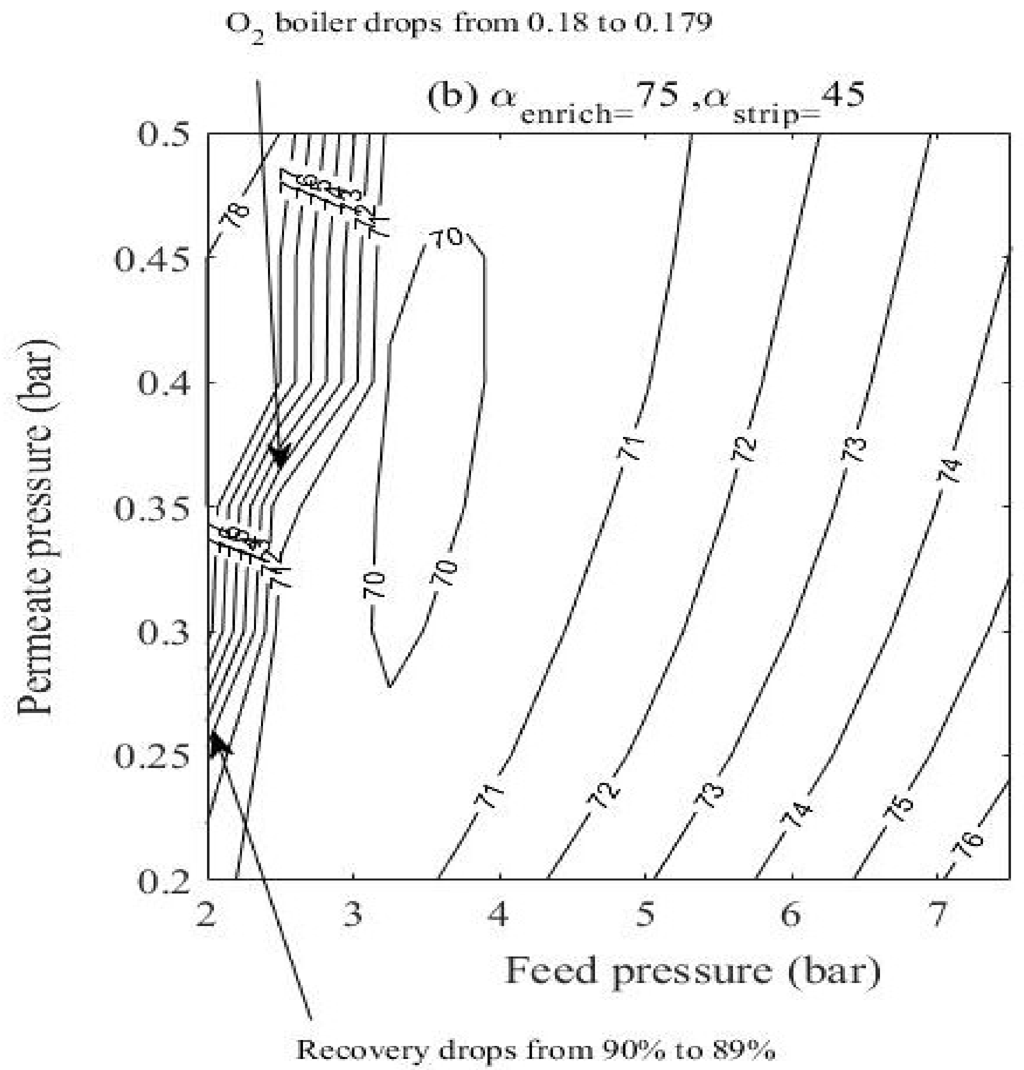
"Real" performance observed – simulation requires model development

MEMBRANE CARBON CAPTURE

- Air feed sweep system (MTR process)

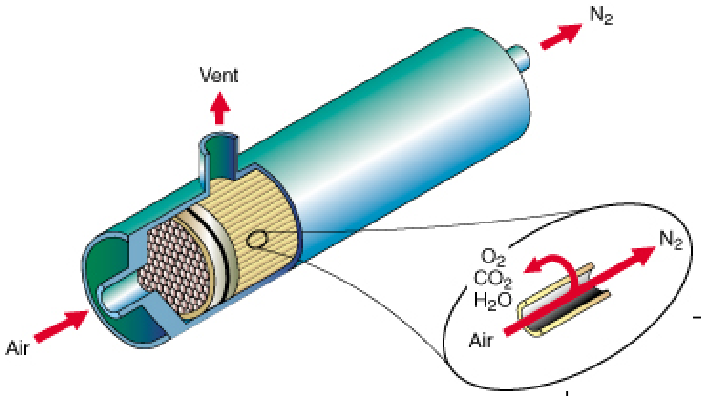


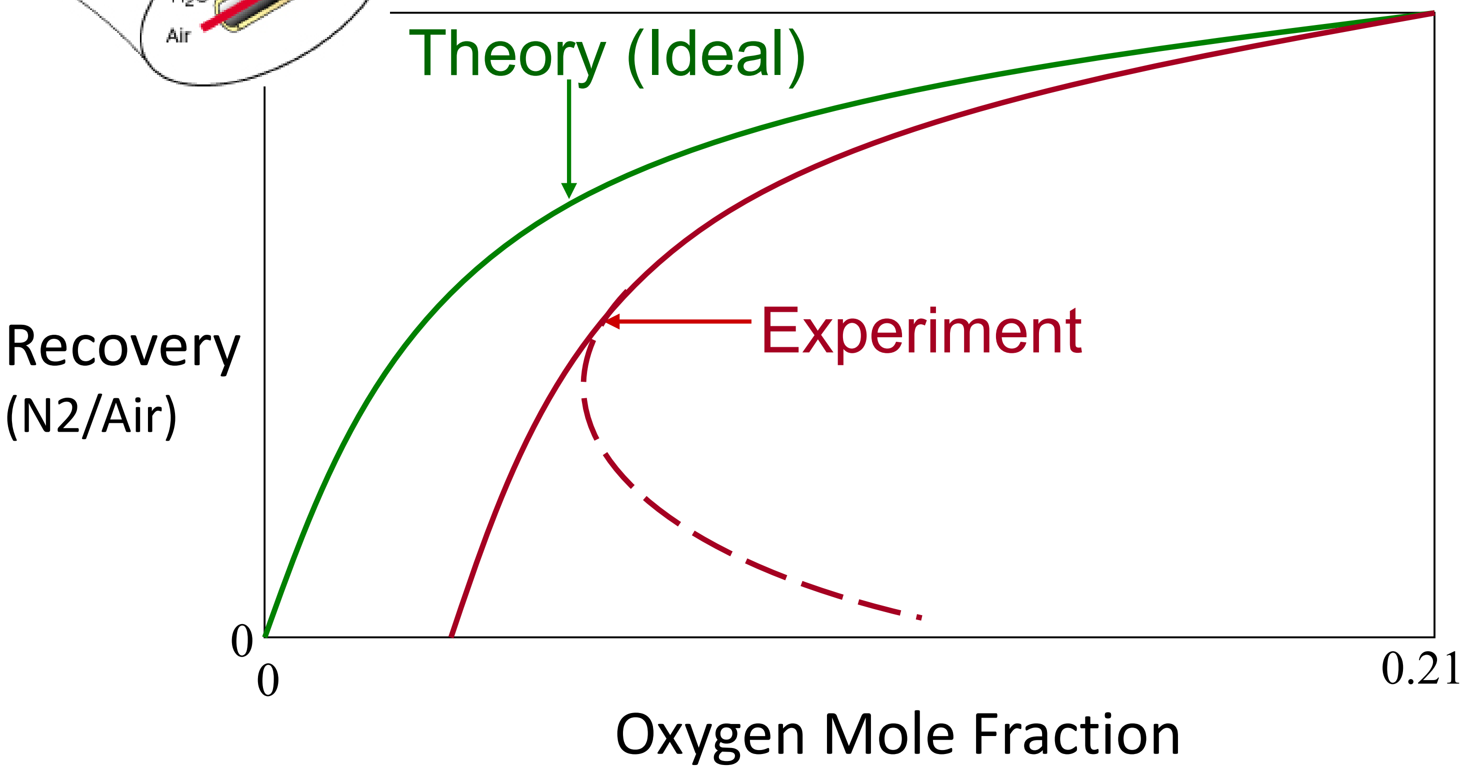
IDEAL PROCESS OPTIMIZATION



Che Mat and Lipscomb, 2017, 2019

REAL MODULE (HF) PERFORMANCE



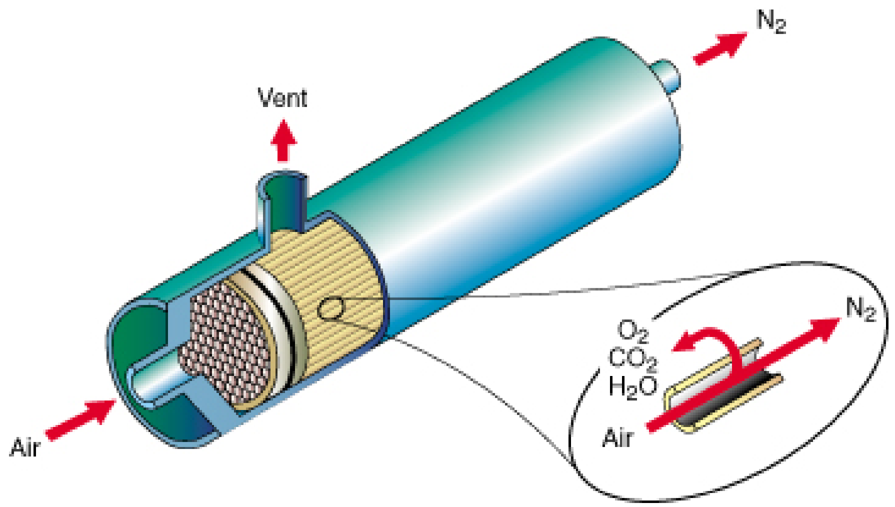


ORIGINS OF INEFFICIENCY

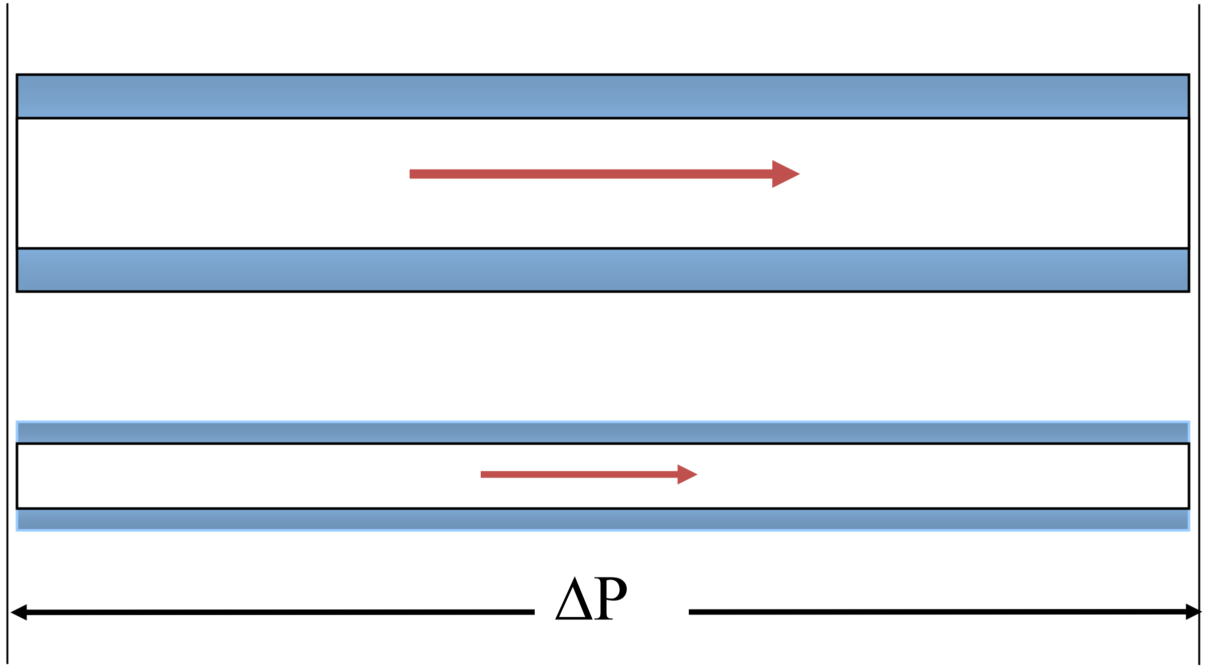
- Thermal
- Flow distribution
- Spacer design

FLOW DISTRIBUTION EFFECTS

- Tubesheet imperfections
  – Flow between shell and lumen
- Fluid distribution into lumen
  – Header distribution
  – Flow within fibers (fiber property variation)
- Fluid distribution into shell
  – Header distribution
  – Flow within bundle



EFFECT OF FIBER PROPERTY VARIATIONS



J. Lemanski and G. G. Lipscomb, J. Membrane Sci. 167 (2000) 241-252.
B. Liu, G. G. Lipscomb, and J. A. Jensvold, AIChEJ 47 (2001) 2206-2219.
S. Sonalkar, P. Hao, and G. G. Lipscomb, IEC Res., 49 (2010) 12074–12083.

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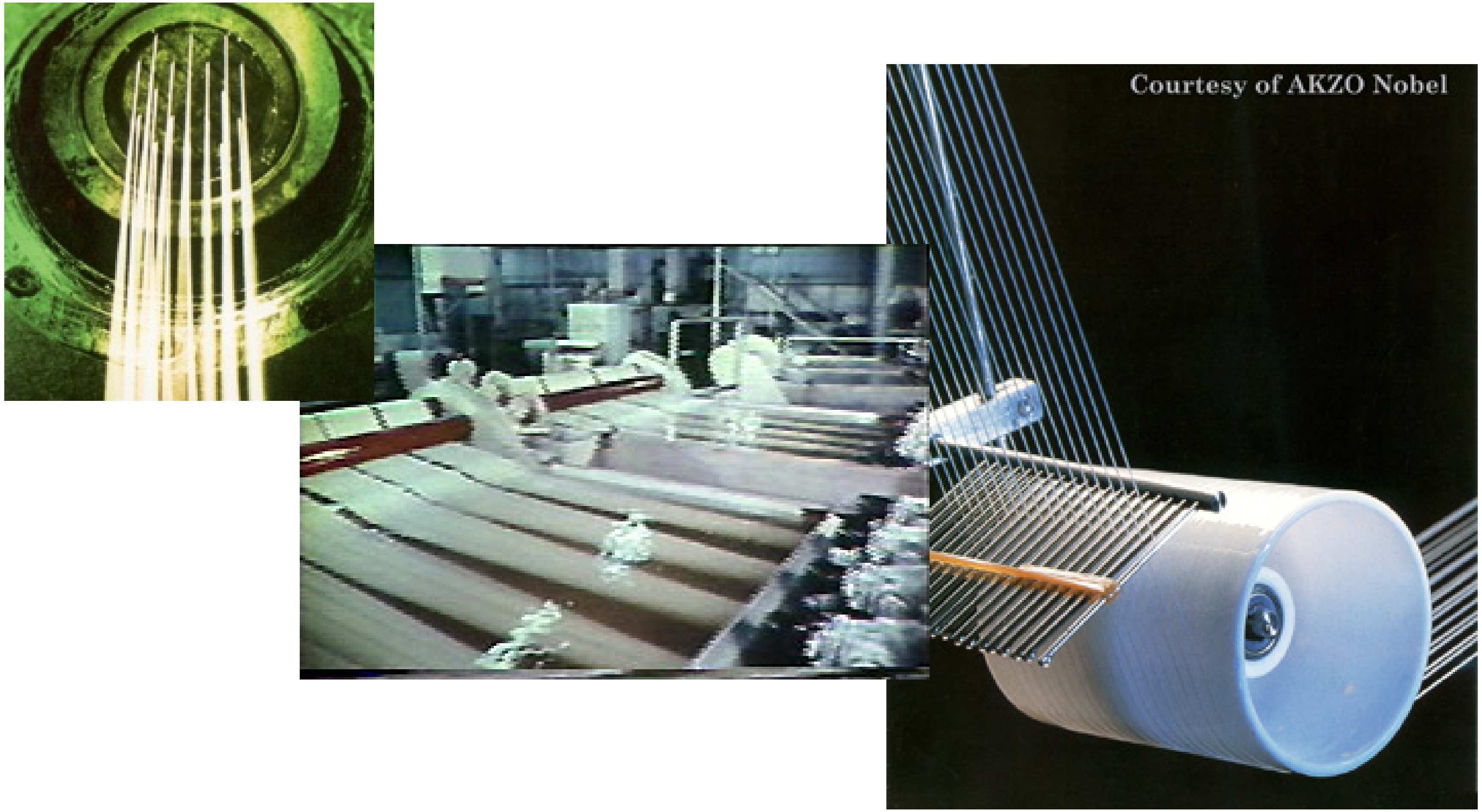


http://www.fibersource.com/f-tutor/techpag.htm

EFFECT OF FIBER PROPERTY VARIATIONS

- Gaussian distribution:

$$g(\phi)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{(\phi-\bar{\phi})^2}{2\sigma^2}\right]$$

- Average flow
  - Gauss-Hermite approx.

$$\bar{f}=\int_{ID_{\min}}^{ID_{\max}}\int_{Q_{2,\min}}^{Q_{2,\max}}\int_{\alpha_{\min}}^{\alpha_{\max}} fg\,(dID)(dQ_2)(d\alpha)$$

- Retentate/Permeate mass balances

$$\frac{d\theta_R}{dz}=\frac{d\theta_P}{dz}=-(J_1+J_2) \qquad \frac{d(x\theta_R)}{dz}=\frac{d(y\theta_P)}{dz}=-J_1$$

$$J_1=\alpha N^h(x-\gamma y)$$

$$J_2=N^h[(1-x)-\gamma(1-y)]$$

- Pressure drop

$$\frac{d\Pi^2}{dz}=-N^p\theta_R$$

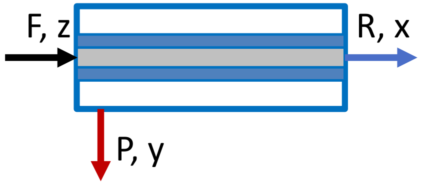
- Boundary conditions
  - Inlet
  - Outlet

$$x=x_f \qquad \theta_R=1$$

$$y=\frac{J_1}{J_1+J_2} \qquad \theta_P=P/F=0$$

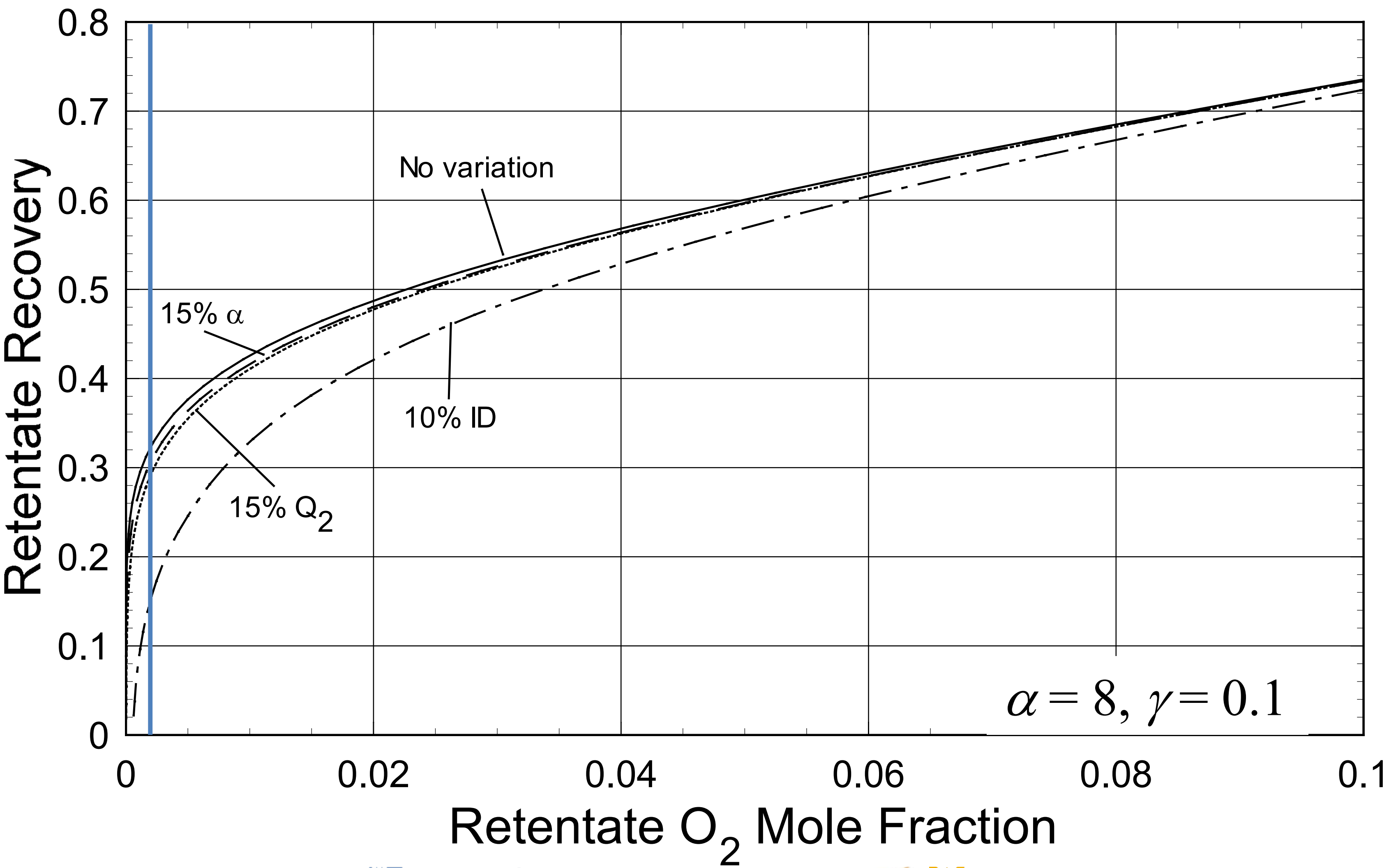
- For given ΔP, determine flow in each fiber that gives same ΔP

RETENTATE RECOVERY

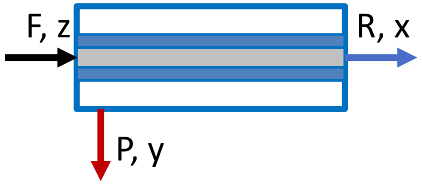


Retentate Recovery = R/F

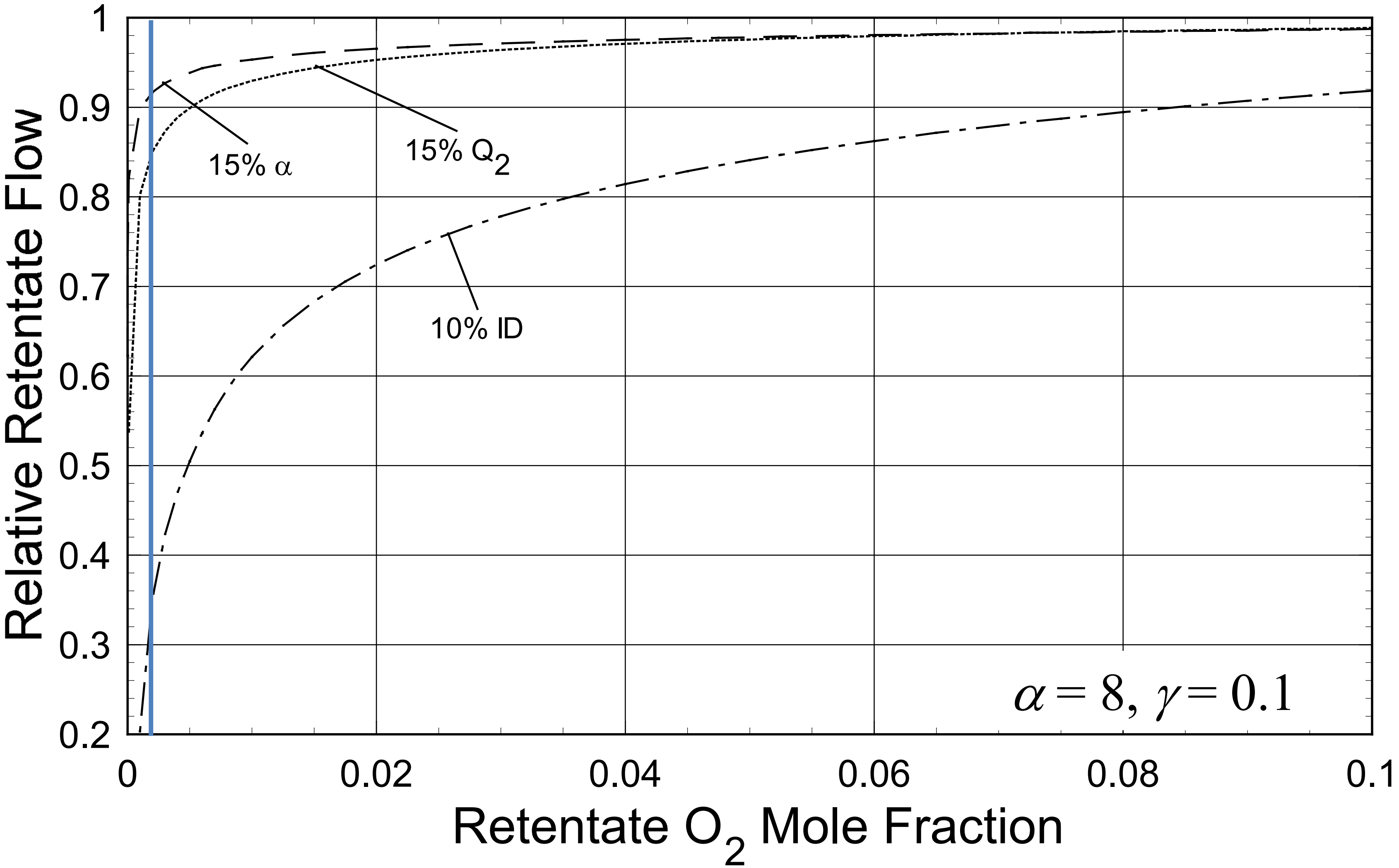
Retentate O_2 = x



MODULE PRODUCTIVITY

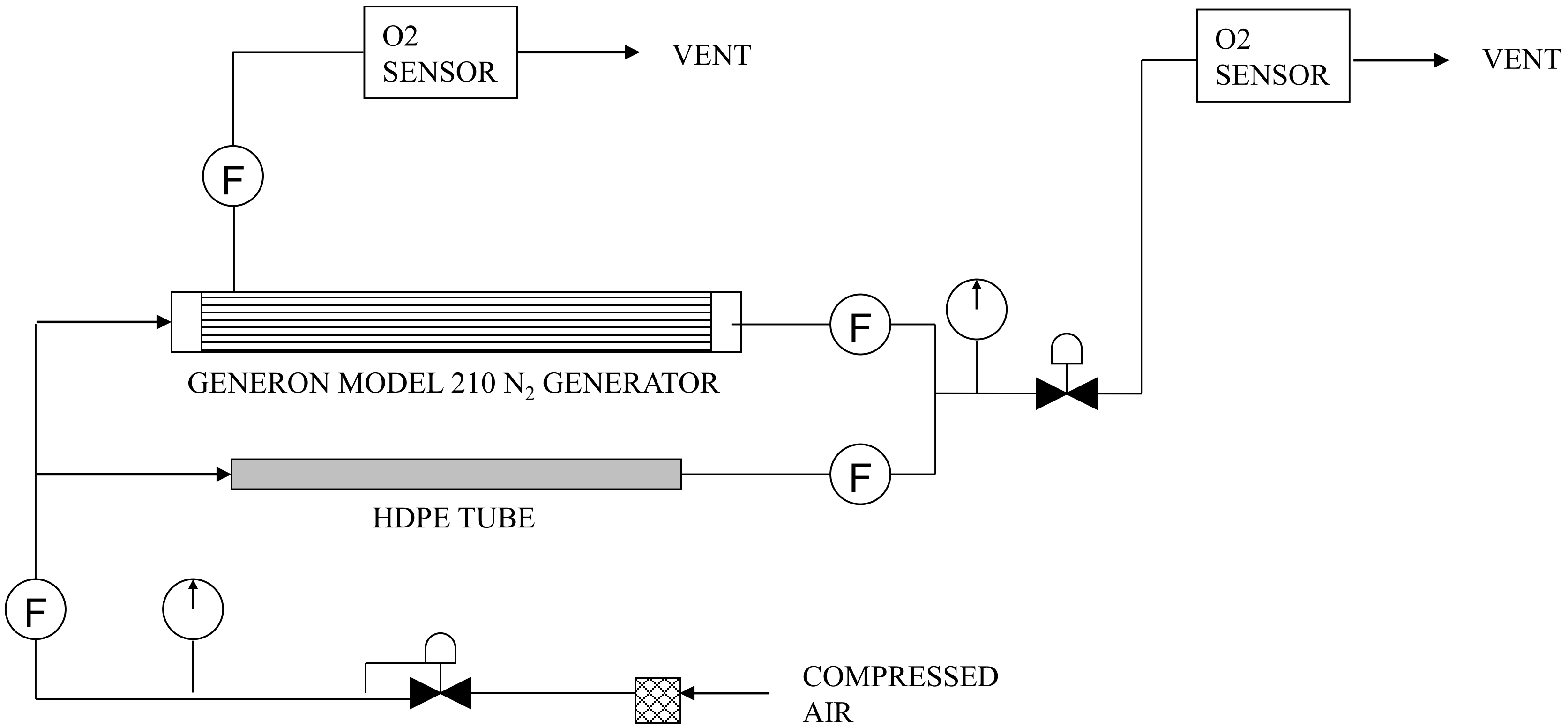


Relative Flow = R/R_{ideal}
Retentate O_2 = x



EXPERIMENTAL OBSERVATIONS

- Generon, Model 210



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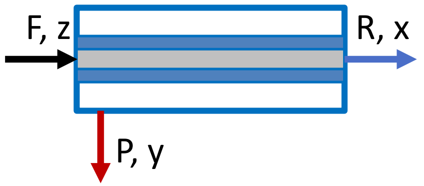

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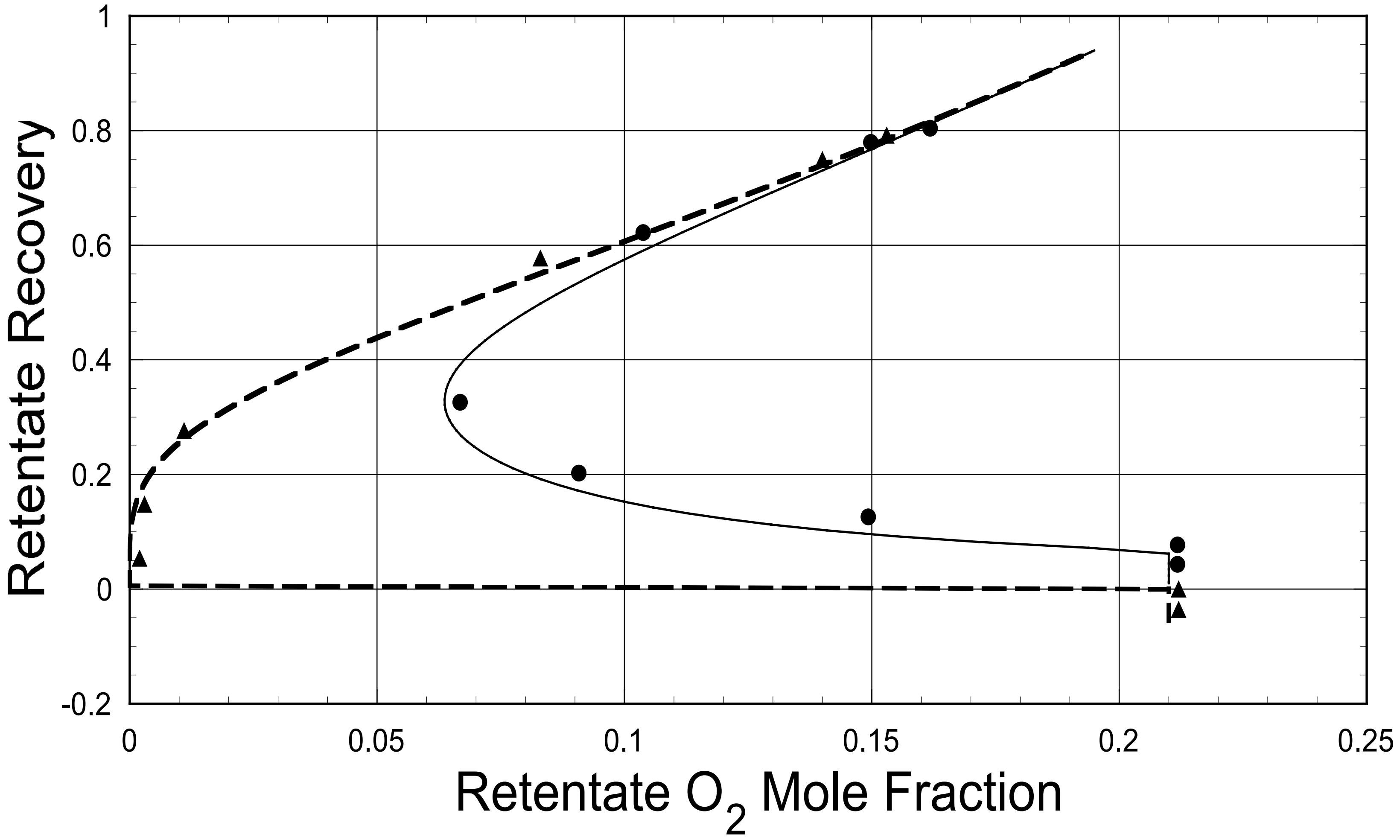

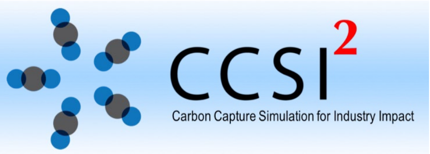

EXPERIMENTAL OBSERVATIONS

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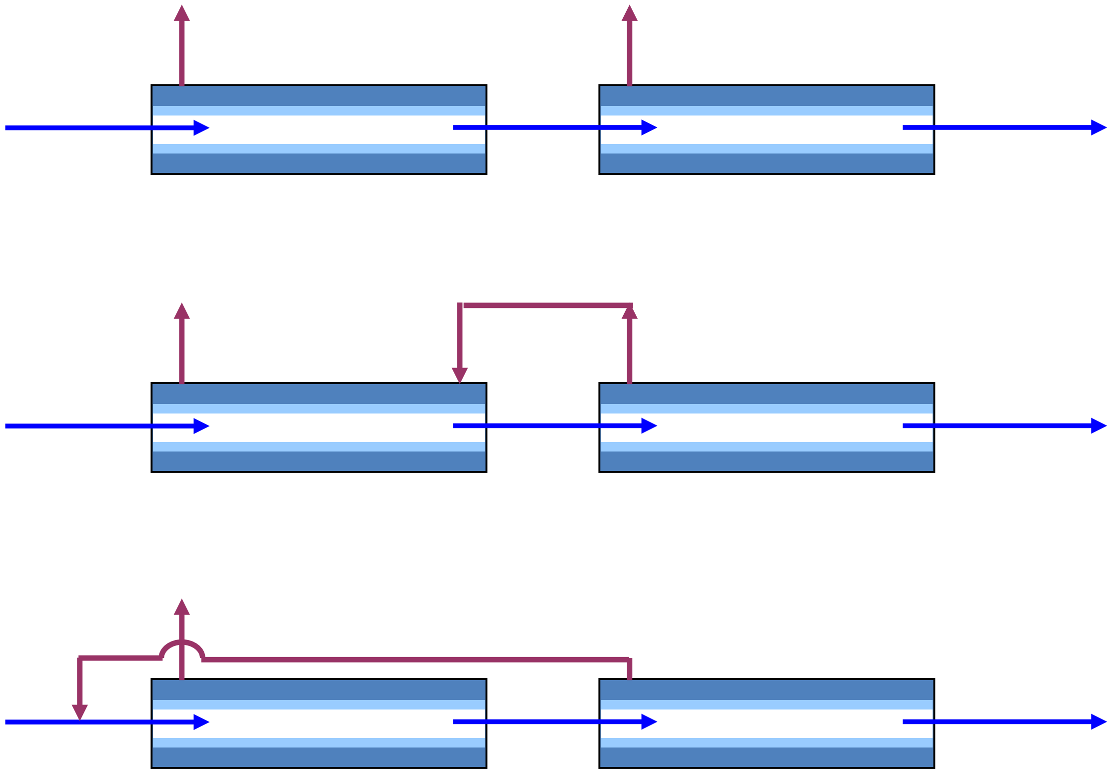
Permeate Venting

Recycle as Sweep

Recycle to Feed



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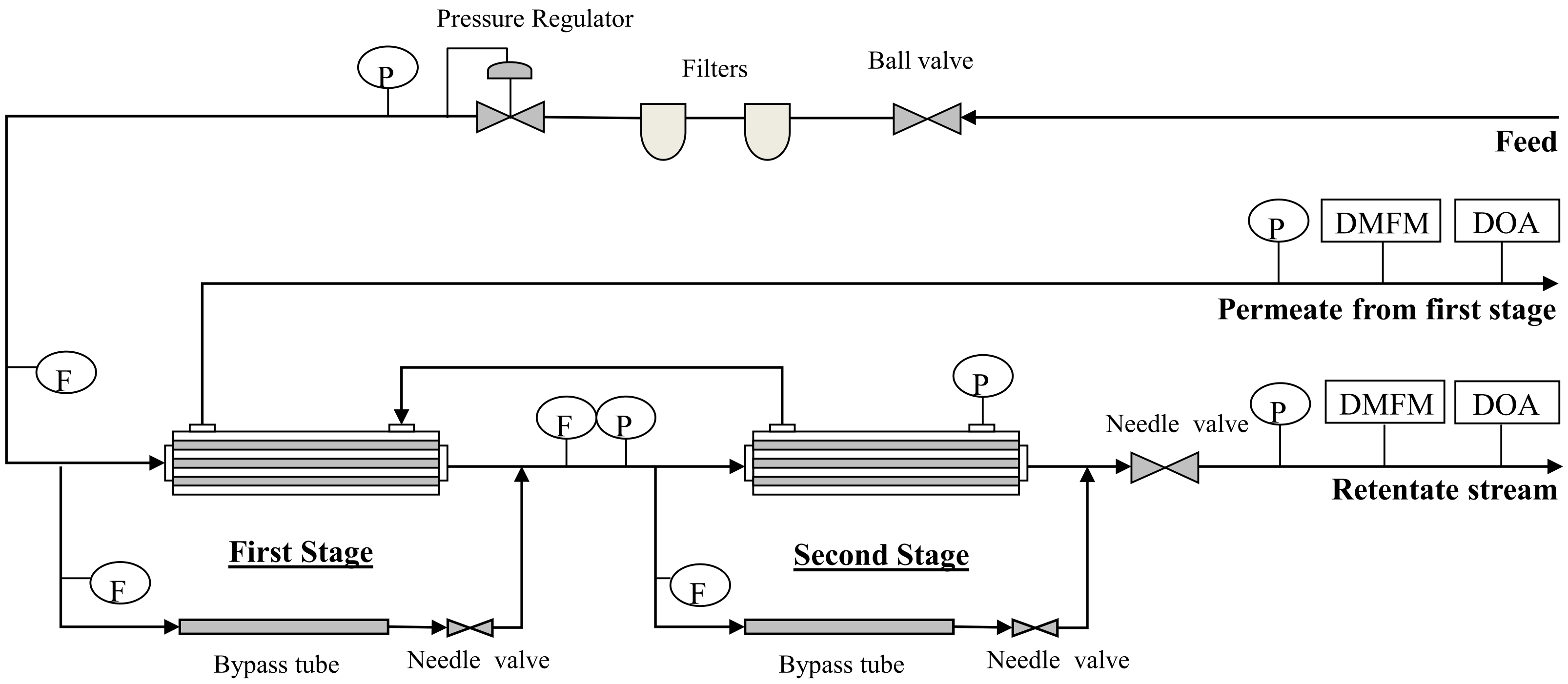
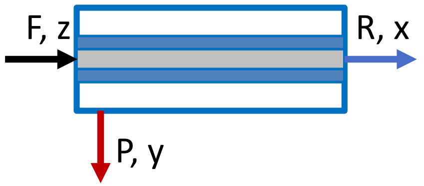


DMFM: Digital mass flow meter
DOA: Digital oxygen analyzer
P: Pressure indicator
F: Flow meter

EXPERIMENTAL OBSERVATIONS



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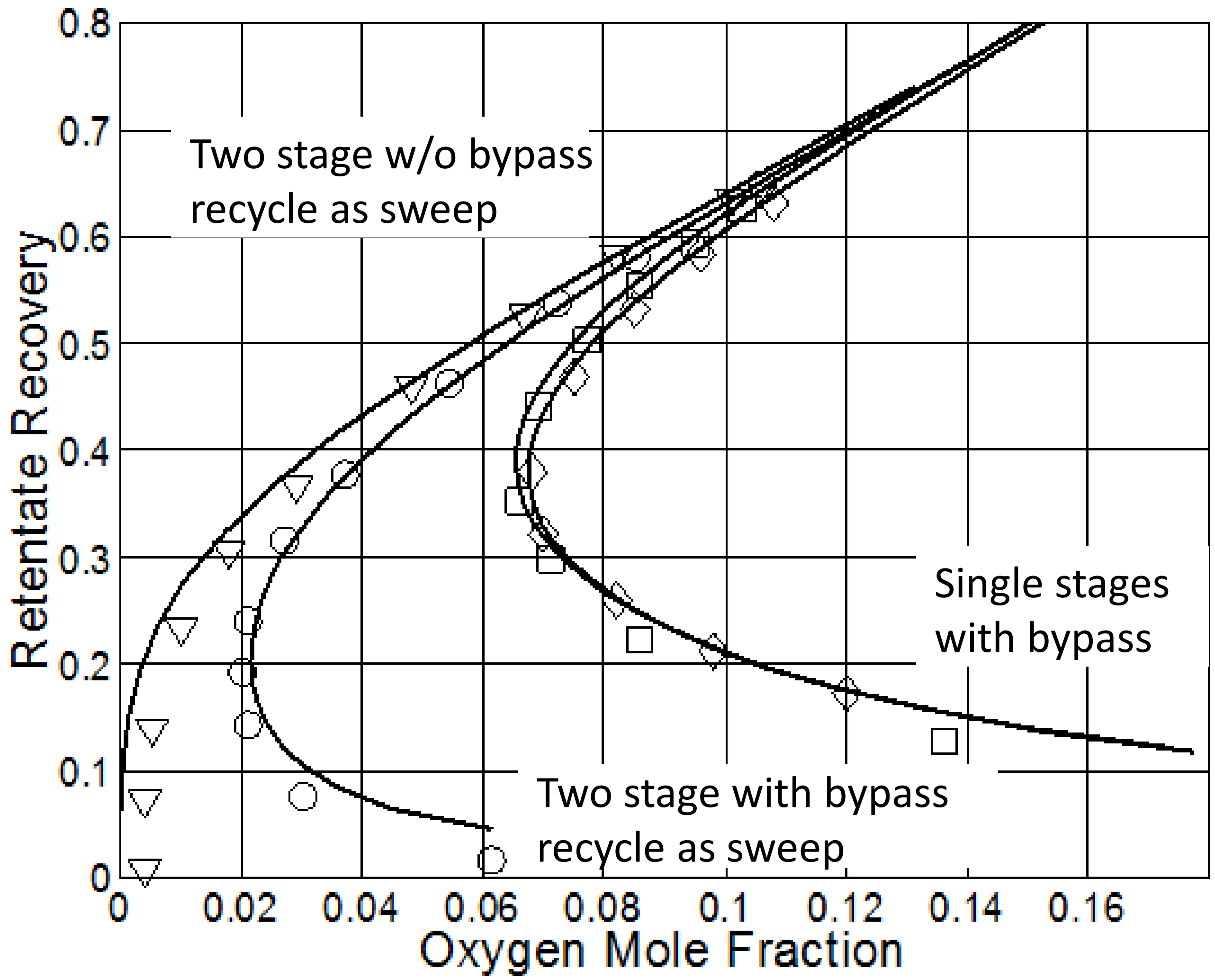
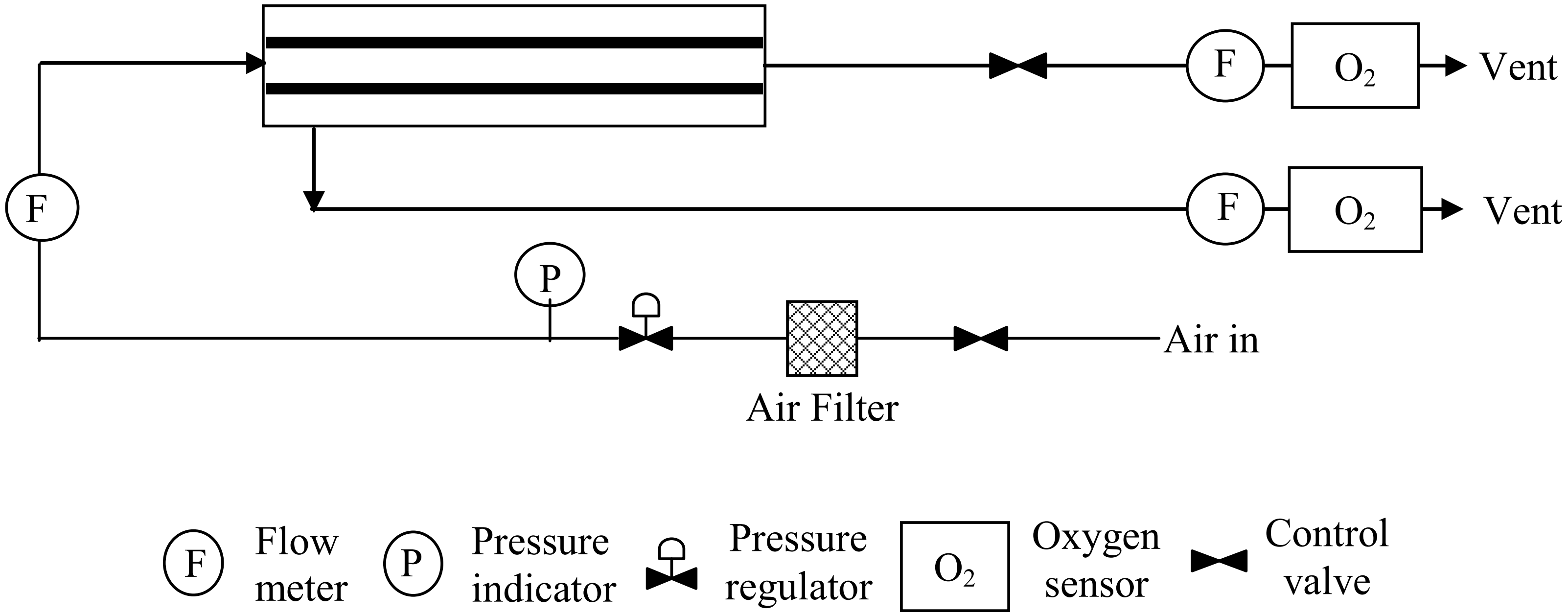
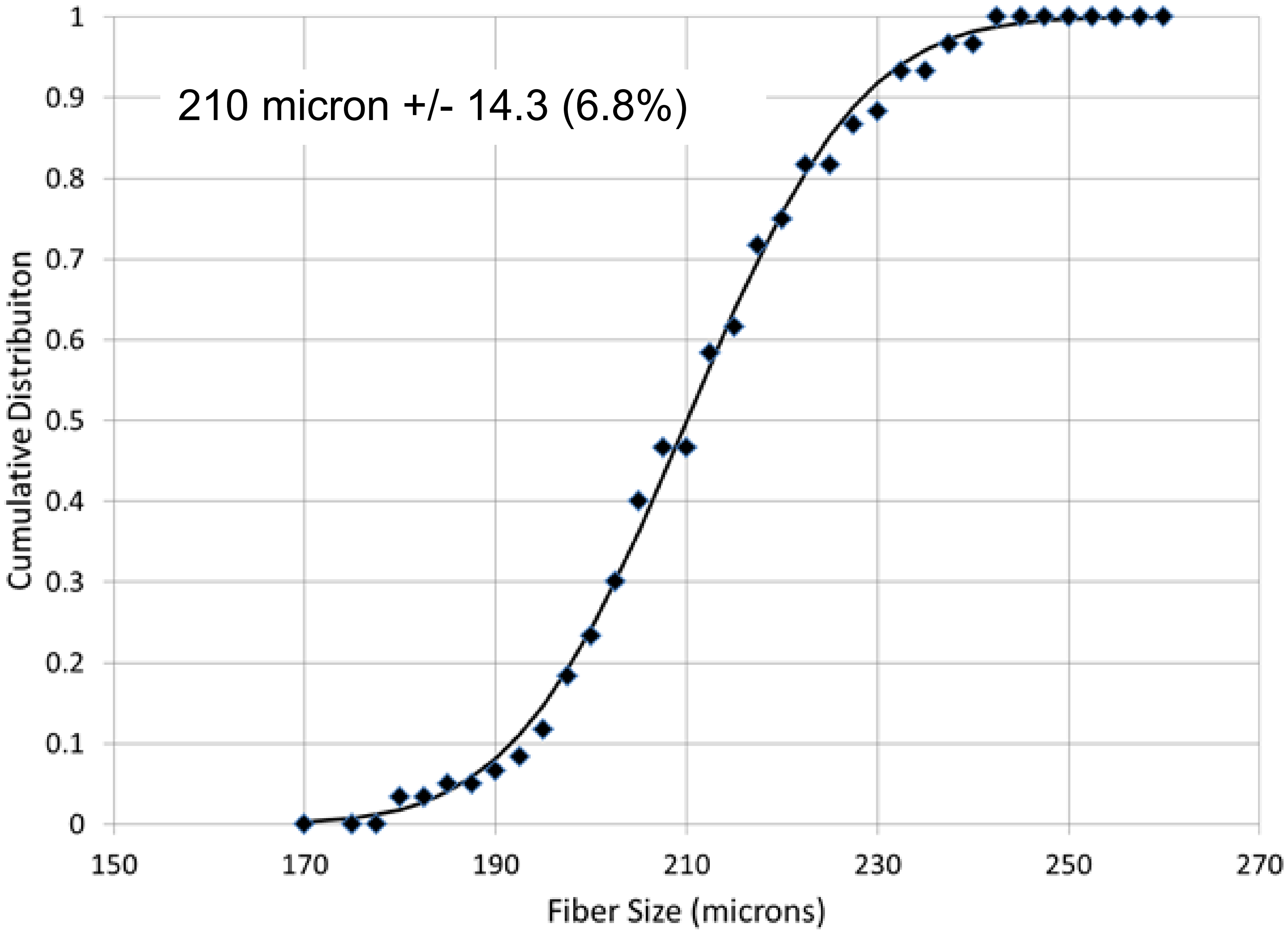


OXYGEN PRODUCTION

- Permea, Inc., Model PPA-22AD



FIBER SIZE DISTRIBUTION



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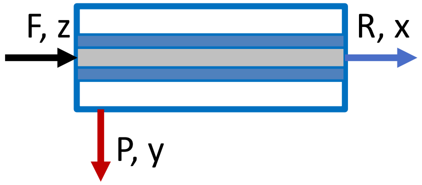
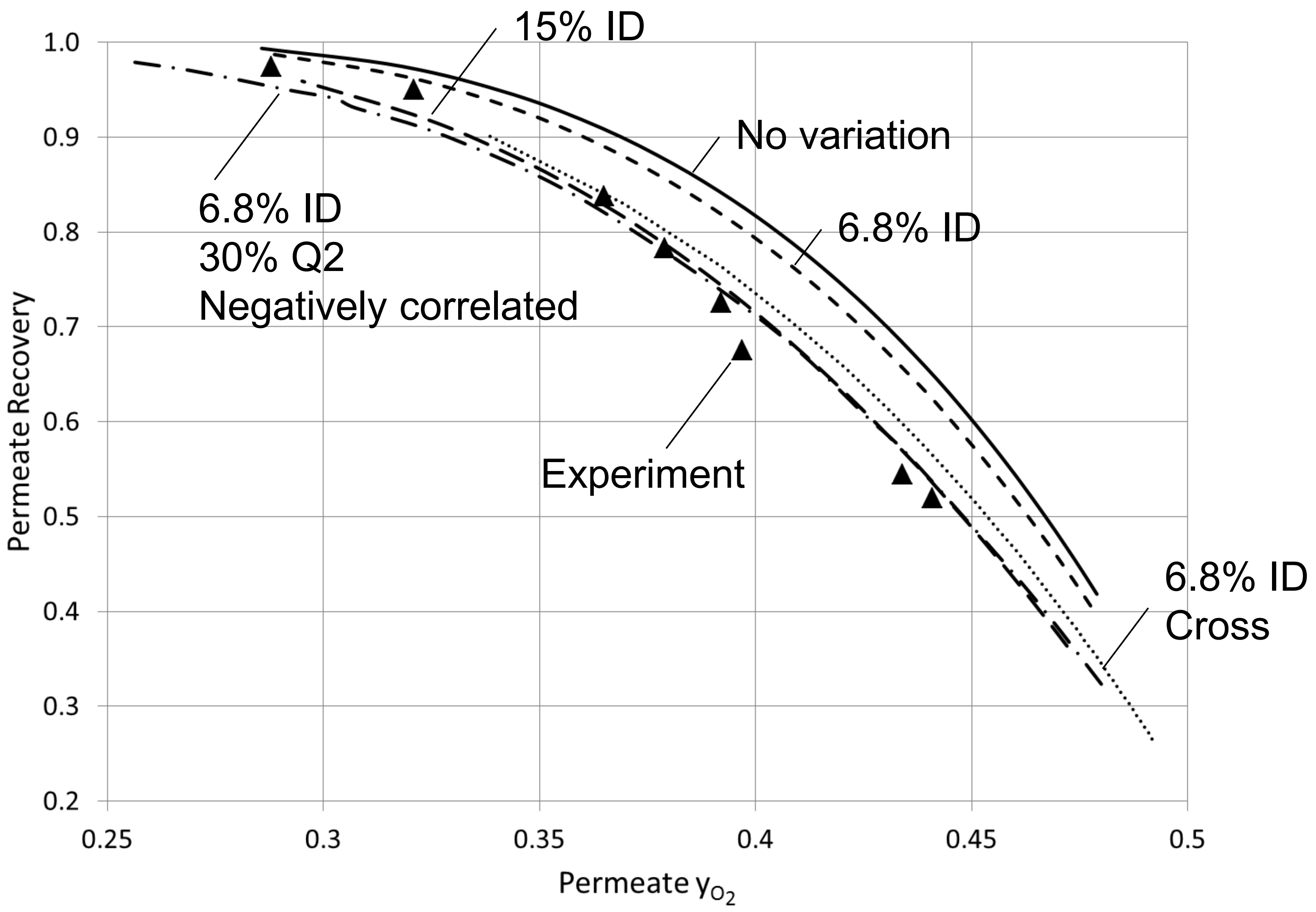


Permeate Recovery = P/F

Permeate O_2 = y



CONCLUSIONS

- Process development typically with ideal module models – real module performance may differ
- For HF modules:
  - Fiber variations are detrimental to performance: ID variations have greatest effect
  - Staging can dramatically improve performance
  - Similar behavior for permeate or retentate product
- Simulation can be used to establish manufacturing QC guidelines
- Additional efforts to advance module simulation …

ON GOING WORK

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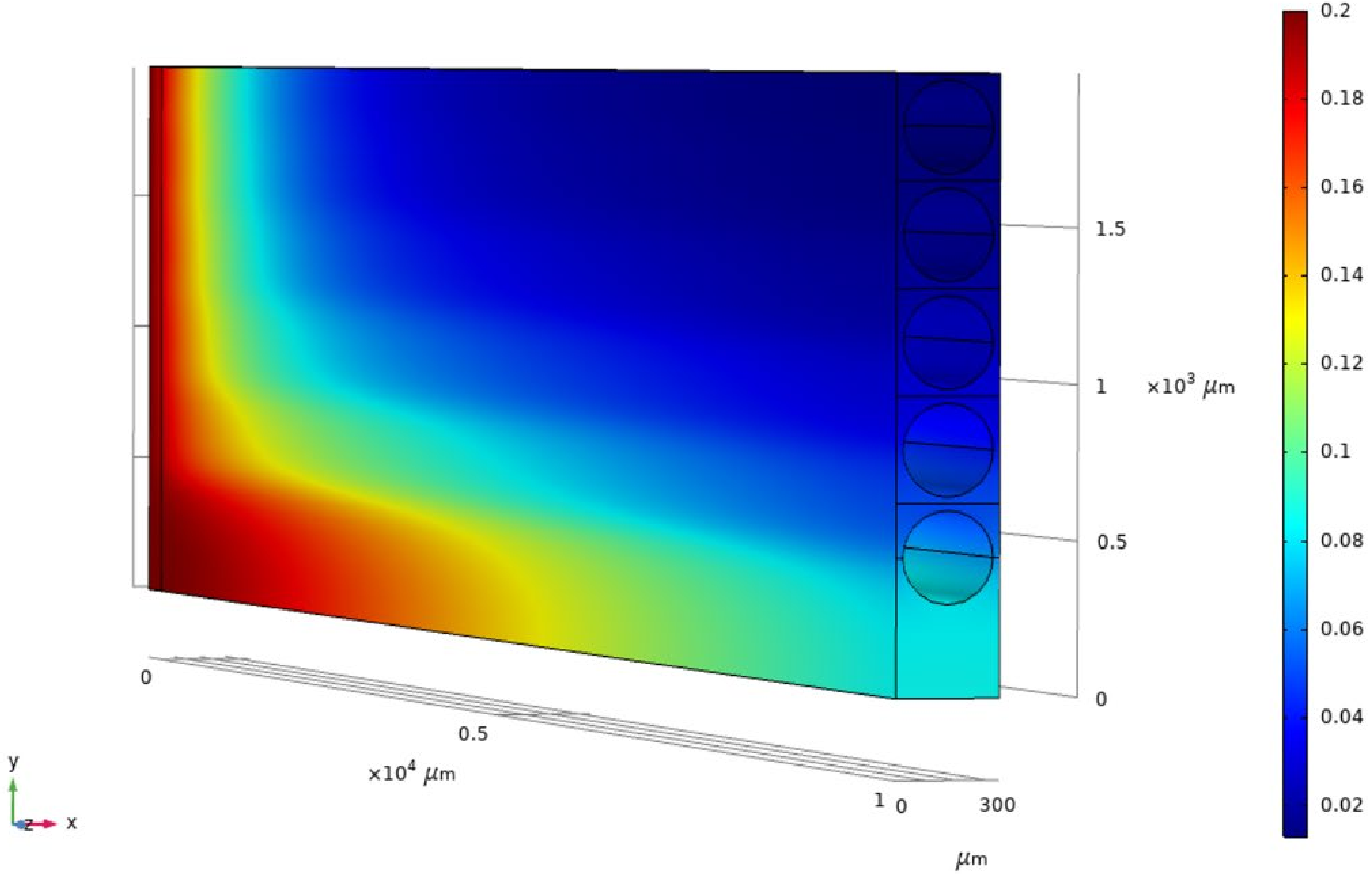

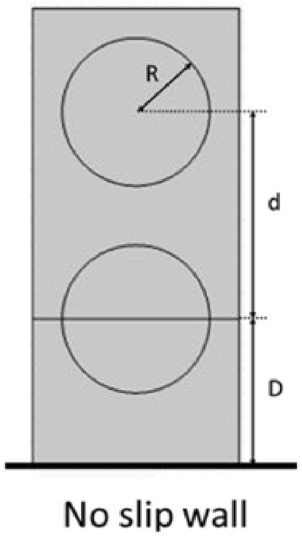

FUTURE WORK

- Effect of fiber variability for multicomponent streams
- Flow distribution from header
- Effect of porous support

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For more information

https://www.acceleratecarboncapture.org/

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