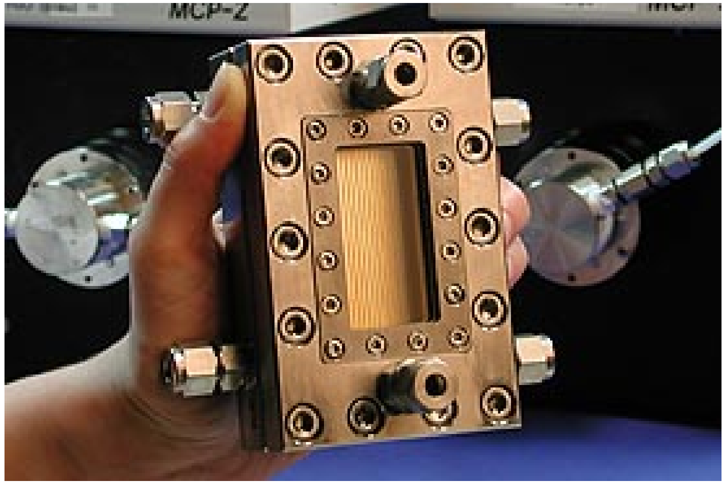
Presented at the COMSOL Conference 2008 Hannover

Process Intensification in a Falling Film Microreactor Based on Pseudo 3-D Simulation

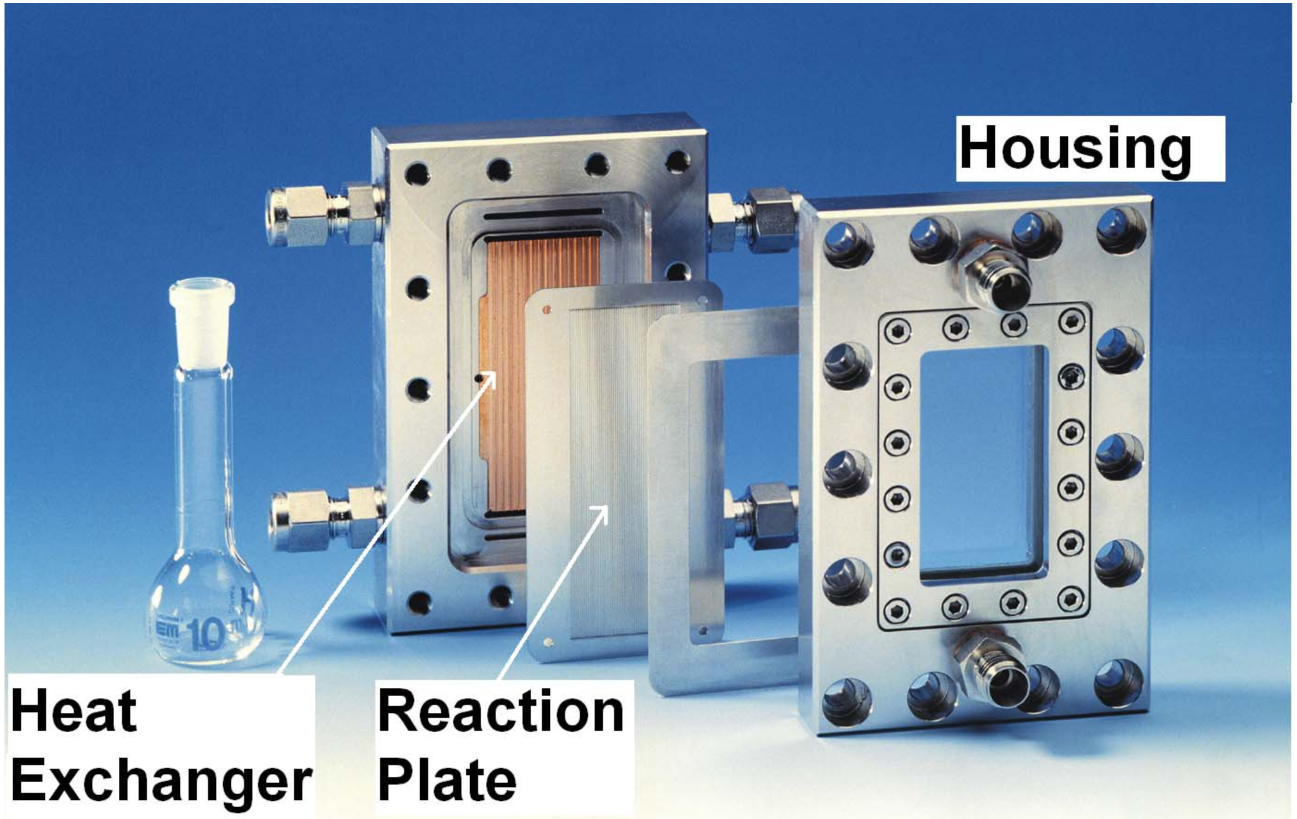
Technische Universiteit Eindhoven University of Technology

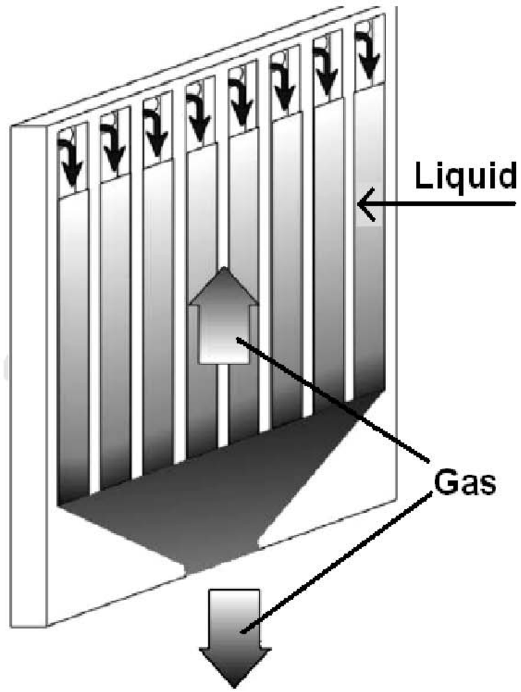


<u>Ma'moun Al-Rawashdeh</u>, Volker Hessel, Patrick Löb, Friedhelm Schönfeld, Bhanu Kiran Vankayala, Ulrich Krtschil, Christian Hofmann

Introduction

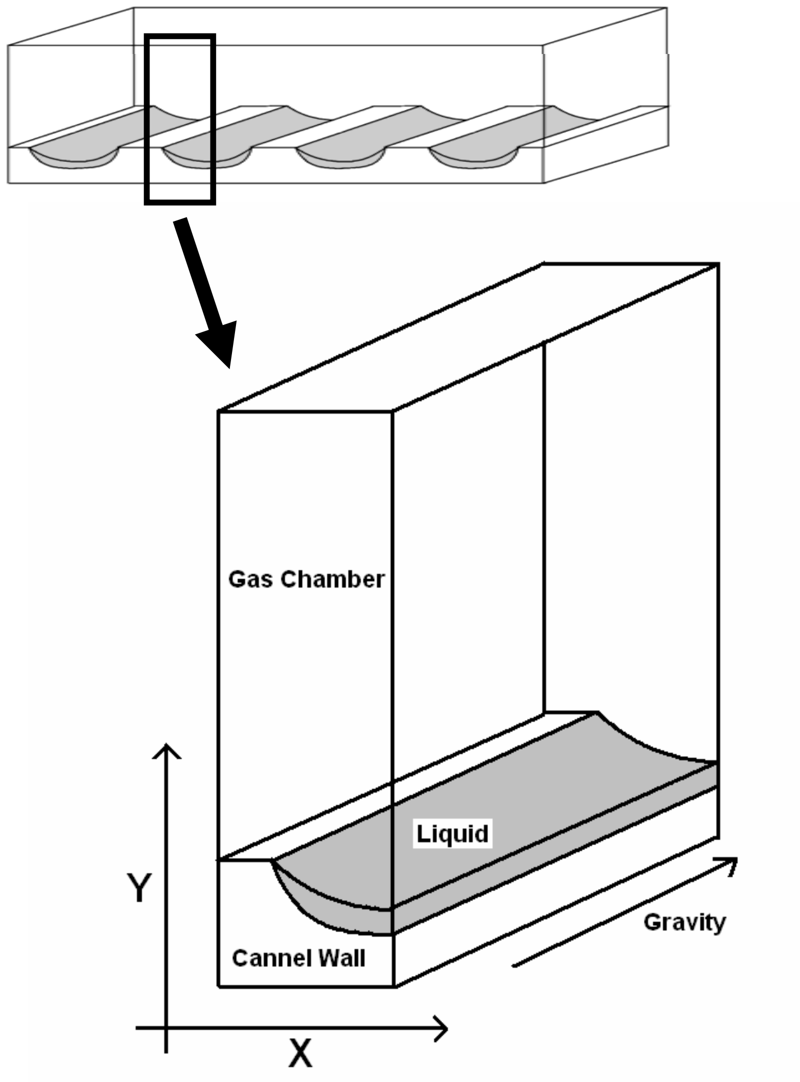
- **High surface area to volume ratio**
- **Low liquid hold-up**
- **Scale up by scale out**
- **Applications (Ex: Ozonolysis, Sulfonation, Photochlorination, Ethoxylation, Hydrogenation)**

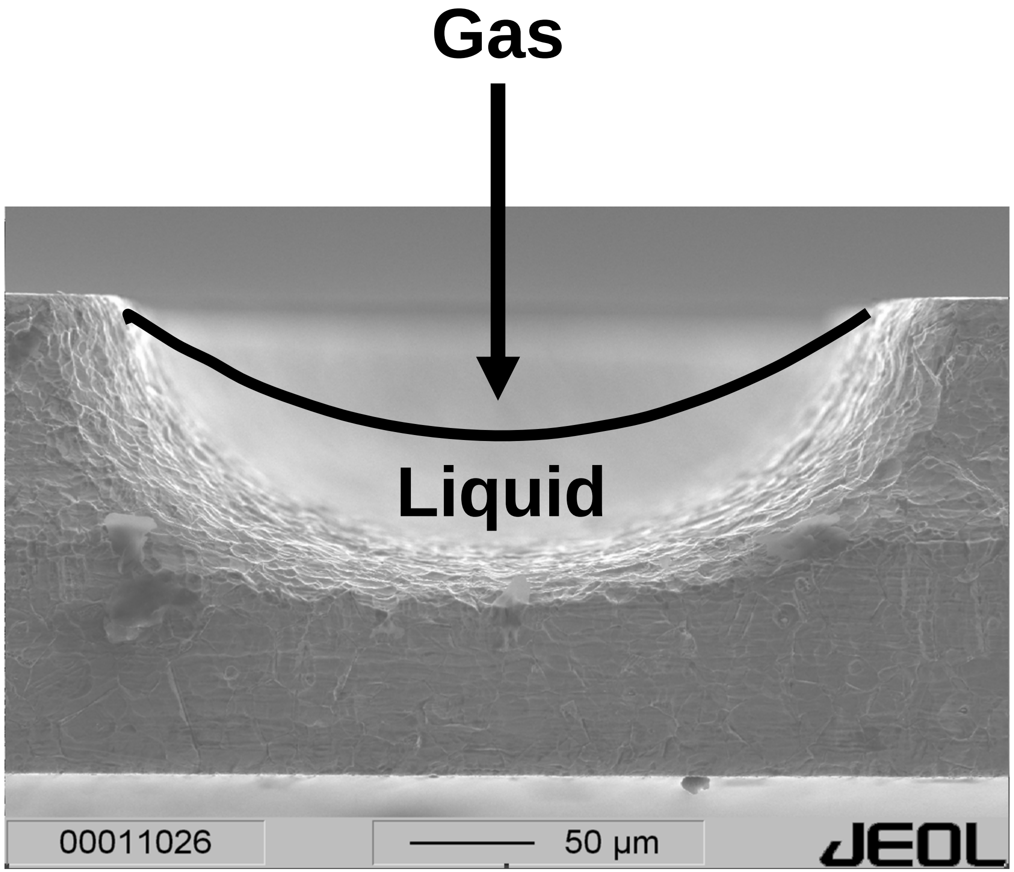




Modeling Challenge

Pseudo 3-D Model





- Channel geometry
- Liquid meniscus
- Flow rate vs. meniscus

Technische Universiteit Eindhoven University of Technology

Modeling & Simulation

- **Reaction Model**

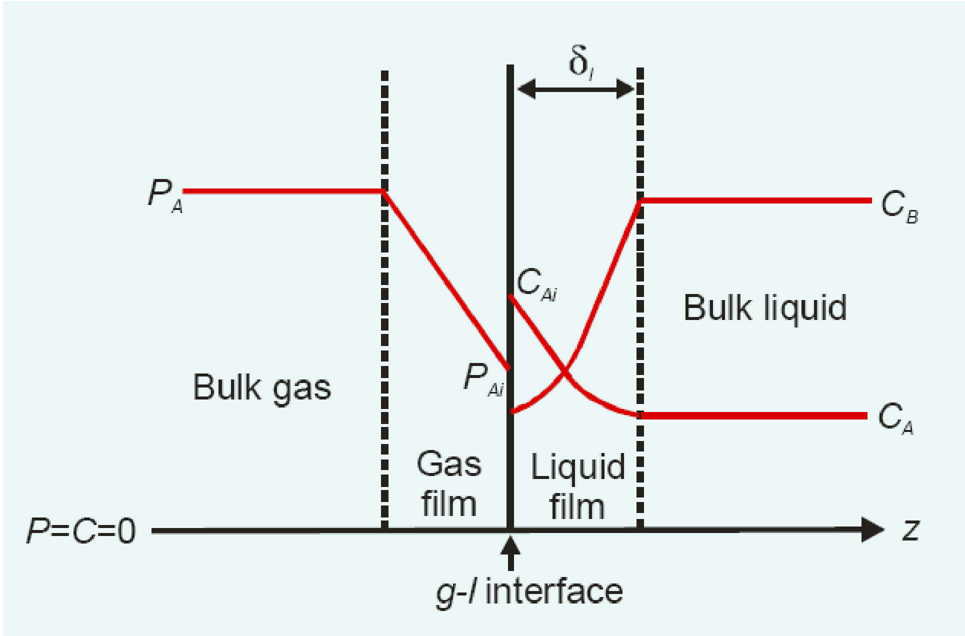
$$CO_{2(g)} \rightleftarrows CO_{2(l)}$$

$$CO_{2(l)} + OH^- \rightleftarrows HCO_3^-$$

$$HCO_3^- + OH^- \rightleftarrows CO_3^{2-} + H_2O$$

$$2NaOH + CO_2 \rightarrow Na_2CO_3 + H_2O$$

Reaction rate = k_{OH} x C_{OH} x C_{CO2}



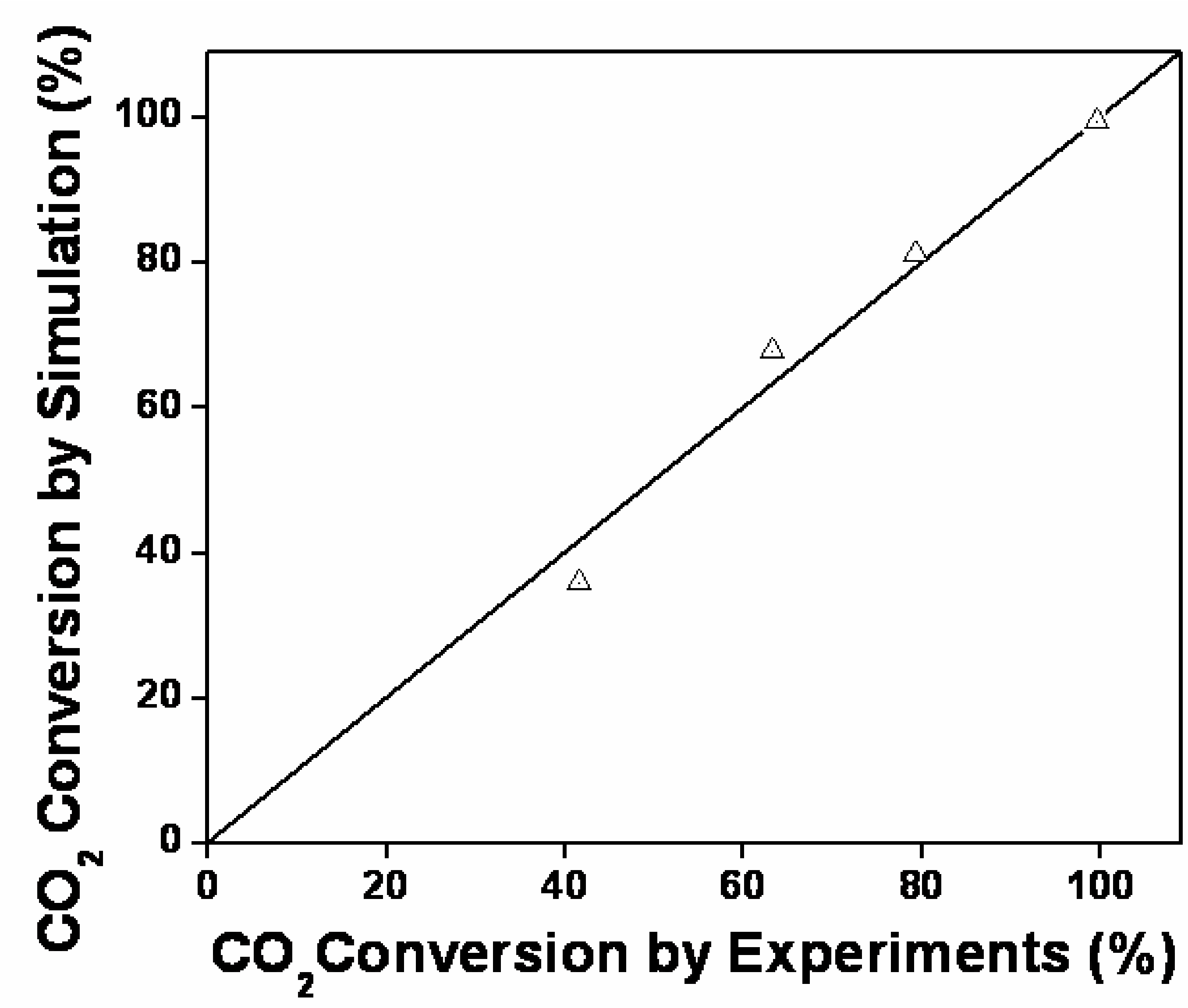
Modeling

	Liquid	Gas
Momentum	$-\mu_l\left(\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}\right)=\rho_l g$	$-\mu_g\left(\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}\right)=\frac{\partial P}{\partial z}$
Material	$v_{l,z}\frac{\partial c_i}{\partial z}=D_i\left(\frac{\partial^2 c_i}{\partial x^2}+\frac{\partial^2 c_i}{\partial y^2}\right)+R_i$	$v_{g,z}\frac{\partial c_{g,CO_2}}{\partial z}=D_{g,CO_2}\left(\frac{\partial^2 c_{g,CO_2}}{\partial x^2}+\frac{\partial^2 c_{g,CO_2}}{\partial y^2}\right)$

$$i = CO_2, OH^-, CO_3^{2-}$$

Technische Universiteit Eindhoven University of Technology

Model Validation

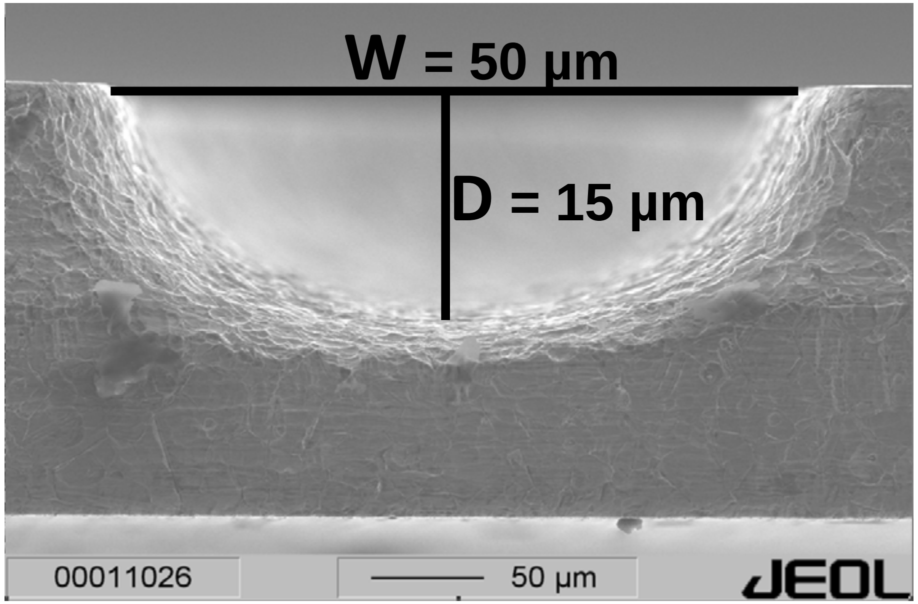


Characterization - Fabrication Precision

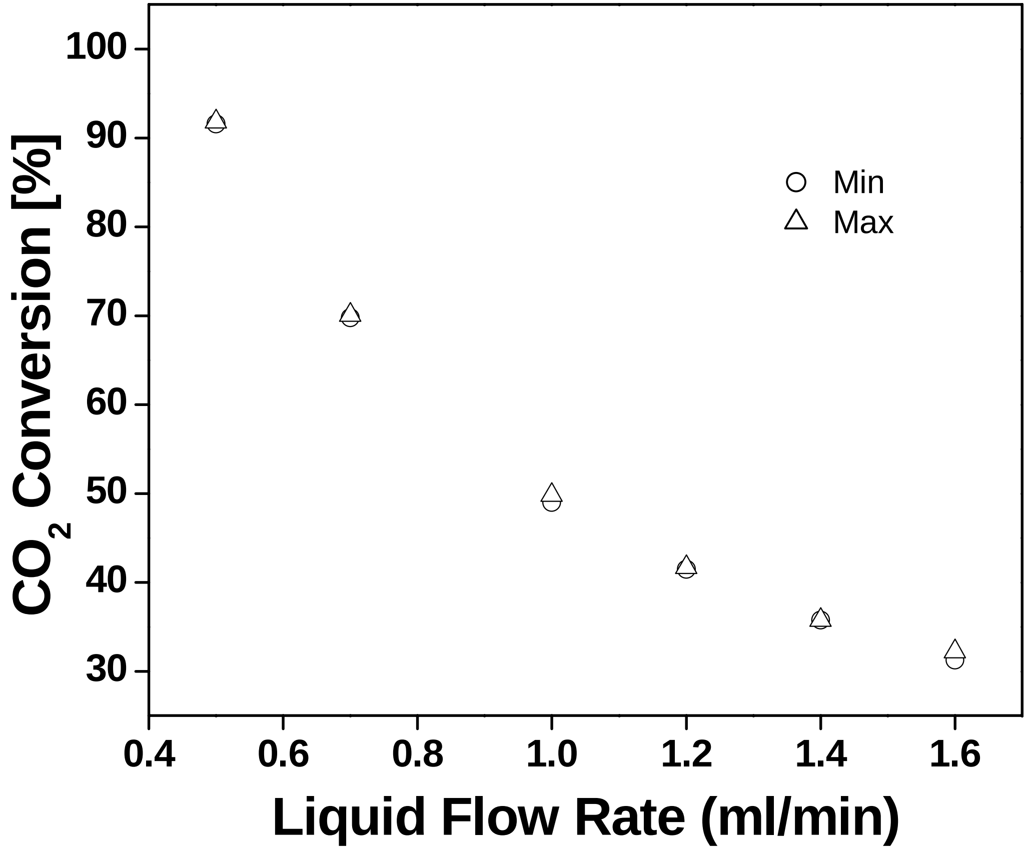
Ch. Depth = 400 μm

Ch. Width = 1200 μm

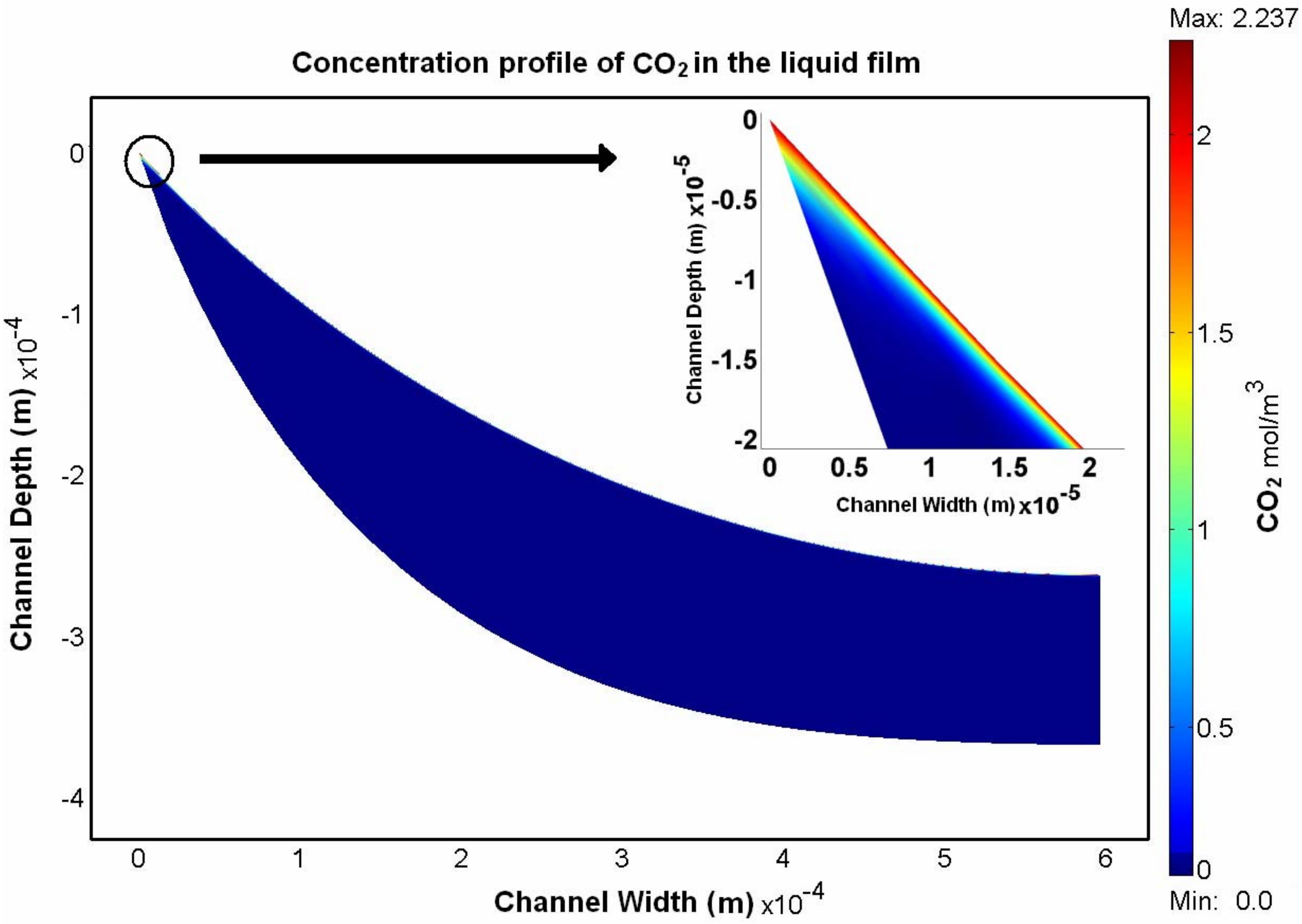
Manufacturing Tolerance



Effect of Channel Fabrication Precision on Reaction Conversion

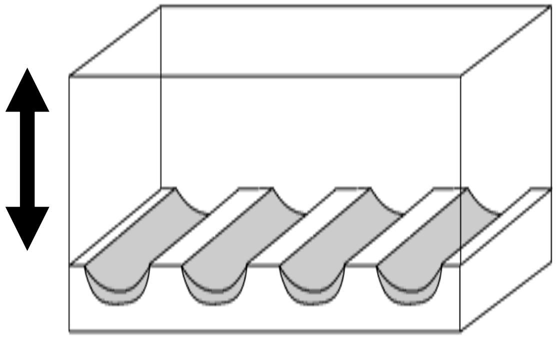


Characterization - Fabrication Precision

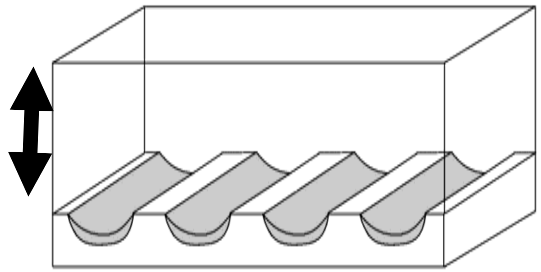


Gas Chamber Reduction

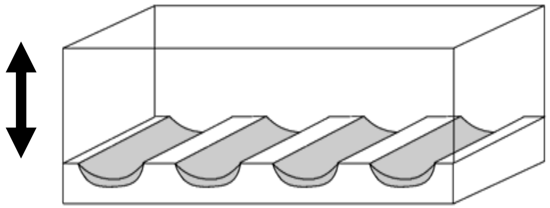
H = 5.5 mm



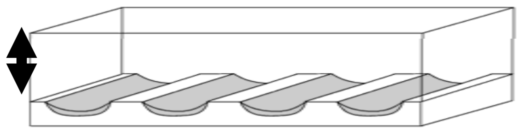
H = 2.6 mm



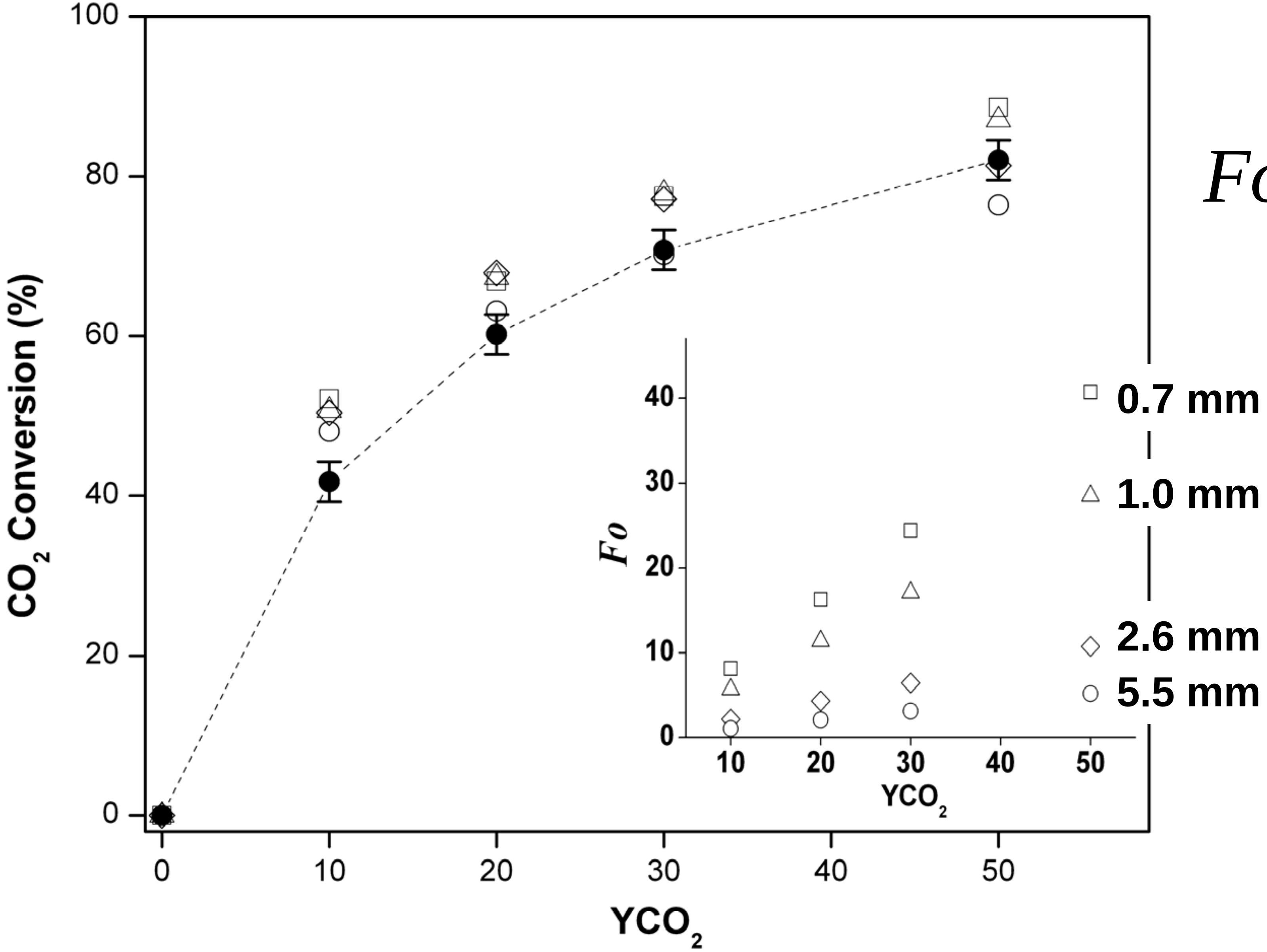
H = 1 mm



H = 0.7 mm

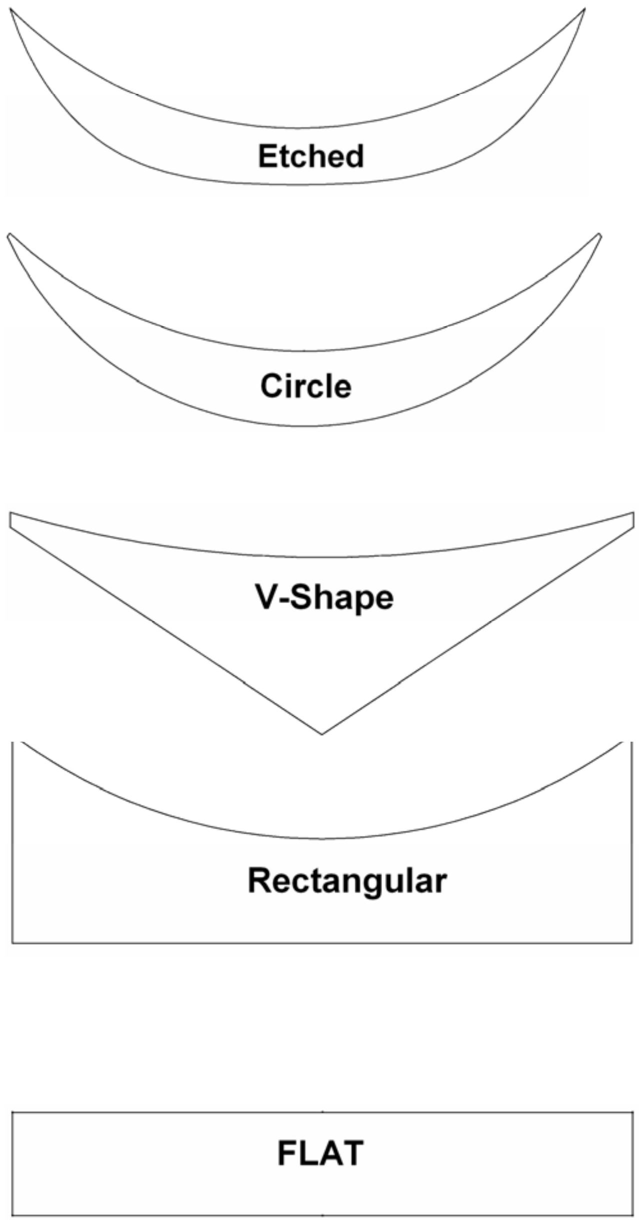


Gas Chamber Reduction



$$Fo = \frac{t_g}{\tau_d}$$

Channel Geometry Analysis



Evaluation Techniques

Intensification factor

- Adjust channel length to achieve 95% CO_2
- Structured area = channel width x channel length
- Intensification factor = liquid flow rate / structured area

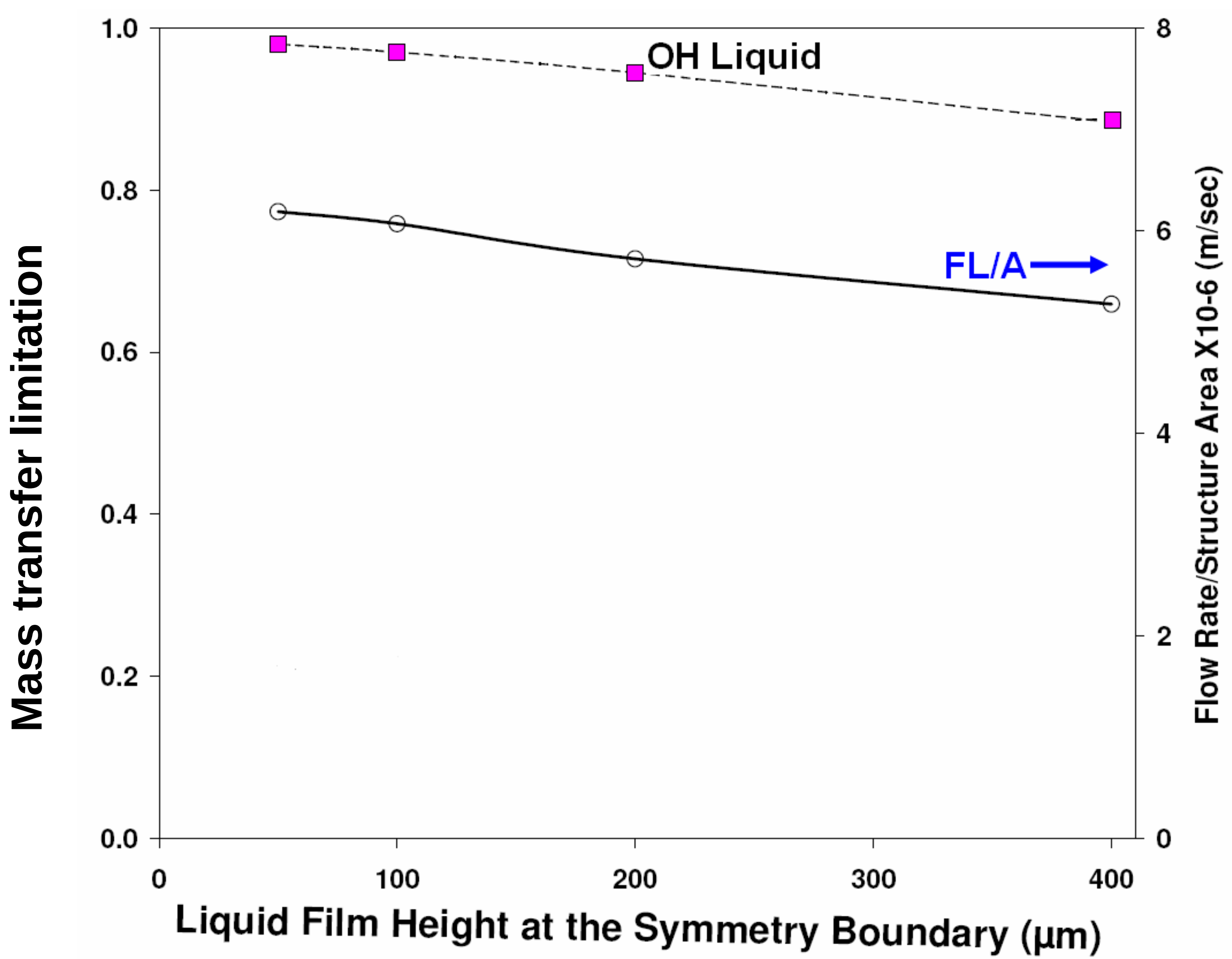
Limitation to mass transfer

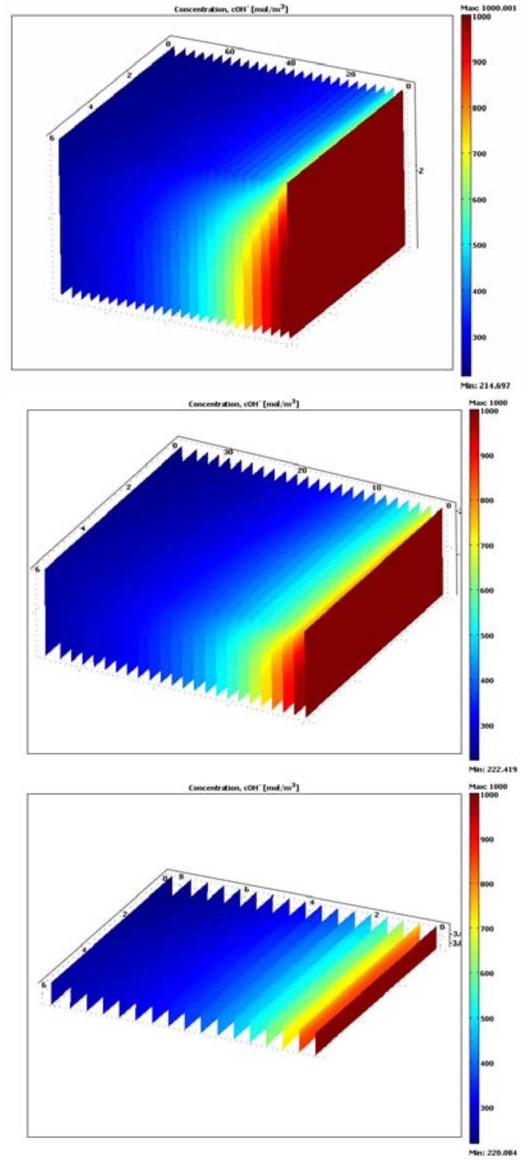
- Increase the diffusivity by a factor of 100
- Adjust channel length to achieve 95% CO_2
- Mass transfer limitation = $\dfrac{\text{Channel Length of Diffusivity x 100}}{\text{Channel Length of Actual Diffusivity}}$

Operating condition kept the same

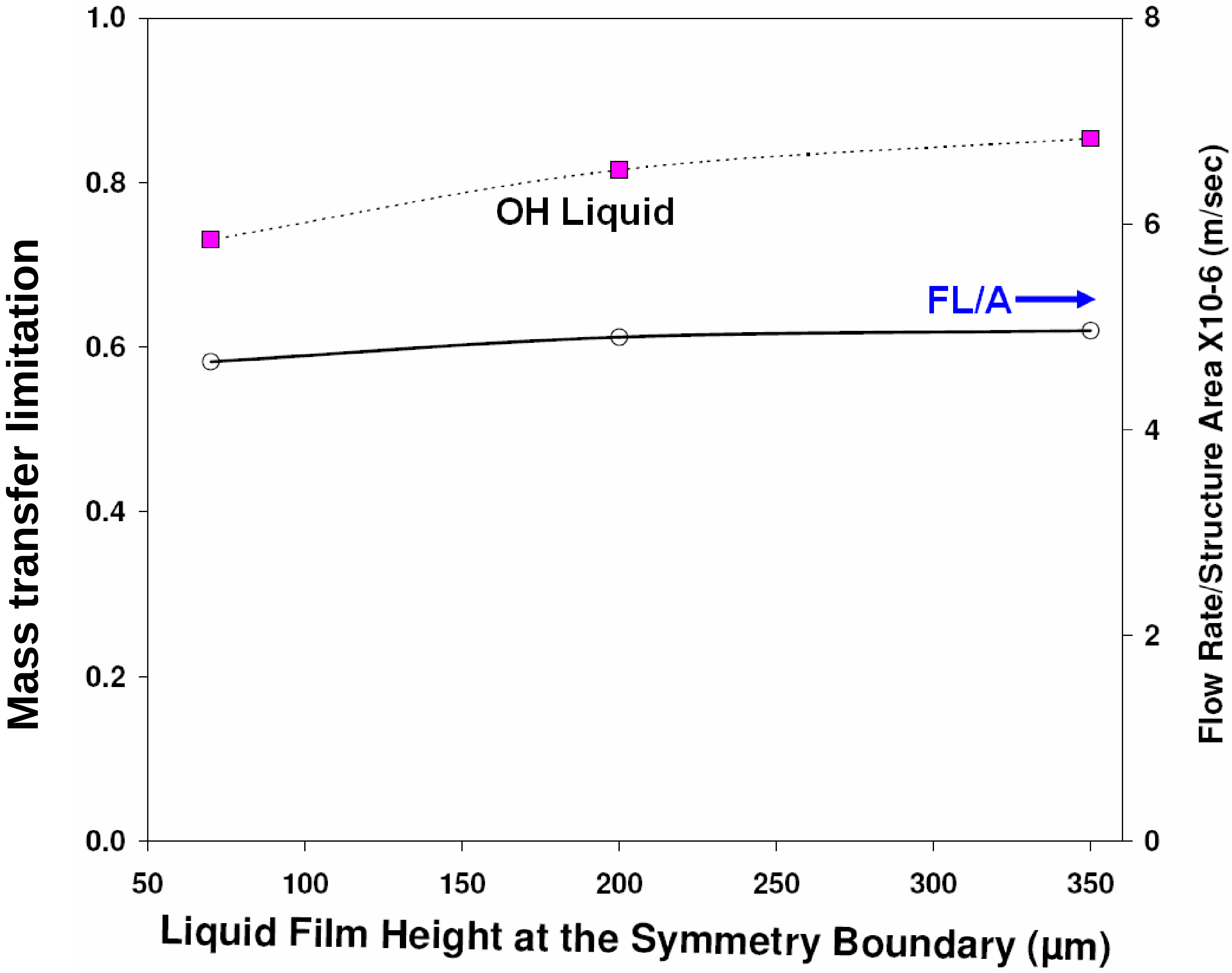
T = 298 K , P = 1 bar, CNaOH = 1M , YCO_2 = 0.1, nCO_2/nNaOH = 0.4

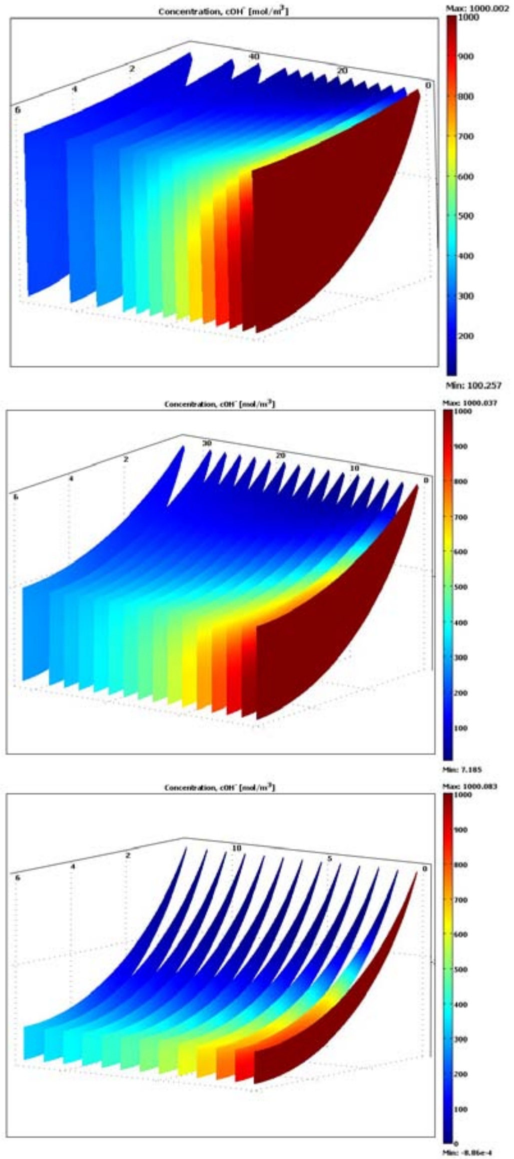
Channel Geometry Analysis– Flat Geometry



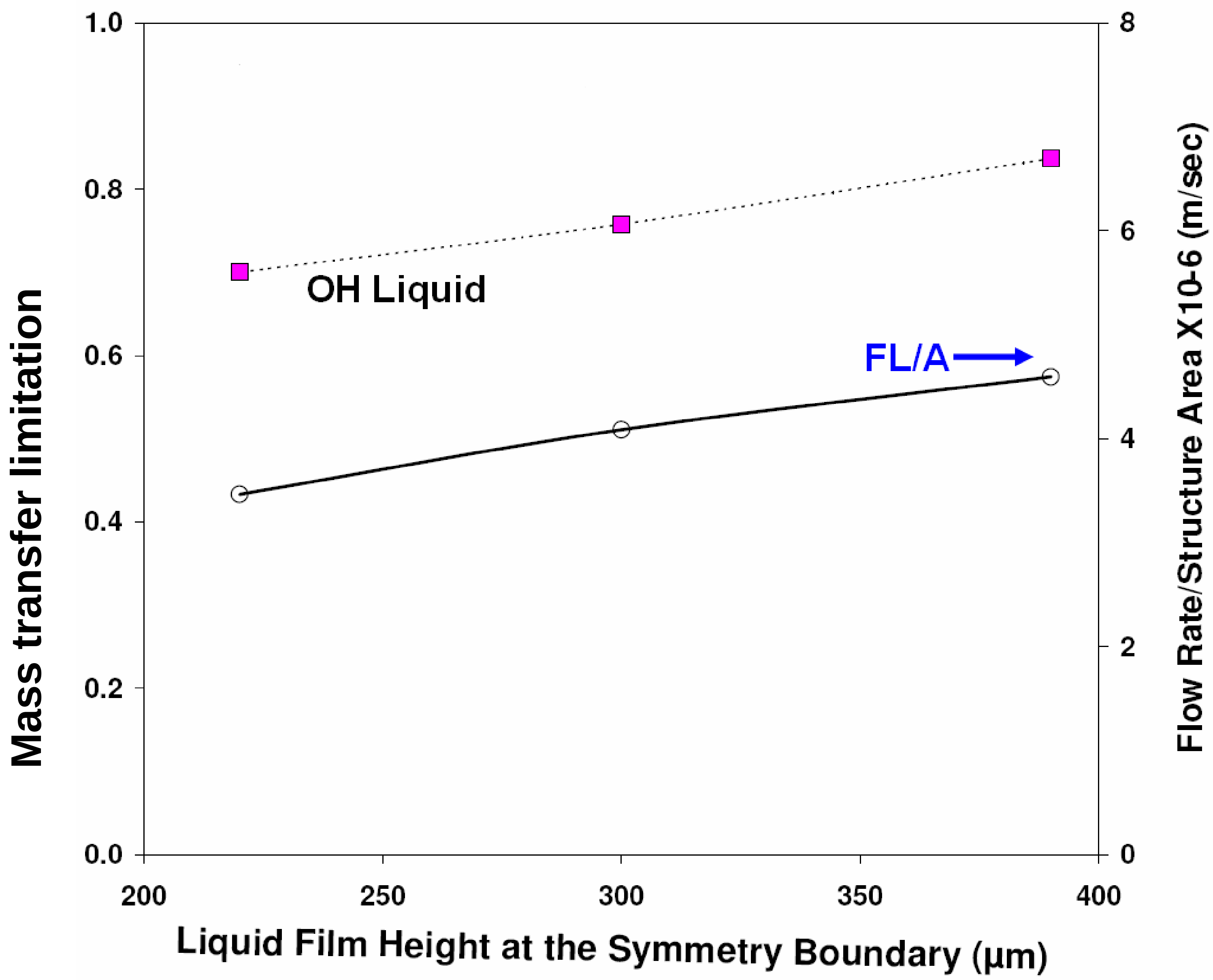


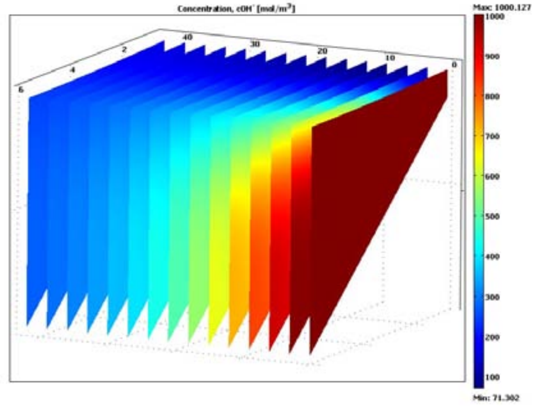
Channel Geometry Analysis– Circle Geometry

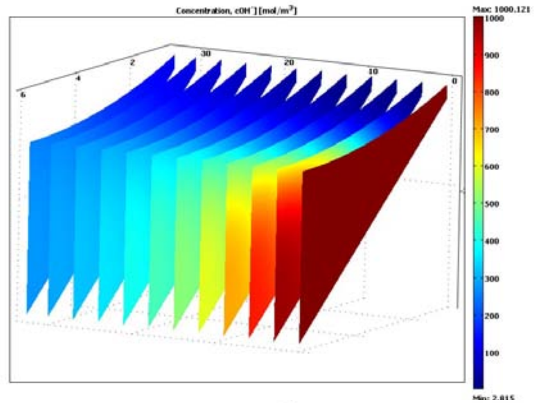


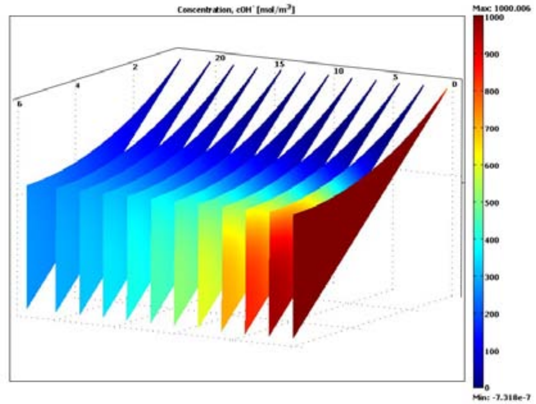


Channel Geometry Analysis– V-Shape

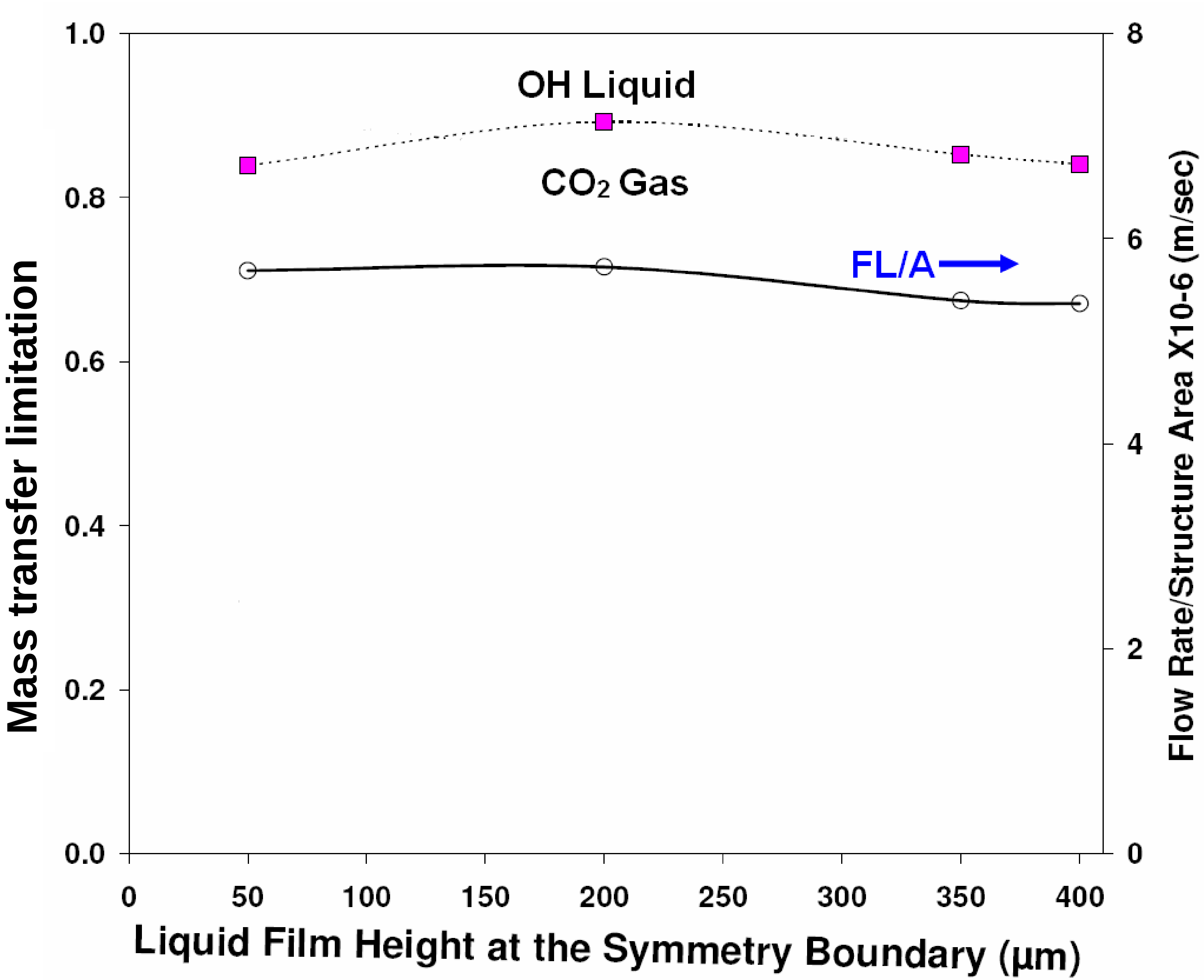


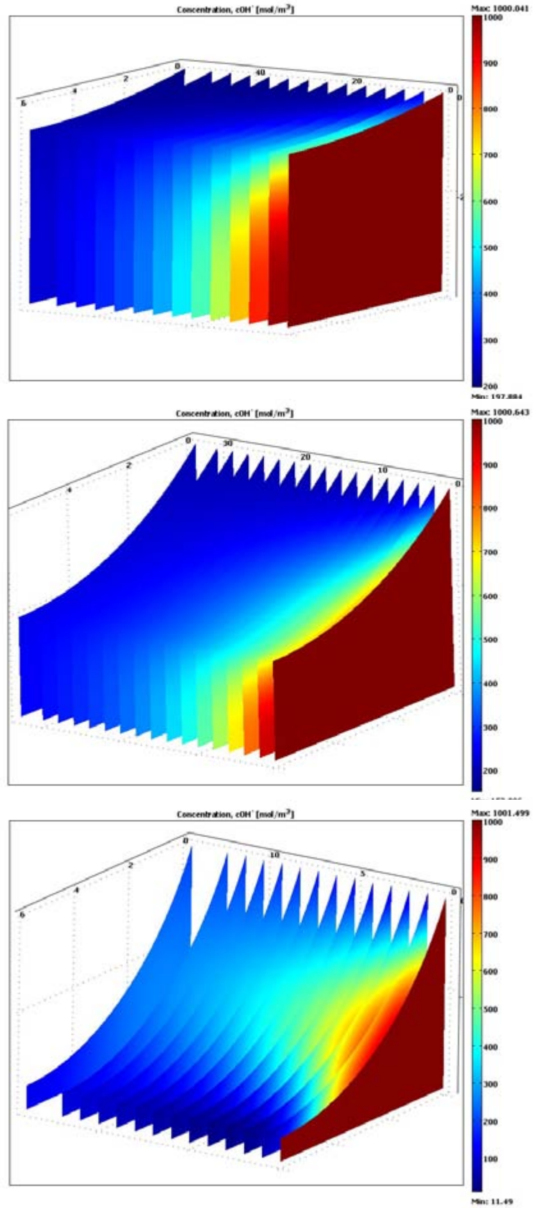






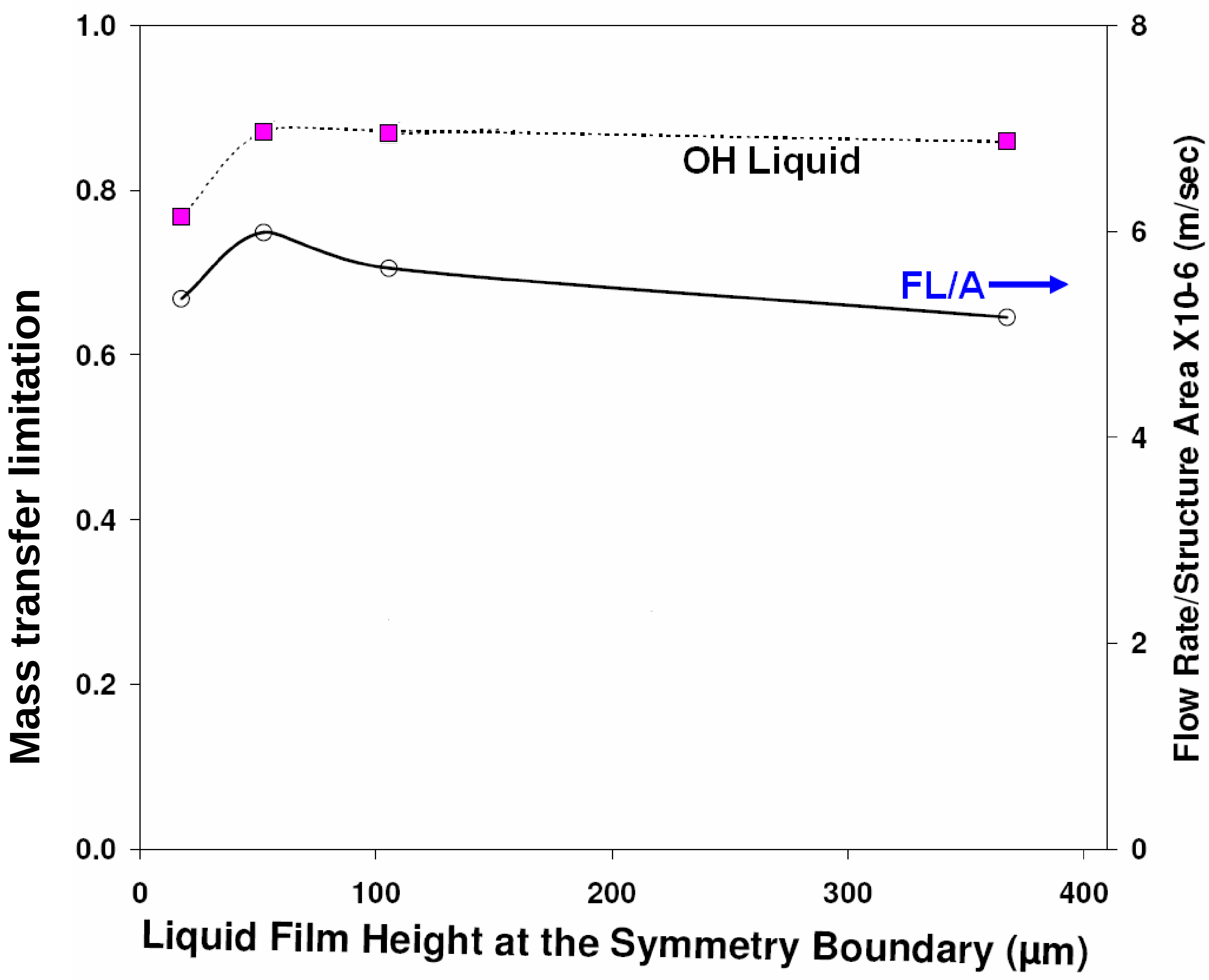
Channel Geometry Analysis– Rectangular

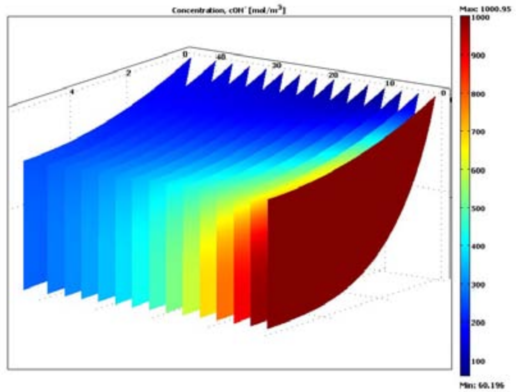


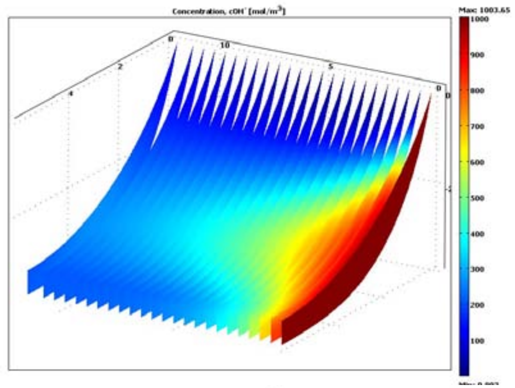


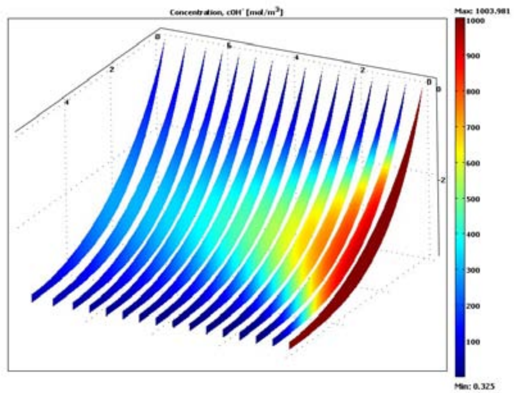
Technische Universiteit Eindhoven University of Technology

Channel Geometry Analysis– Etched

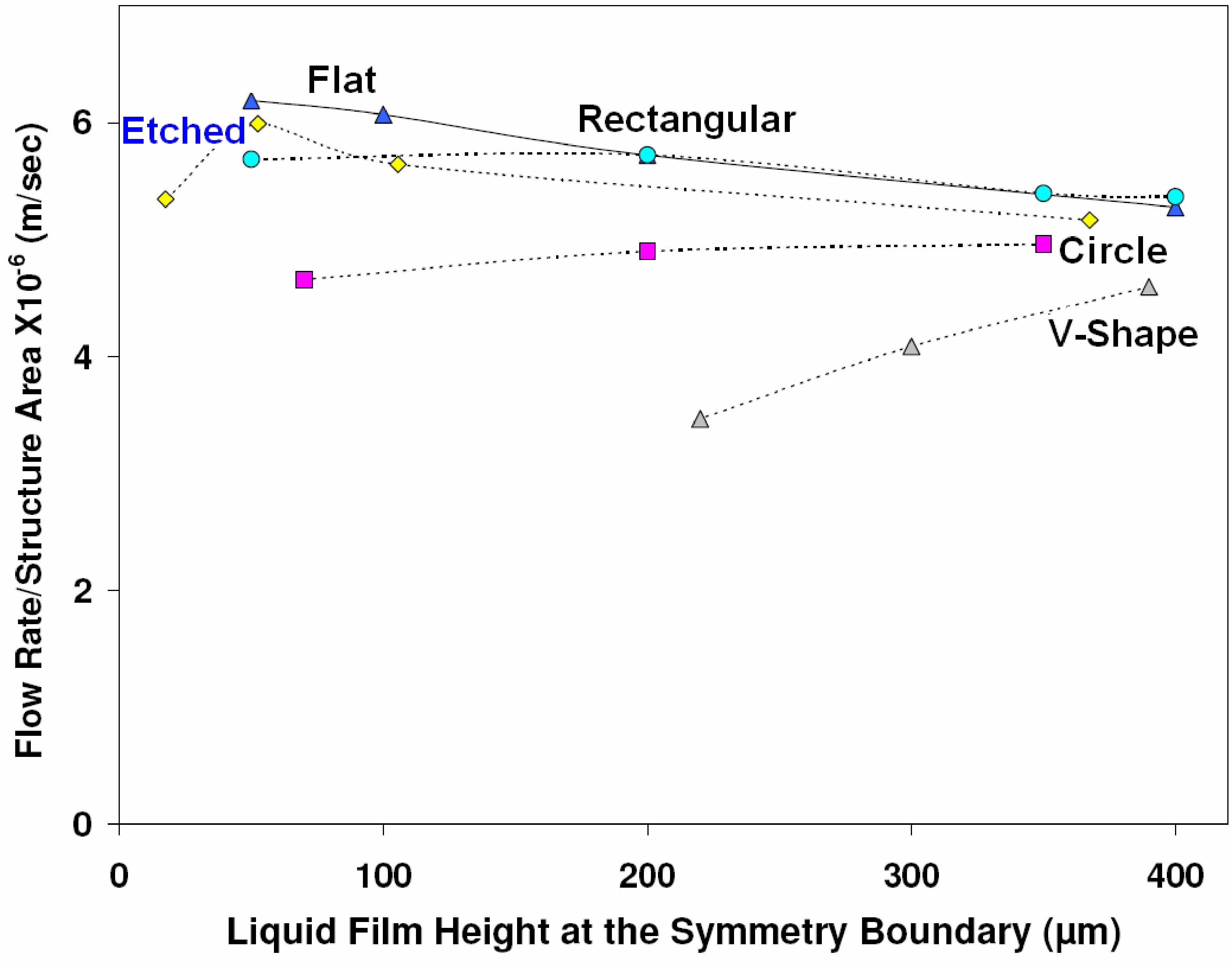








Channel Geometry Analysis - Conclusion



Conclusion

- **Pseudo 3-D model for gas/liquid system coupled with reaction is developed**
- **Fabrication imprecision currently is fine**
- **Reduction of gas chamber height slightly improve the performance**
- **Best reactor performance achieved with minimum uniform liquid film thickness**

Technische Universiteit
Eindhoven
University of Technology

Questions