Numerical Simulation of Film Flow over an Inclined Plate: Effects of Solvent Properties and Contact Angle

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Multiphase Flow Science Workshop

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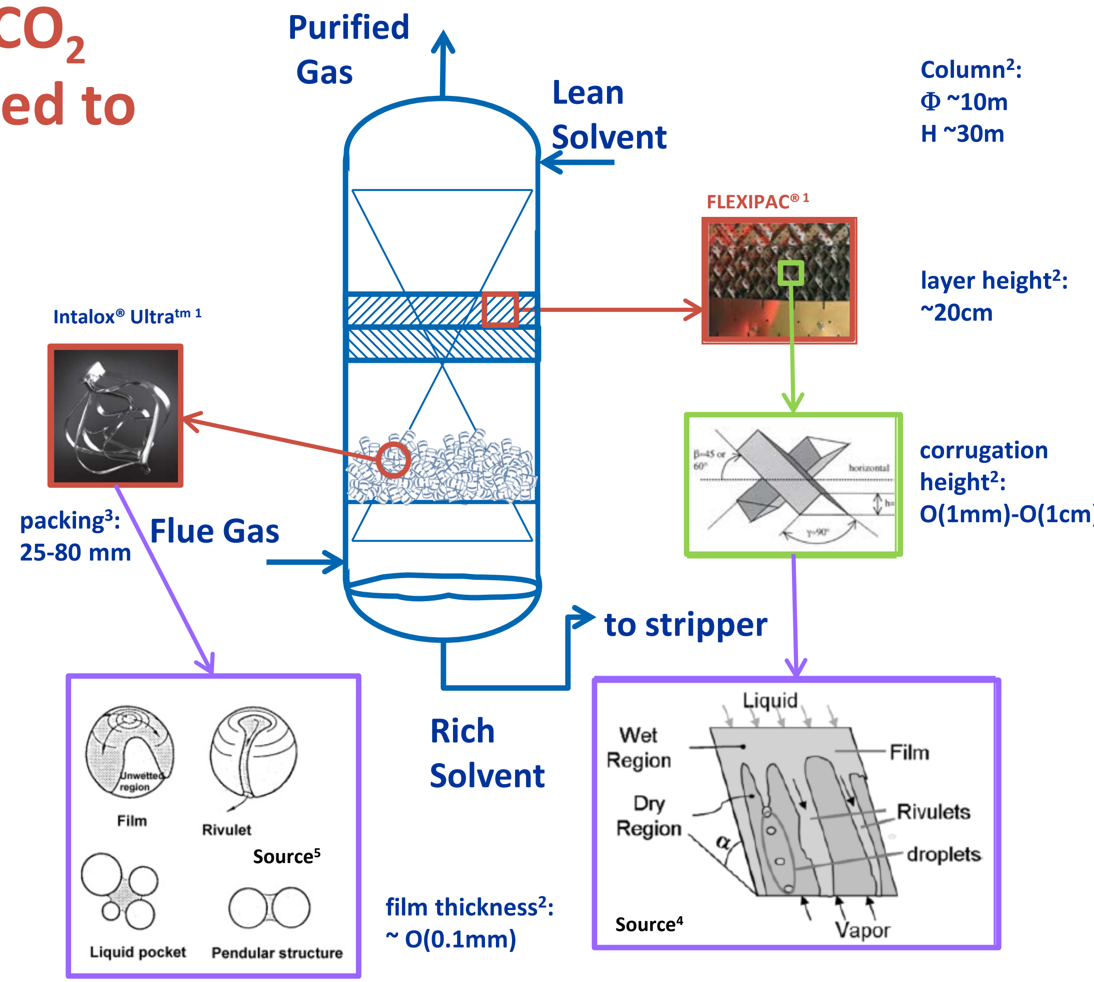
CFD Modeling of Solvent Absorption

Motivation: efficiency of CO_2 absorption is closely related to local flow behavior

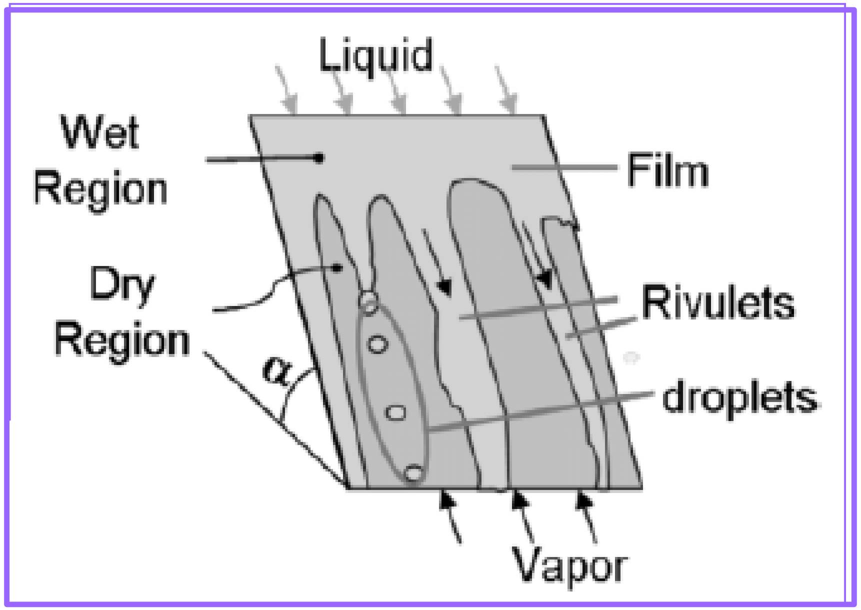
Challenges:

- Cannot model entire column focusing in on all physical phenomenon
- Multi-scale approach required
- Suitable closure models for interphase interactions have not been developed



(1) Koch-Glitsch: http://www.koch-glitsch.com/default.aspx; (2) Raynal & Royon-Lebeaud, CES, 2007; (3) Mackowiak, Fluid Dynamics of Packed Columns, Springer, 2010; (4) Xu et al., Chem. Eng. Tech., 2008; (5) Maiti et al., IECR, 2006

Liquid Films



Features depend upon various flow parameters and liquid properties

Current Goal: study the impact of solvent properties, contact angle, flow rates, inclination angle on hydrodynamics

- film thickness
- wetted area
- interfacial area
- flow regime

Method: Volume of Fluid Simulations

Volume of Fluid (VOF)[1] Multiphase Model

Governing Equations

- Continuity and momentum equation of average phase

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla P + \nabla \cdot \tau + \rho \mathbf{g} + \mathbf{F}$$

$$\rho = \rho_G \varepsilon_G + \rho_L \varepsilon_L \qquad \mu = \mu_G \varepsilon_G + \mu_L \varepsilon_L$$

- Transport equation for volume fraction

$$\frac{\partial \varepsilon_L}{\partial t} + \mathbf{u} \cdot \nabla \varepsilon_L = 0$$

$$\varepsilon_L + \varepsilon_G = 1$$

Stress : turbulence neglected

$$\boldsymbol{\tau} = -\mu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right)$$

Interfacial forces

- Force at interface resulting from surface tension

Challenges

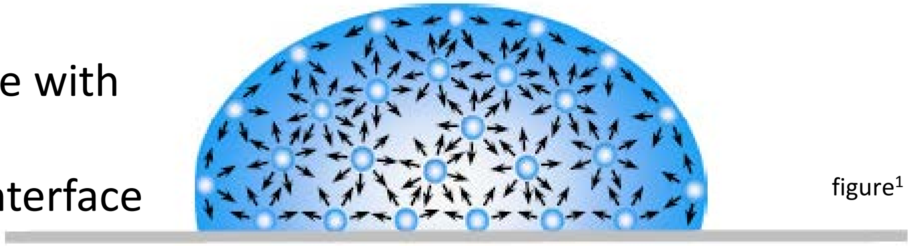
- preserving a sharp boundary between immiscible fluids
- computations of surface tension

[1]Hirt & Nichols, J. Comput. Phys, 1981

Computation of Interfacial Force

Surface tension force acts only at surface and is required to maintain equilibrium

- balances inward intermolecular attractive force with outward pressure gradient force
- minimizes free energy by decreasing area of interface



figure[1]

Continuum surface force model – Brackbill et al., J. Comput Phys., (1992):

→ Other techniques are available[2]

- Force at surface expressed as volume force using divergence theorem

$$\mathbf{F} = \sigma \frac{\rho \kappa \nabla \varepsilon_G}{0.5(\rho_L + \rho_G)}$$

<= For two phase flow

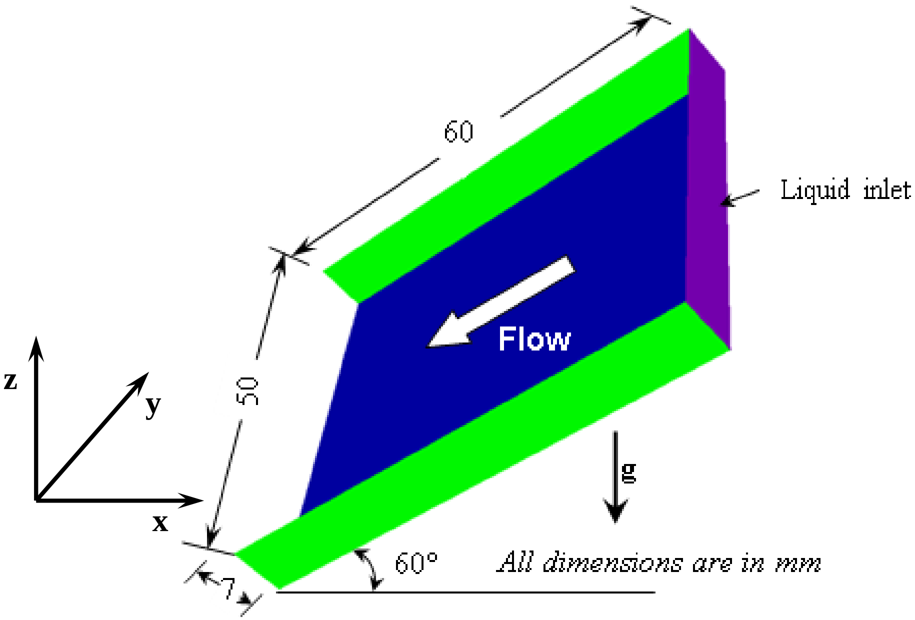
- Surface curvature is computed from local gradients in the surface normal to the interface

- Effects of wall adhesion at fluid interfaces in contact with boundaries is also estimated within the CSF model

  The contact angle that the fluid is assumed to make with the wall is used to adjust the surface normal in cells near the wall

[1]Yuan, Y. and Lee, T. R., Contact Angle and Wetting Properties, in Surface Science Techniques , Bracco, G., and Holst B. (eds), 2013.
[2]Haroun et al., CES, 2010

Liquid Film Down Inclined Plate



Inlet: constant velocity (through plane)
Outlet: pressure (0 Pa)
Plate: smooth wall (no slip)
Sides: smooth walls (no slip)
Top: pressure outlet (0 Pa)

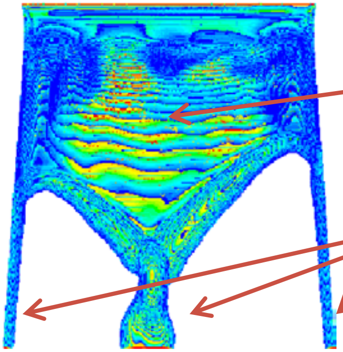
$1.05\text{x}10^{-6} \leq Q_{in} \leq 1.05\text{x}10^{-5}$ kg/m^3
$0.003 \leq v_{in} \leq 0.03$ m/s
$0.03 \leq We_N \leq 1.49$
$23.5 \leq Re_N \leq 235$

Base case

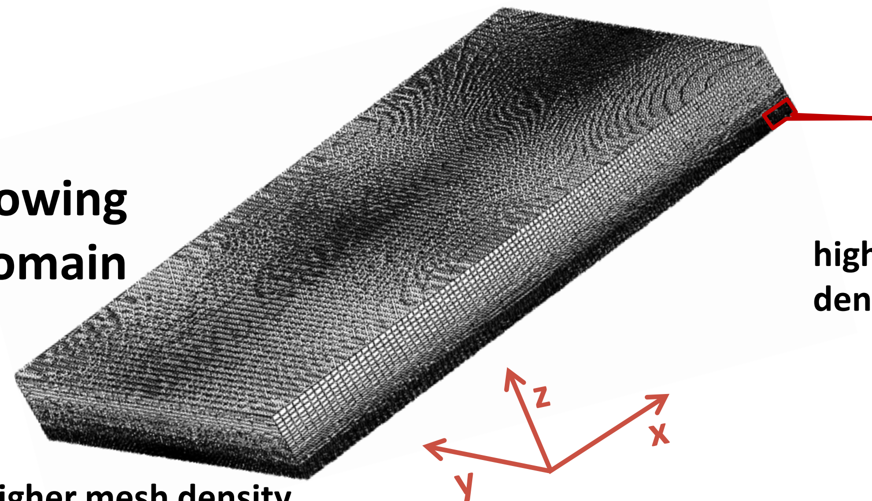
Physical Properties	Air	Water
Density ρ (kg/m^3)	1.185	997
Viscosity μ (Pa.s)	$1.831\text{x}10^{-5}$	$0.8899\text{x}10^{-3}$
Surface Tension σ (N/m)	–	0.0728
Static contact angle with air-steel γ (°)	70	

Computational Domain

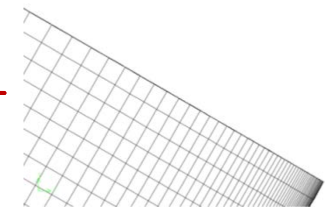
Fine mesh required to resolve rivulets



3D view showing mesh of domain



higher mesh density near center line



higher mesh density near plate

Simulations conducted for pseudo-steady state

$\Delta t = 1\times10^{-5} - 1\times10^{-4}$ (Co=0.50)

Fails to correctly predict flow behavior

Number of elements: 1.15M*

(Literature: 1.0 – 1.5M elements)

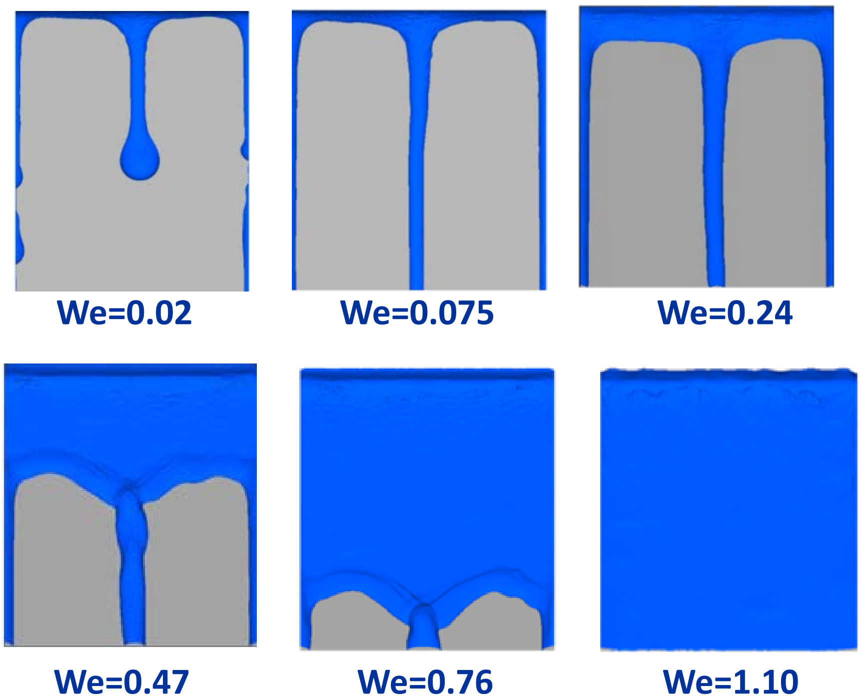
Typical Run Times

Case	No of Cells	Simulation time	Wall Time	No of Processor
Coarse	500K	**2s**	24hrs	32
Fine 1	1.12M	2s	48 hrs	128
Fine 2	1.37M	2s	48 hrs	128

Comparison with Experiments

Impact of inertia on flow transition & wetted area

Snapshot of Interface ($\varepsilon_L = 0.5$)

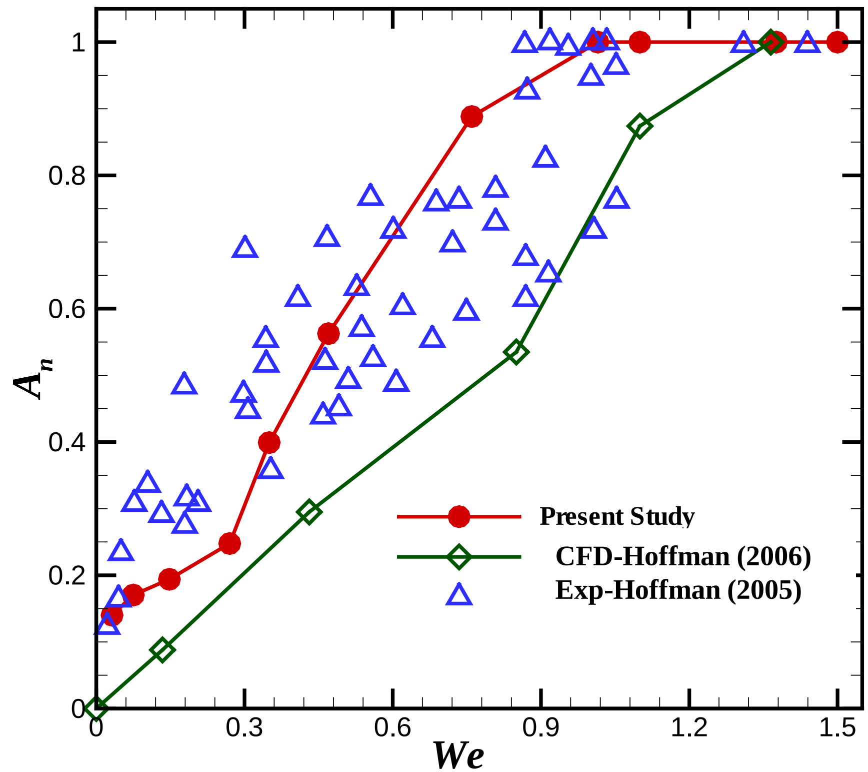


Increasing We

$$We_{lN} = \frac{\rho_l {V_{lN}}^2 \delta_{lN}}{\sigma}$$

Droplet → Rivulet → Full Film

Specific Wetted Area $A_n = \frac{\text{Wetted Area}}{\text{Geometrical Area}}$



Excellent Match with Experiments

Effect of Solvent Properties on Hydrodynamics

- Film thickness
- Wetted area
- Interfacial area

- Kapitza Number only depends on fluid properties
- Fixed for each solvent
- Independent of flow rate

$$Ka = \sigma_l \left(\frac{\rho_l}{g \mu_l^4} \right)^{1/3}$$

- Low Ka ↔ high solvent viscosity

Solvent	μ_l (Pa-s)	ρ_l (kg/m³)	σ_l (N/m)	ν_l	Ka
Water	0.00089	997.0	0.07280	8.92578E-07	**3969.04**
30% MEA	0.00252	1013.0	0.05480	2.48766E-06	**749.71**
26.7% AMP	0.00270	995.80	0.04301	2.71136E-06	**533.65**
40% MEA	0.00371	1015.3	0.05500	3.64917E-06	**450.42**
0.075m MPZ	0.00556	1005.3	0.05442	5.53489E-06	**258.27**
48.8% MDEA	0.00925	1016.6	0.04756	9.09896E-06	**116.60**
0.51m MPZ	0.01336	946.41	0.03437	1.41165E-05	**49.72**
0.41m MPZ	0.02348	962.20	0.03589	2.44022E-05	**24.62**
0.31m MPZ	0.03642	981.31	0.03840	3.71137E-05	**14.77**

Flow rate computation

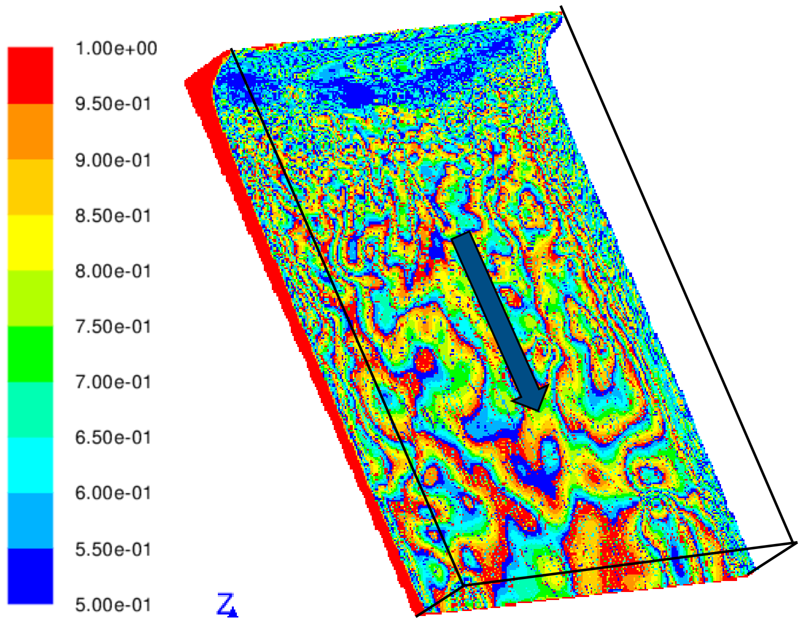
$$Q = W \left(\frac{3We^3}{g \sin \alpha} \right)^{0.2} \left(\frac{\mu_l}{\Delta \rho} \right)^{0.2} \left(\frac{\sigma_l}{\rho_l} \right)^{0.6}$$

Q_l = liquid flow rate
We = Weber number
W = Width of plate
ρ_l = density of liquid
$\Delta\rho$ = $\rho_l - \rho_g$
μ_l = viscosity of liquid
σ_l = surface tension of liquid
g = gravitational acceleration

Film Thickness for Fully Wetted Plate

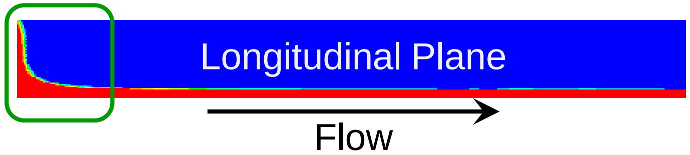
Fixed Q = 1.053×10^{-5} m^3/s

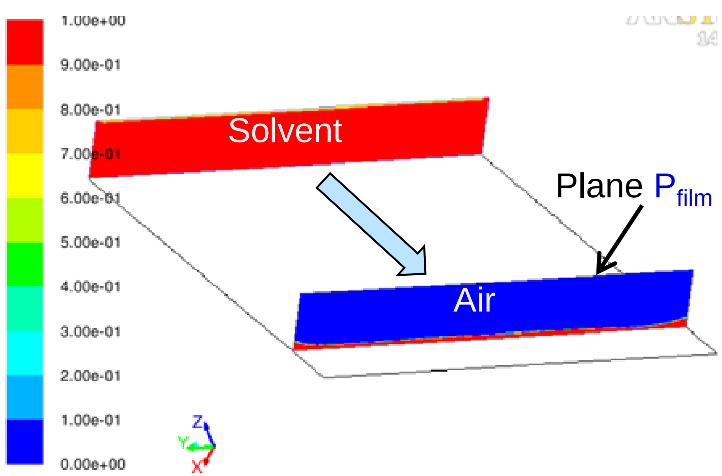
To yield fully wetted plate



Volume Fraction of Water

Snapshot of liquid and gas distribution in the central xz-plane

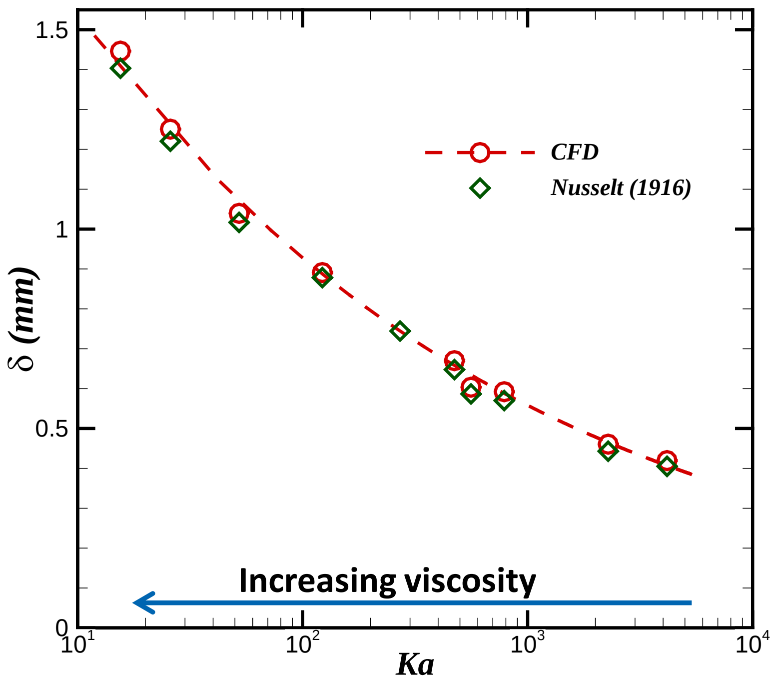


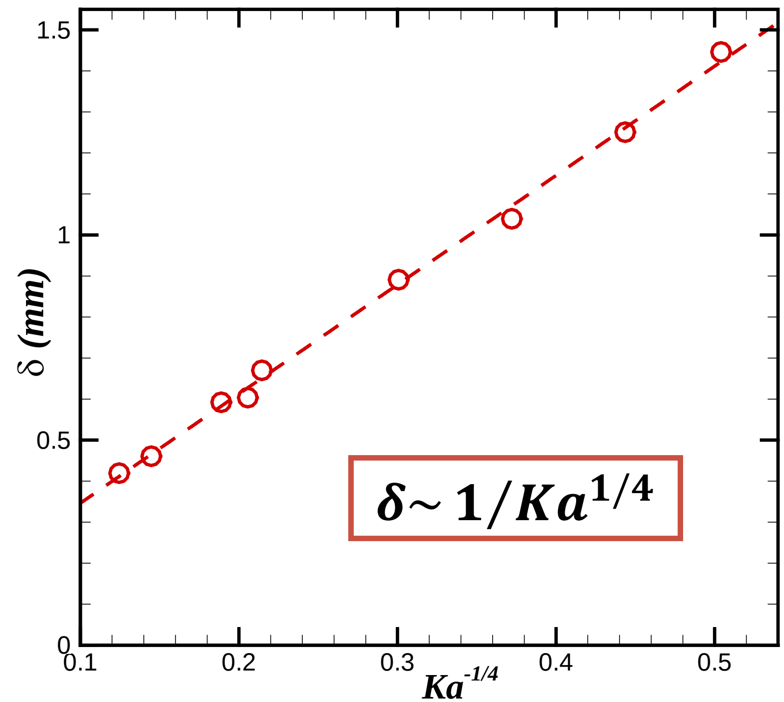


$$\delta = \frac{\text{Entrained area of Solvent in } P_{film}}{\text{Width of plate}}$$

Film Thickness for Fully Wetted Plate
Impact of solvent properties

- δ decreases with increase Ka



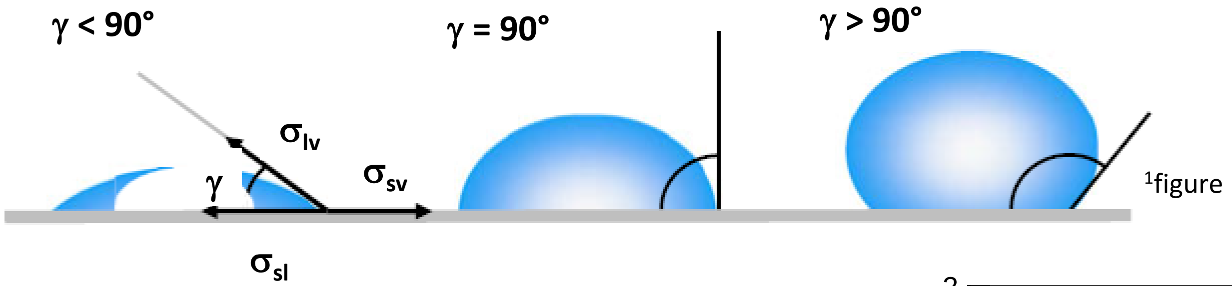


Excellent agreement with Nusselt theory

Flow rate: $\delta \sim Q^{1/3}/Ka^{1/4}$

Film Thickness for Fully Wetted Plate

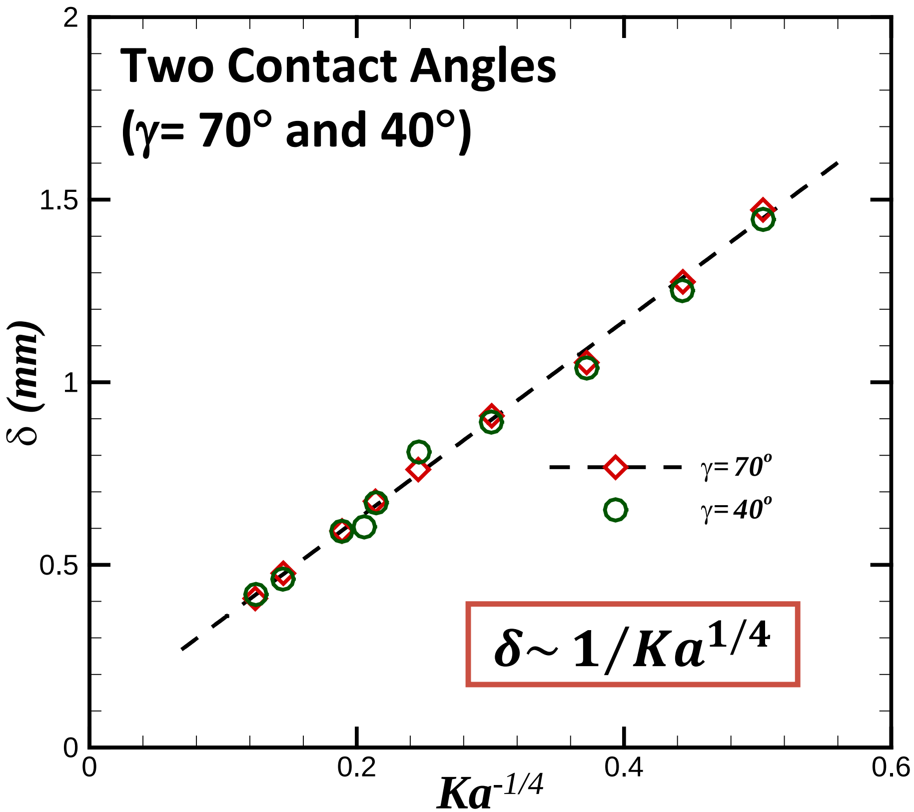
Impact of contact angle



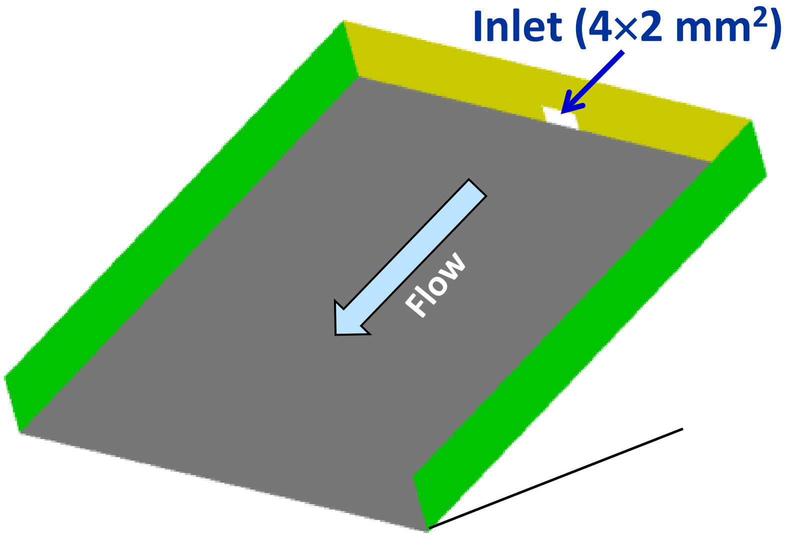
- Characteristics of solid- liquid system in specific environment
- Dictates the wetting behavior of solvent

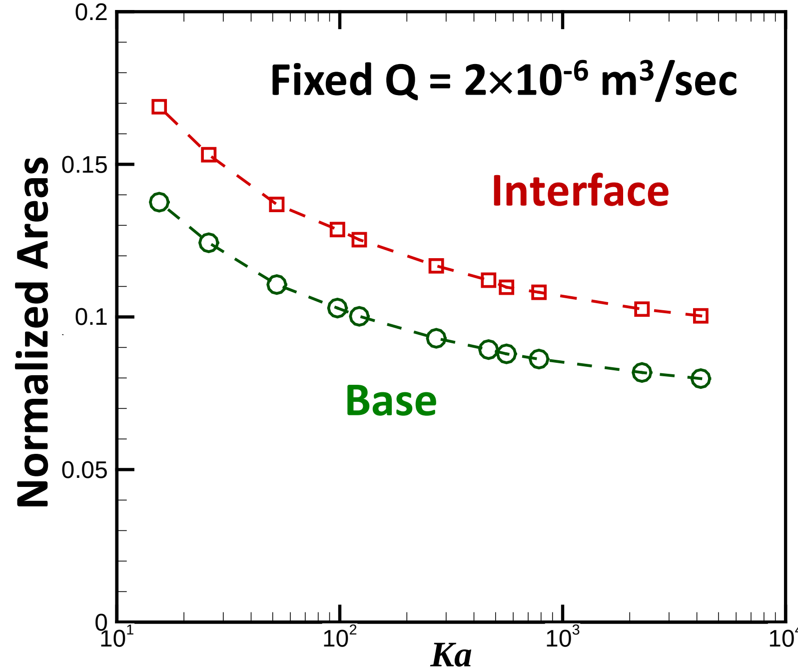
- Film thickness unaffected by contact angle for fully wetted plate

What about for partially wetted plate?

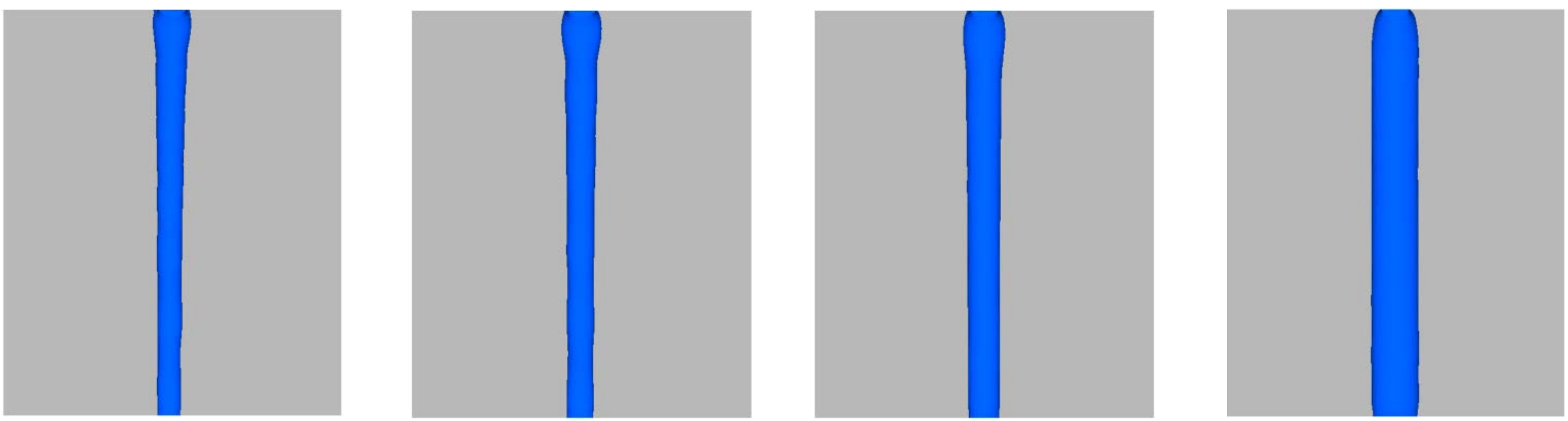


Modified Setup for Rivulet Flow





Snapshot of Interface (ε_L = 0.5)

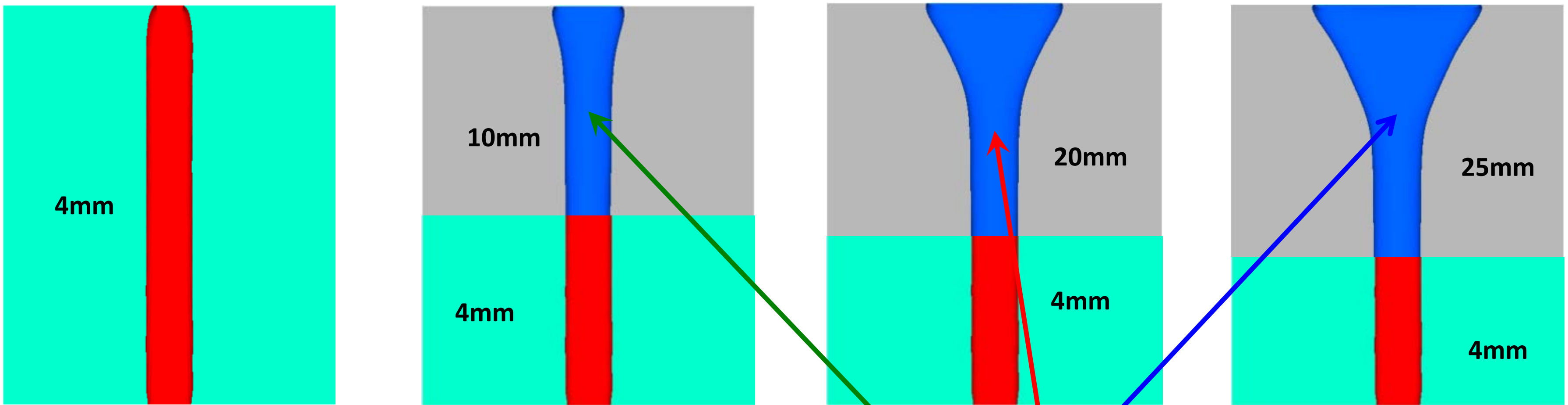


Water Ka=3969	30MEA Ka=749	48MDEA Ka=116	31MPZ Ka=15

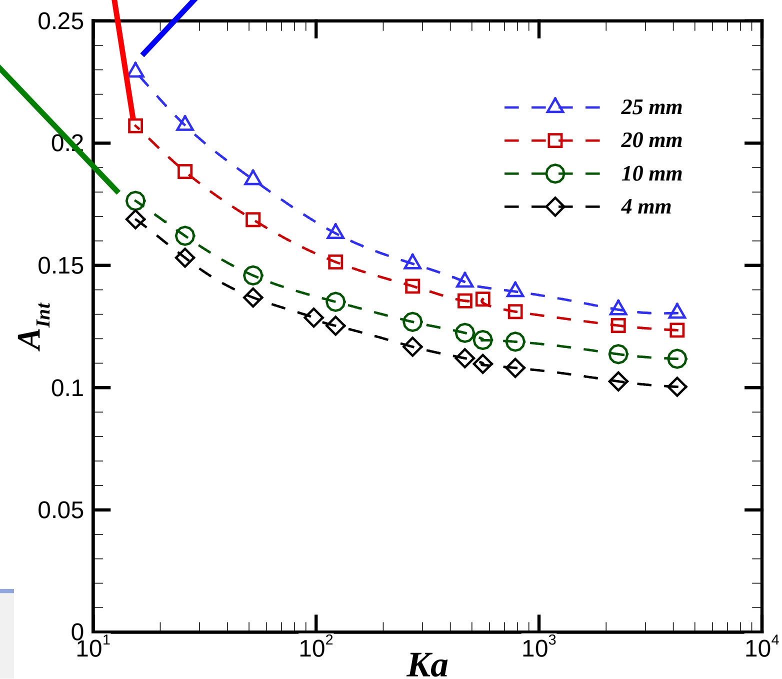
Interfacial Area for Rivulet Flow

Impact of inlet size and solvent property

Interface at ε_L = 0.5 for 0.31m MPZ (Ka=15)

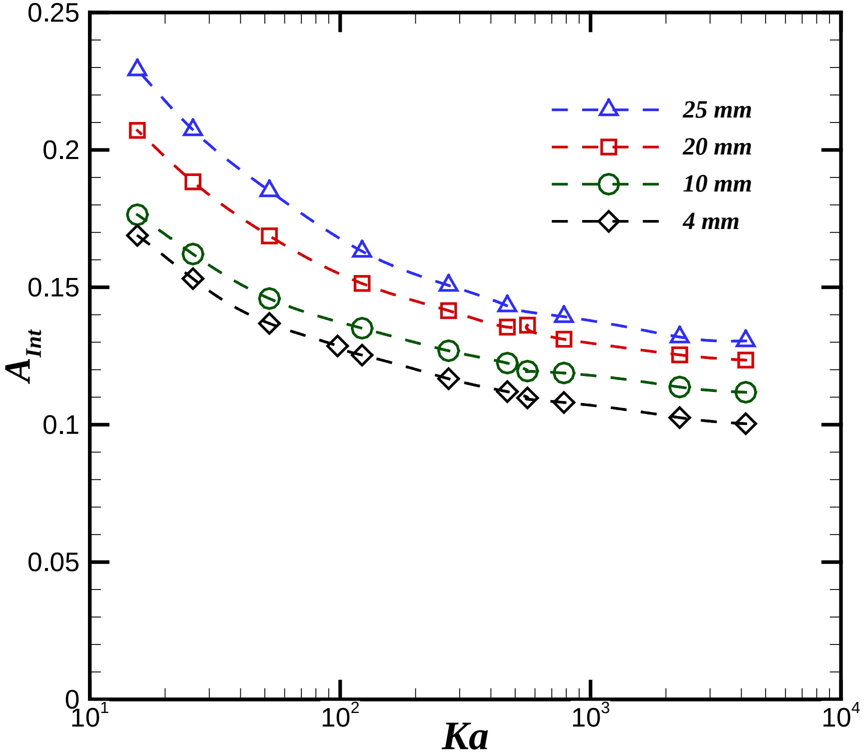


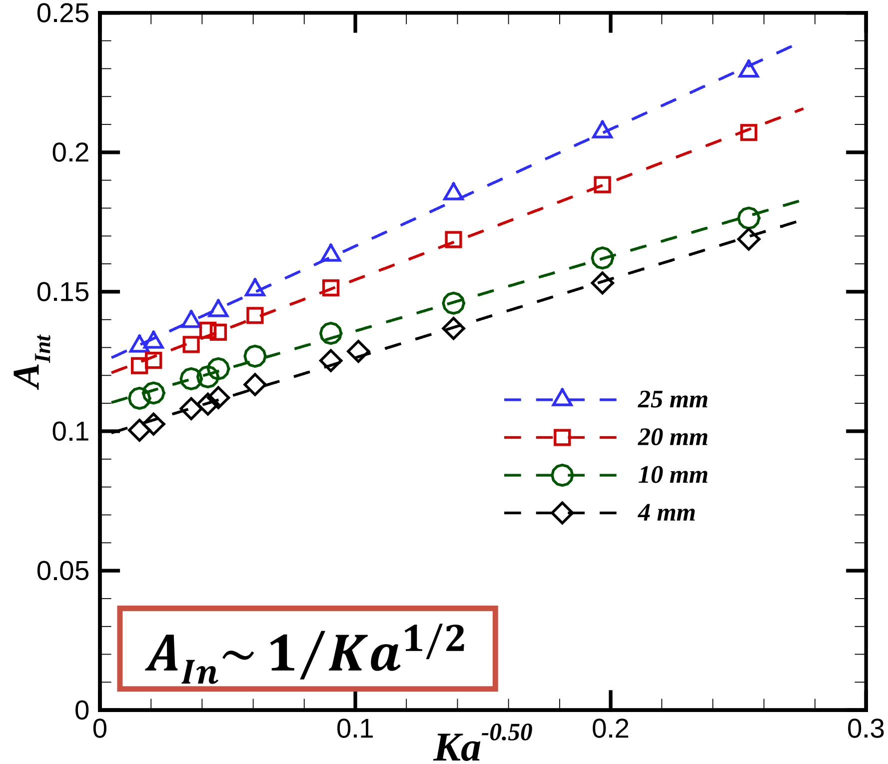
- **Developed width of rivulet remains constant at a fixed Q**
- **Developed width only depends on Q**
- **Slight increase in interfacial area is due to entrance effects**
- **A_{In} decreases with increased Ka**



Interfacial Area for Rivulet Flow

Impact of inlet size and solvent property



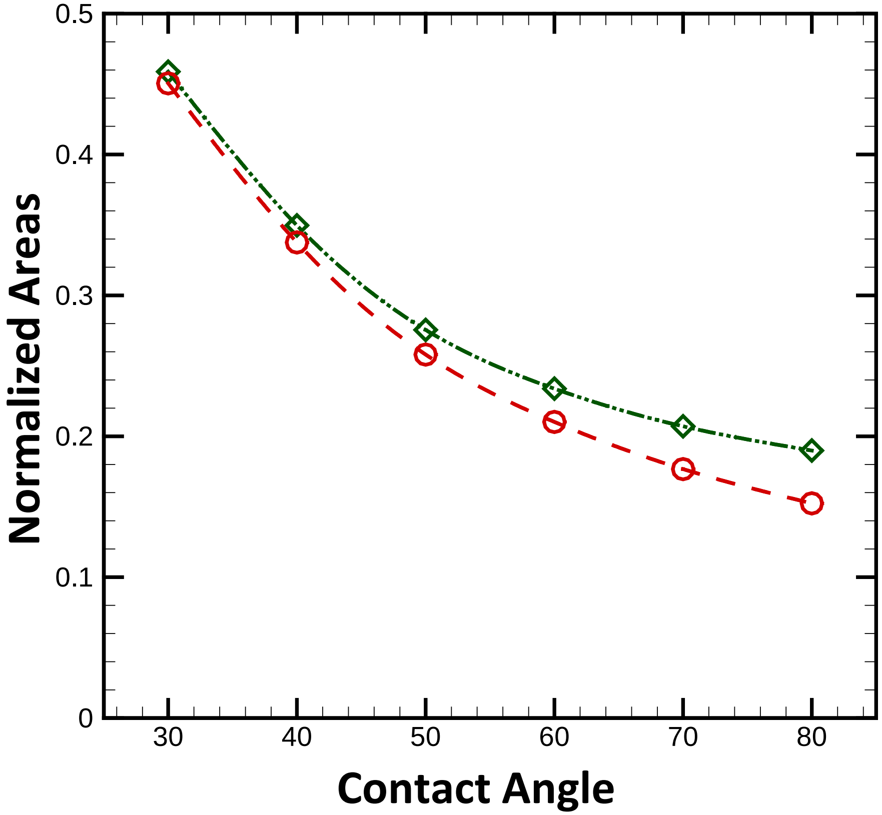


Flow rate: $A_{In} \sim Q^{1/3}/Ka^{1/2}$

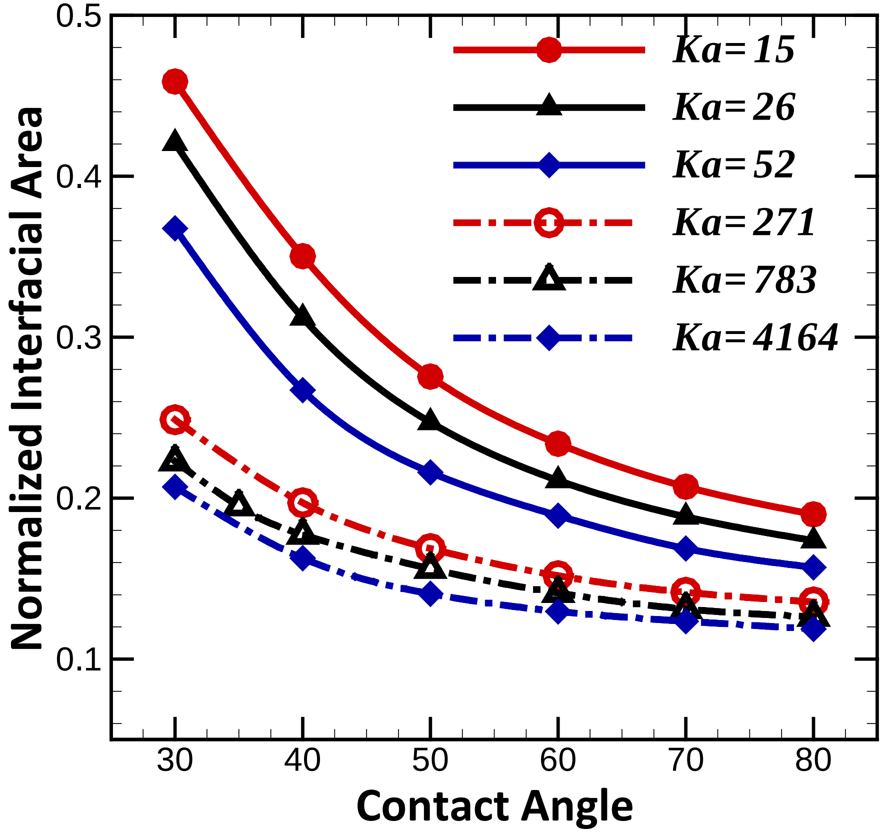
Wetted/Interfacial Areas for Rivulet Flow

Impact of contact angle

For 0.31m MPZ (Ka=15)



For all solvents



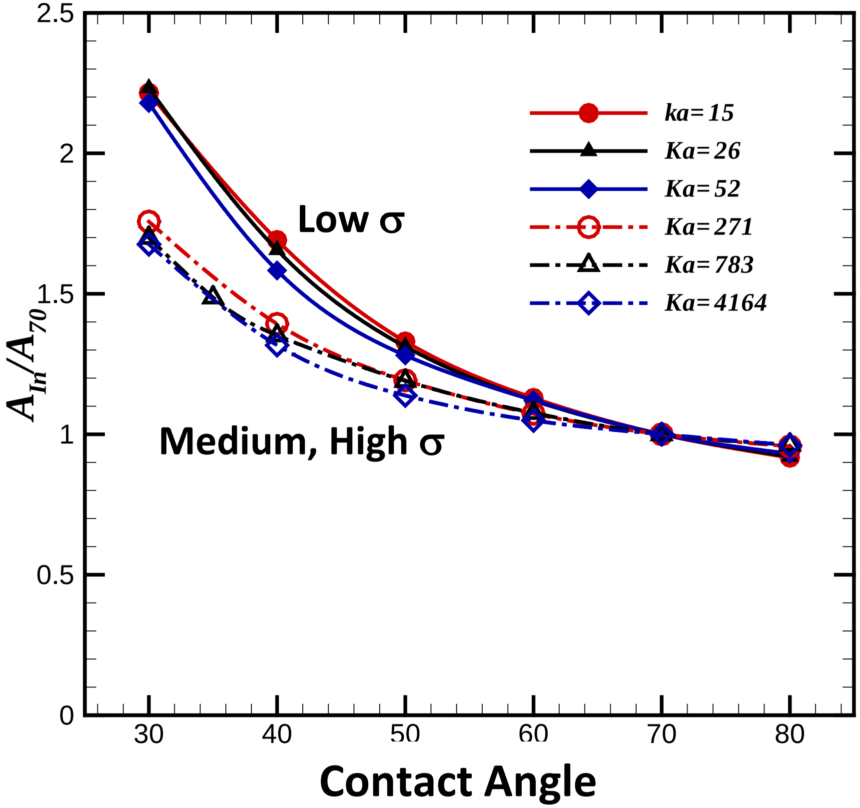
- Wettability decreases with increased γ
- Impact is greater on wetted area
- Leads to increase in δ with increased γ

Re-normalized Interfacial Areas for Rivulet Flow

Impact of contact angle

$$A_0 = \frac{A_{In}}{A_{70}}$$

A_{70} = Interfacial area at γ = 70°



Pioneering work of Zisman and co-workers[1] found[2]:

- For given solid, contact angle (γ) does not vary randomly with liquid
- The change of cos γ vs surface tension (σ) falls in a linear trend
- Lower values of σ corresponds to smaller γ

Two regimes are evident for

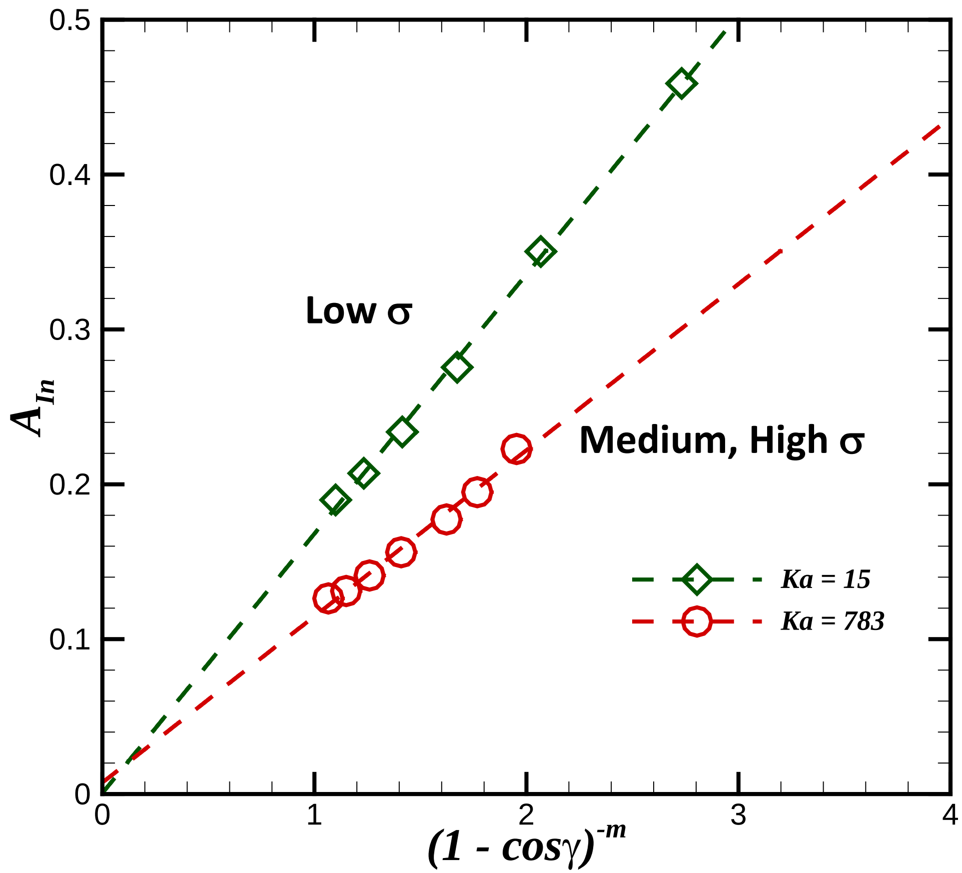
- **Low σ (< 50 mN/m)**
- **Medium & High σ (>50 mN/m; 70 mN/m)**

[1]*Yuan, Y. and Lee, T. R., Contact Angle and Wetting Properties, in Surface Science Techniques , Bracco, G., and Holst B. (eds), 2013.*

2W.A. Zisman, in *Contact Angle, Wettability and Adhesion: Advances in Chemistry Series*, vol. 43, ed. by R.F. Gould (ACS, Washington, 1964), p. 1

Interfacial Area for Rivulet Flow

Impact of contact angle



Areas scale as

$$A \sim 1/(1-\cos\gamma)^m$$

- **Interfacial Area (A_{In})**

  m **= 0.50** **σ < 50mN/m**

  = 0.33 **≥ 50mN/m**

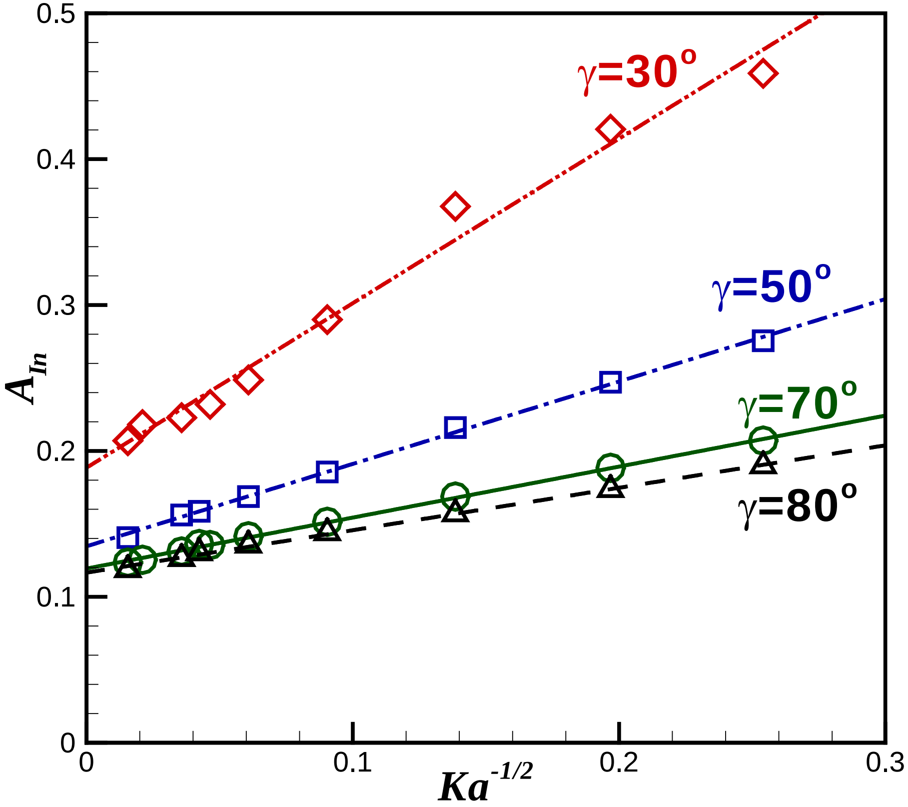
- **Wetted Area (A_n)**

  m **= 0.60** **σ < 50mN/m**

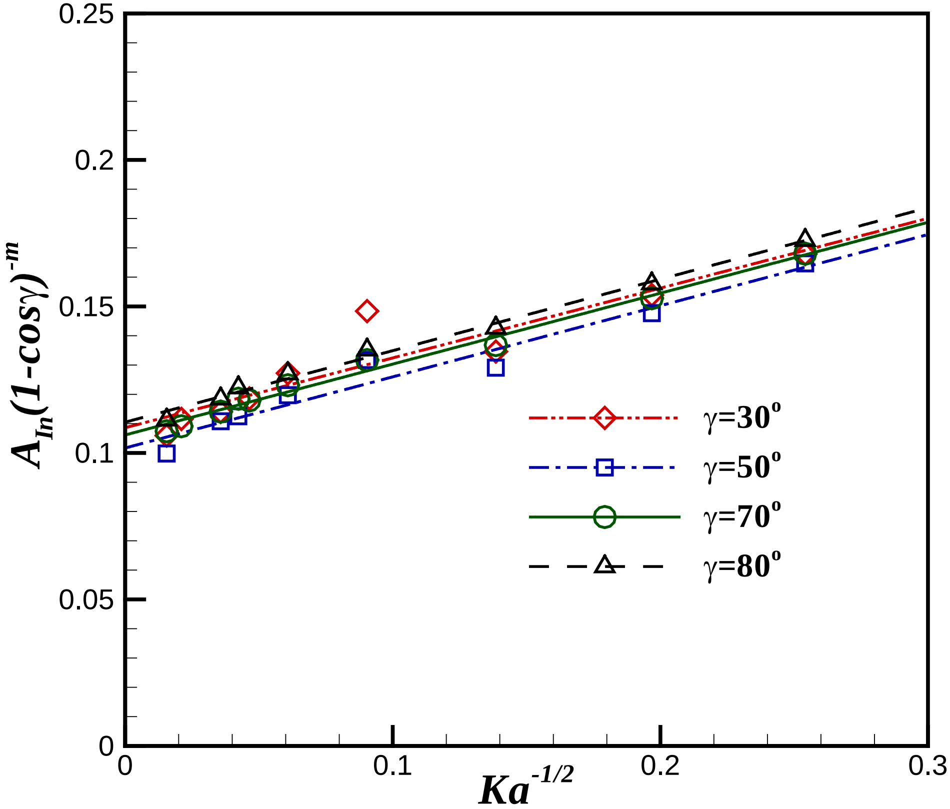
  = 0.45 **≥ 50mN/m**

Interfacial Area for Rivulet Flow

Impact of Ka at various γ



Impact of Ka and γ



$$A_{In} \sim 1/Ka^{1/2}$$

Valid for all γ

$$A_{In} = C\frac{Q^{1/3}}{Ka^{1/2}(1-\cos\gamma)^m}$$

Summary & Conclusions

- **Multiphase flow VOF simulations can be used to explore film flow down a plate**
- **Results presented in terms of the Kapitza number**

$$Ka = \sigma_l \left(\frac{\rho_l}{g\mu_l^4}\right)^{1/3}$$

- **Scaling relations were obtained to describe impact of solvent properties and contact angle on interfacial area**
  - **Full Film Flow:**
    - **Film thickness decreases with increase Ka**

$$\delta \sim Q^{1/3}/Ka^{1/4}$$

  - **Rivulet Flow:**
    - **Wetted/Interfacial areas decrease with increased Ka**
    - **Wetted/Interfacial areas decrease with increased γ**

$$A = C\frac{Q^{1/3}}{Ka^{1/2}(1-\cos\gamma)^m}$$

- Work in progress
  - Identifying critical We for flow regime transition
  - Impact of varying inclination angle

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