Guess free evaporation modeling without adsorbed film constraints

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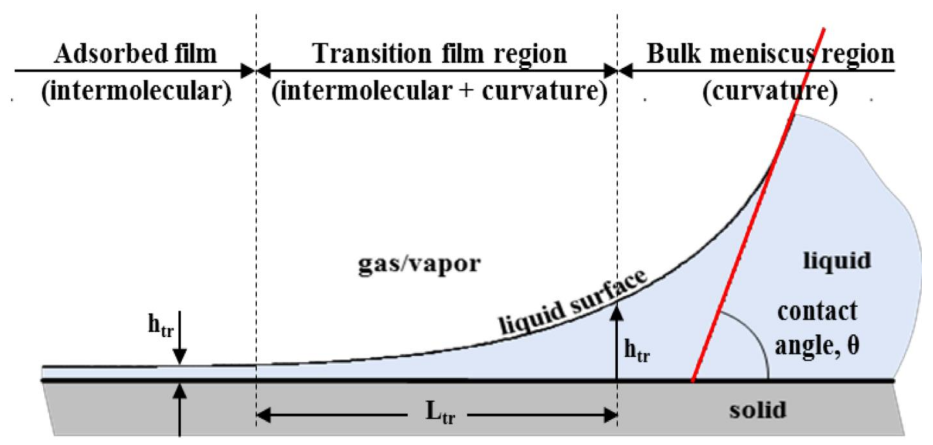
Kinetic Model of Phase Change

$$\dot{m}'' = \frac{2\alpha}{2-\alpha}\sqrt{\frac{m}{2\pi k_b}}\left(\frac{P_{li}}{\sqrt{T_i}} - \frac{P_{vi}}{\sqrt{T_v}}\right)$$

Planar interface:
Maxwellian Distribution with drift velocity



Curved interface:
Pressure and temperature variations result in non-uniform evaporation

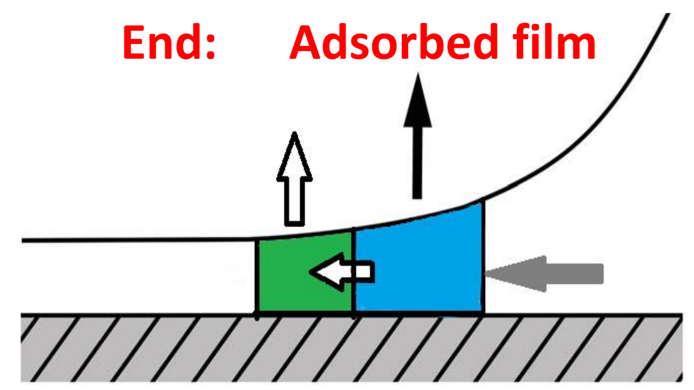
$$\dot{m}'' = \frac{2\alpha}{2-\alpha}\left(\frac{M}{2\pi R T_i}\right)^{1/2}\left[\underbrace{\frac{p_v M h_{fg}}{R T_v T_i}(T_i - T_v)}_{\text{Thermal}} - \underbrace{\frac{v_l p_v}{R T_i}(\Pi + \sigma\kappa)}_{\text{Mechanical}}\right]$$

α: fraction of molecules that undergo phase change

Thin film evaporation

Lubrication Approximation

Start: Bulk meniscus
End: Adsorbed film



Interface Curvature

$$\kappa = \frac{1}{(a/2-h)\left(1+h'^2\right)^{1/2}} + \frac{h''}{\left(1+h'^2\right)^{3/2}}$$

Disjoining Pressure

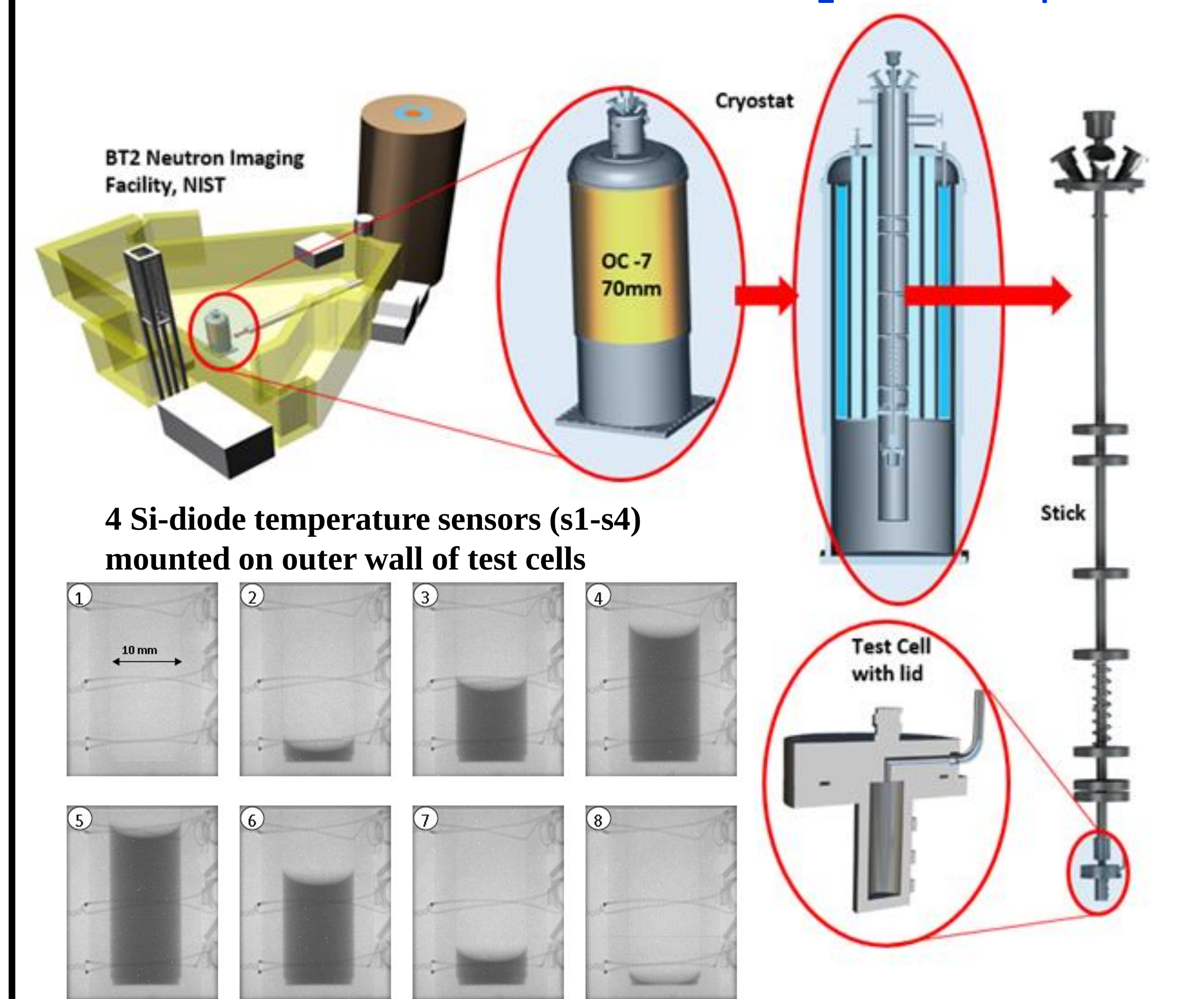
$$\Pi = -\frac{A}{h^3}$$

Combine mass, momentum and energy equations with Kinetic Model:

$$h_{xxx} - \frac{3h_{xx}^2 h_x}{1+h_x^2} - \frac{h_{xx}h_x}{r_{ij}-h} + \frac{h_x(1+h_x^2)}{(r_{ij}-h)^2} + \frac{\gamma}{\sigma}\left\{\frac{1+h_x^2}{r_{ij}-h} + h_{xx}\right\}\frac{dT_i}{dx} + \frac{1}{\sigma}(1+h_x^2)^{\frac{1}{2}}\left(\frac{dp_l}{dx} + \frac{d\Pi}{dx}\right) = 0$$

- 1D cylindrical co-ordinates
- Reversed integration path
- BC tuning is not necessary
- Non-uniform wall temperature
- Thermocapillary accounted

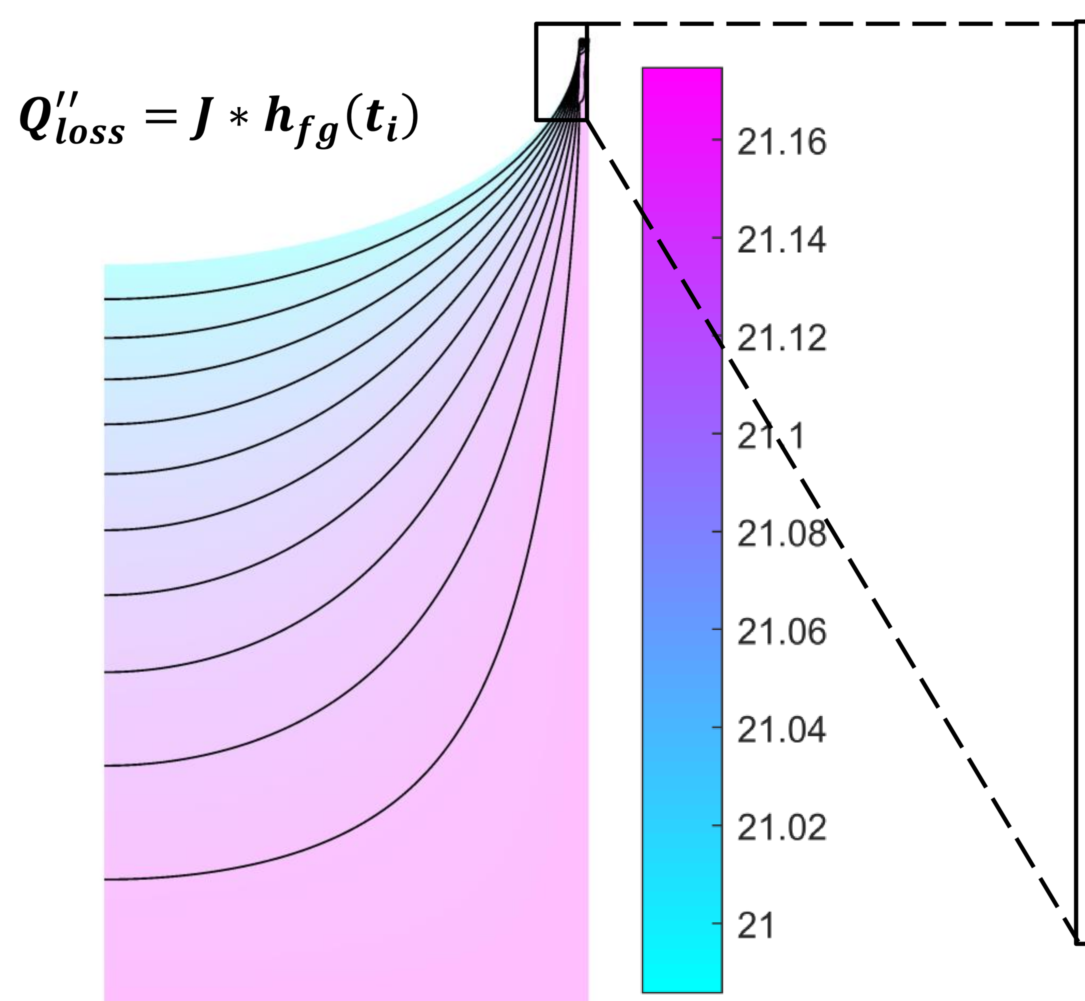
Cryo/neutron experiments with LH_2 and LCH_4

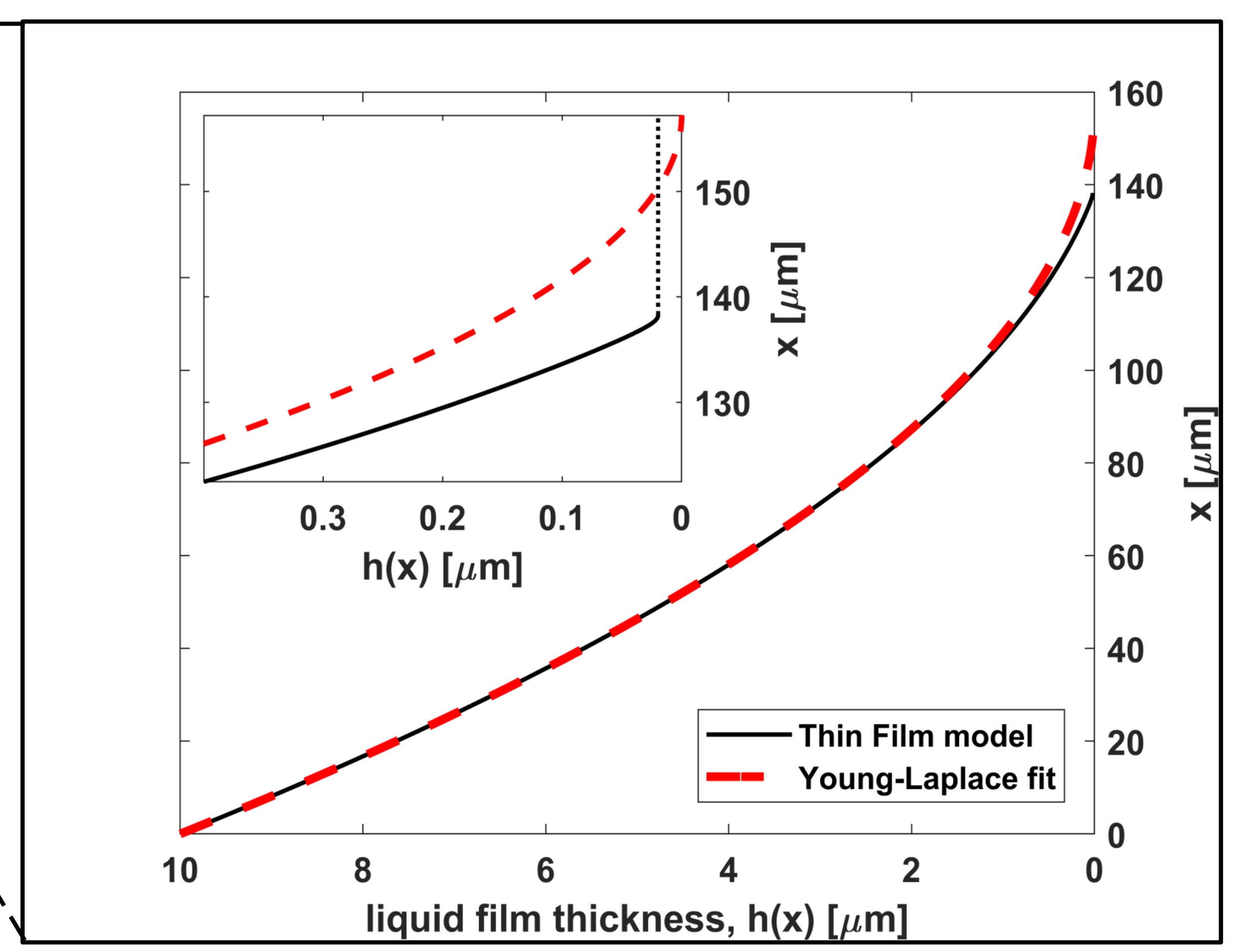


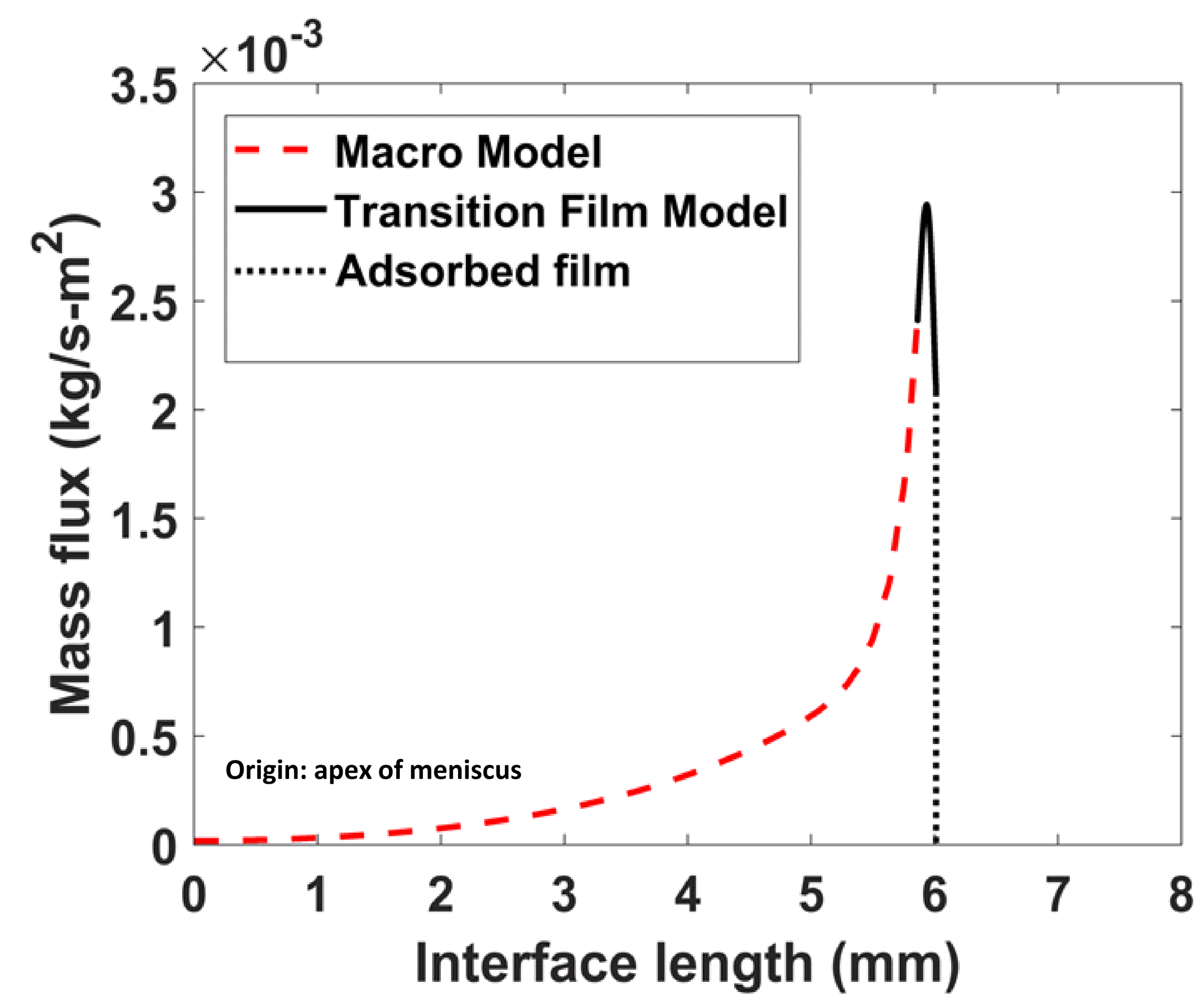
Multi-scale model of phase change

Results with LH_2 saturated at 121 kPa in a 10 mm Al 6061 cell

Macro-scale submodel (2D FEA) + Thin film evaporation model = Coupled multi-scale model







Inputs

Θ, Bo, T_{wall}

Output

Mass flux distribution

- Integrate for total evaporation rate
- Compare with Experimental rate
- Iterate on α to match

- Bulk meniscus accounts for 78-95%
- Adsorbed film not non-evaporating (<1%)
- Flux distribution changes with vapor pressure

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References:

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[2] Bellur et al. *Physical Review Fluids,* 5(2), 2020. LINK
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