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Simulation of Meniscus Motion and Evaporation for Convective Deposition Manufacturing

Junfeng Xiao and Daniel Attinger
Laboratory for Microscale Transport Phenomena,
Department of Mechanical Engineering,
Columbia University, New York, NY 10027

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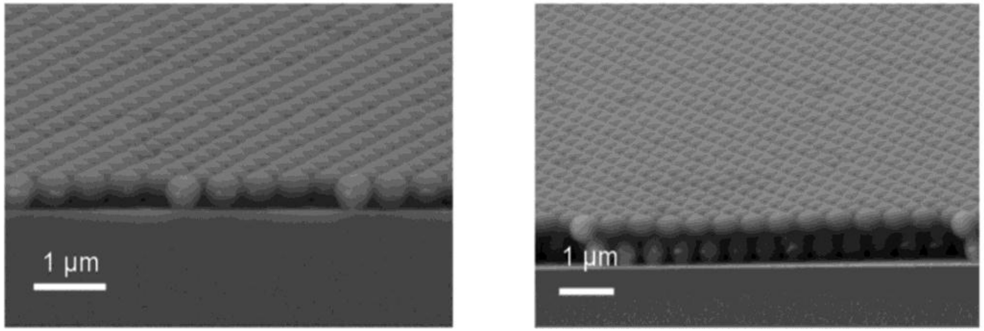
Introduction to Particle Coating

Modify properties of surface

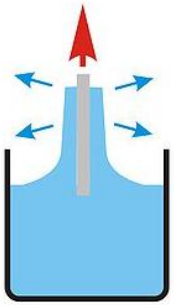
- Optical properties
- Magnetic properties
- Reactivity

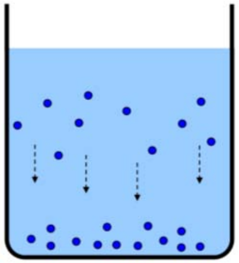


Malaquin, L., et al., *Langmuir*, **23**(23): p.11513-11521, (2007).

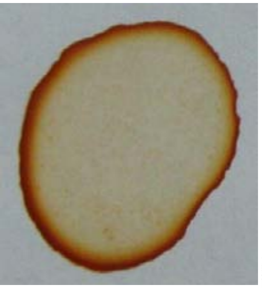
How to fabricate uniform particle coating?

- Dip coating
- Sedimentation
- Spin coating
- Electrostatic assembly
- ……
- Convective deposition

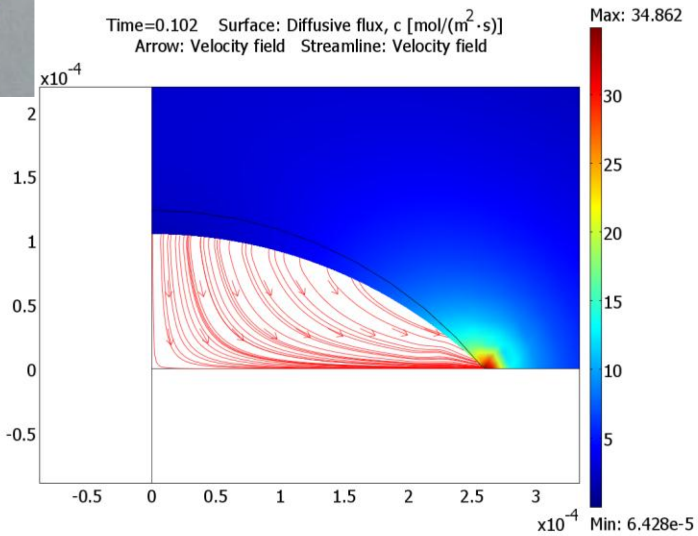




Convective Deposition



coffee ring effect

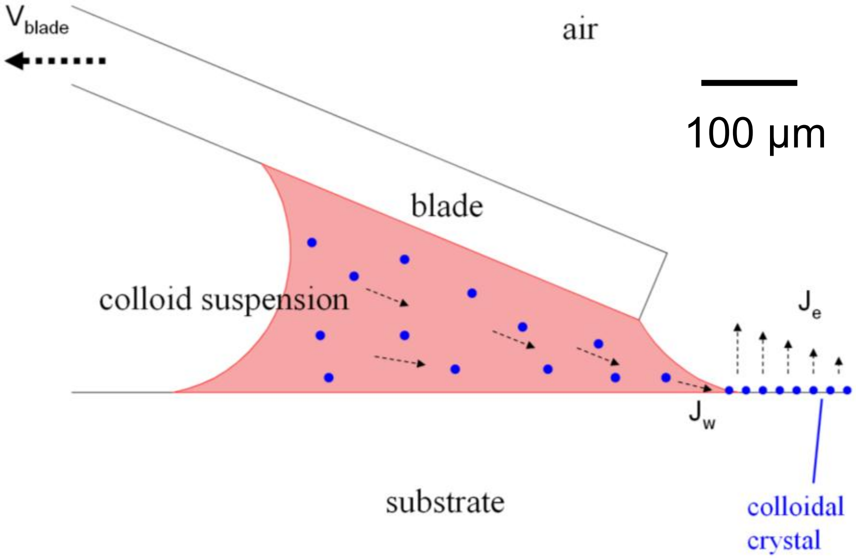


2D axi-symmetrical model of an evaporating droplet

*Deegan, R.D., et al., *Nature*, **389**(6653): p.827-829, 1997.

evaporation-driven convection

$$J_e = J_w$$



Parameters that affect the process:

- Properties of liquid
- Volume fraction of particles
- Particle size
- Particle material

- Velocity of blade
- Height of the blade
- Angle of blade
- Temperature of substrate

- Humidity of air

…

Multiphysics Modeling

	Governing Equations	Initial Conditions
Moving Mesh (ALE) Active in all domains	$\frac{\partial^2 X}{\partial x^2}+\frac{\partial^2 X}{\partial y^2}=0$ $\frac{\partial^2 Y}{\partial x^2}+\frac{\partial^2 Y}{\partial y^2}=0$	x(0) = xinit_ale y(0) = yinit_ale xt(0) = 0 yt(0) = 0
Fluid Dynamics Active in liquid domains	$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=\nabla\cdot\boldsymbol{\sigma}+\mathbf{F}$ $\nabla\cdot\mathbf{v}=\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$	u(0) = 0 v(0) = 0 p(0) = -2γ/r
Heat Transfer Active in liquid and substrate domains	$\rho C\left(\frac{\partial T}{\partial t}+\mathbf{v}\cdot\nabla T\right)=k\nabla^2 T$	Liquid: T(0) = 25°C Substrate: T(0) = T_s
Mass Transport Active in air domains	$D\nabla^2 c=0$	c(0) = 1.3075*RH [mol/m^3]

Multiphysics Modeling

Boundary Conditions

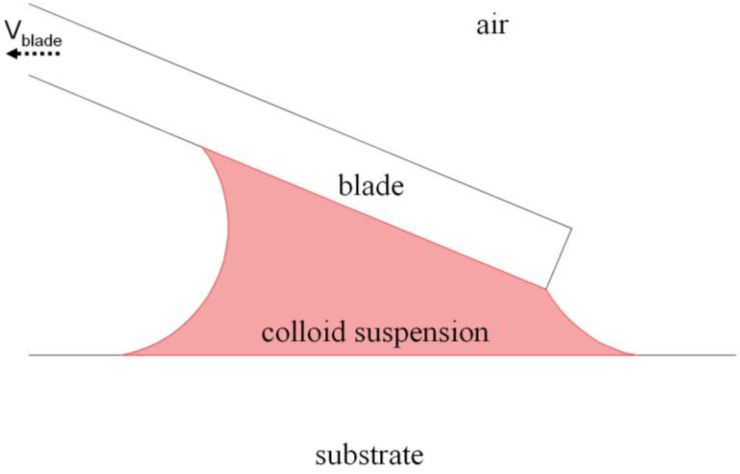
Moving Mesh (ALE)

Horizontal boundaries: dx = 0

Vertical boundaries: dy = 0

Blade: vx = V_blade, vy = 0

Free surface: $\mathbf{v}_{\text{int}} \cdot \mathbf{n} = (\mathbf{v} - \frac{\mathbf{j}}{\rho}) \cdot \mathbf{n}$



Fluid Dynamics

Liquid/substrate : slip/no-slip

Liquid/blade: u = V_blade, v = 0

Free surface: $\boldsymbol{\sigma} \cdot \mathbf{n} = -(2\gamma H + p_0)\mathbf{n}$

Heat Transfer

Far end of substrate: T = T_s

Exposed boundary: thermal insulation

Free surface: $jL = -k\nabla T \cdot \mathbf{n}$

Liquid/substrate: continuity

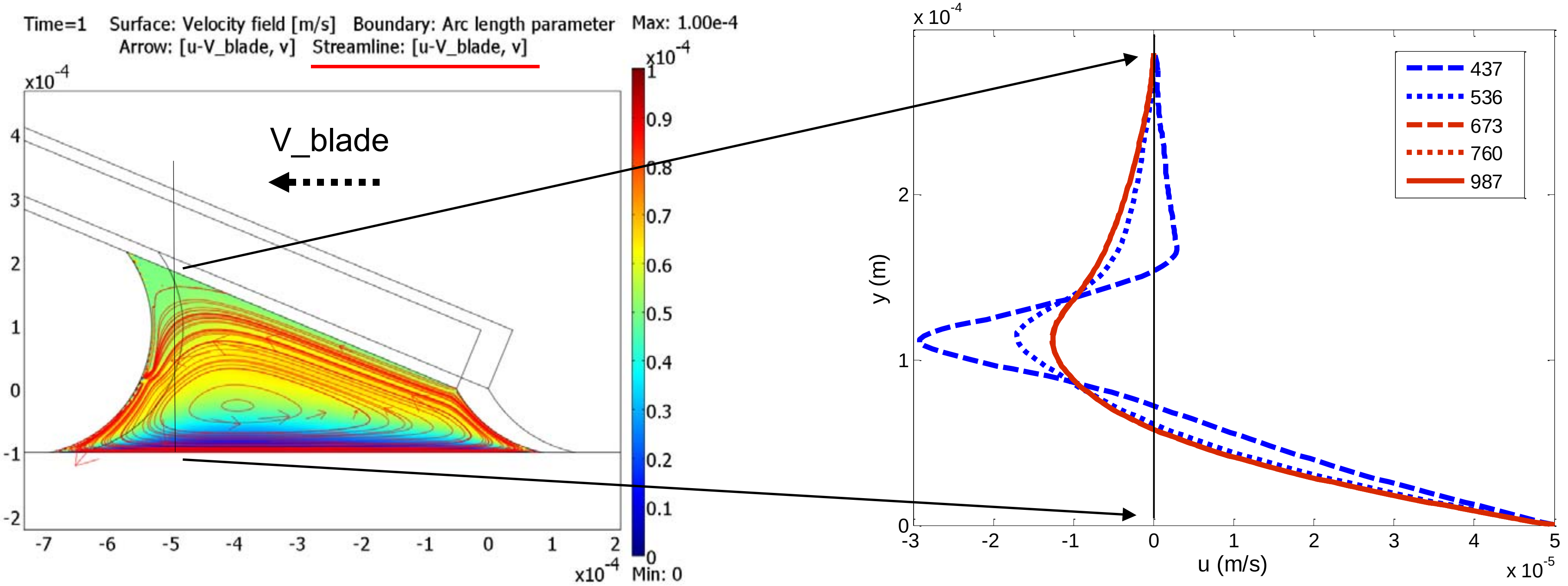
Mass Transport

Far end of air: c = 1.3075*RH [mol/m^3]

Exposed boundary: insulation

Free surface: c = c(t)

Results – Flow Pattern



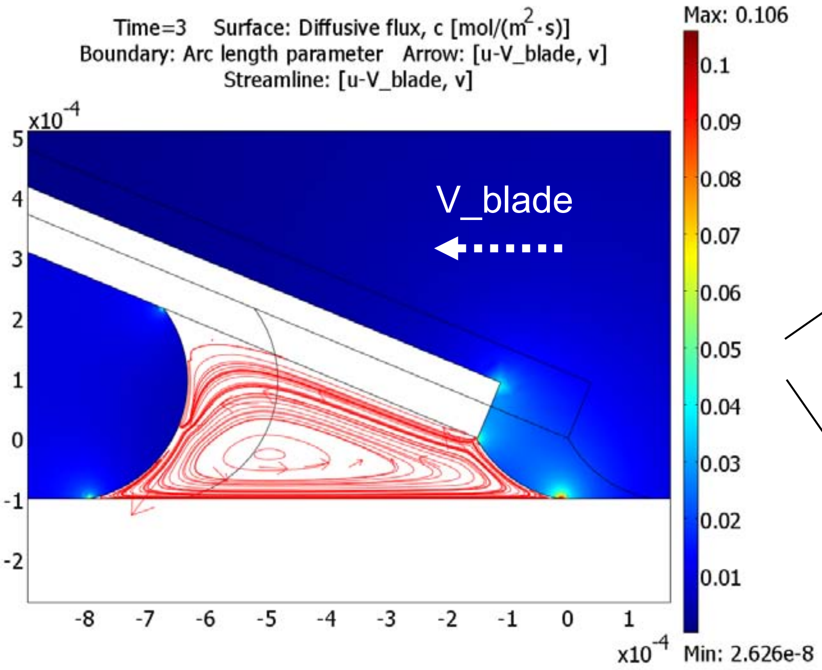
Flow pattern in liquid domain

V_blade = 50 μm/s

Velocity along the red line as a function of mesh size

- Shear flow due to the no-slip boundary conditions on blade and substrate
- Low Reynolds number, Re ~ 0.01

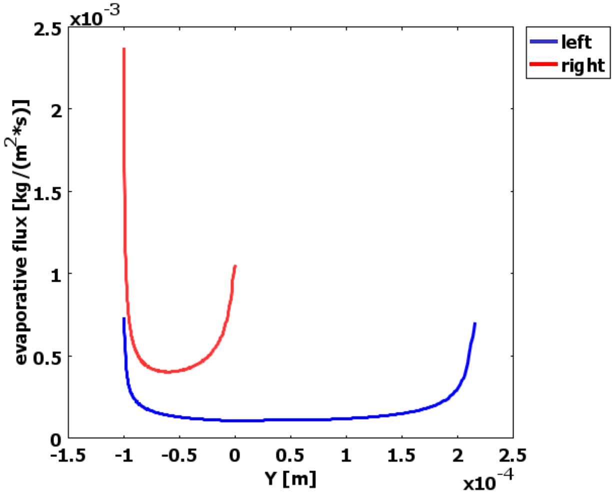
Results – Evaporation Flux



Evaporative flux around free surface

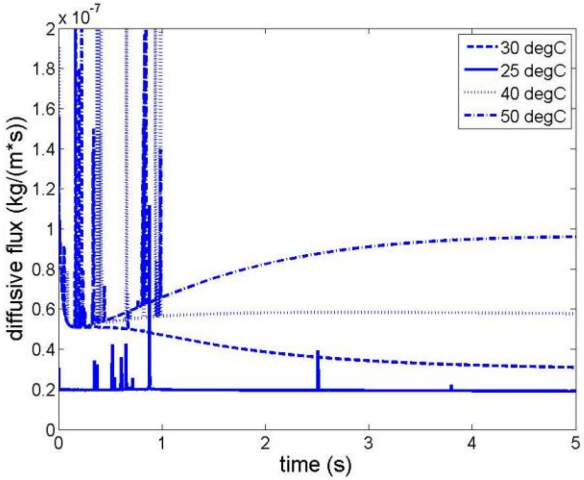
substrate temperature 50°C, V_blade = 50 μm/s, t = 3 s

j(y)



evaporative flux at free surface,
T_s = 50°C, V_blade = 50 μm/s, t = 5 s

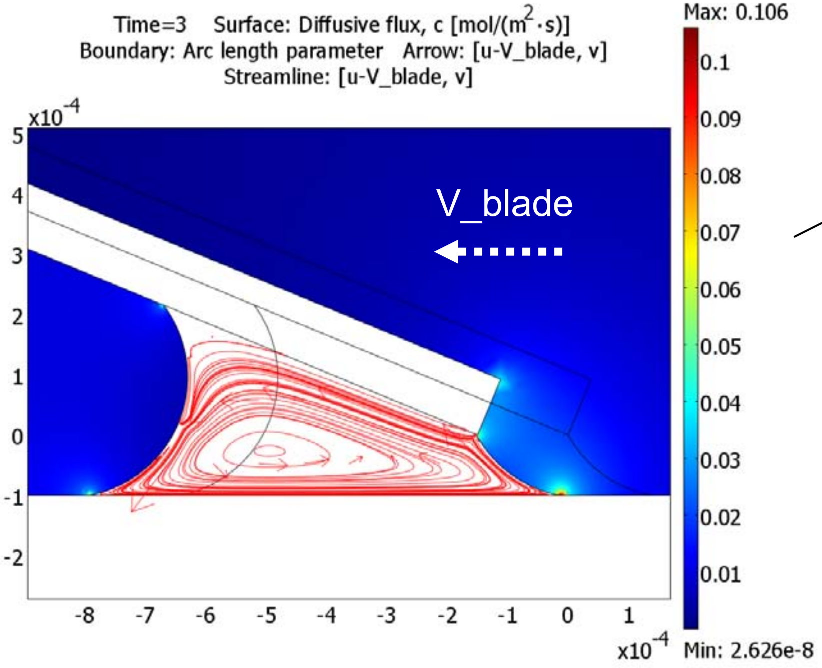
j(T_s)



Boundary integral of evaporative flux at right free surface, T_s = 50°C, V_blade = 50 μm/s

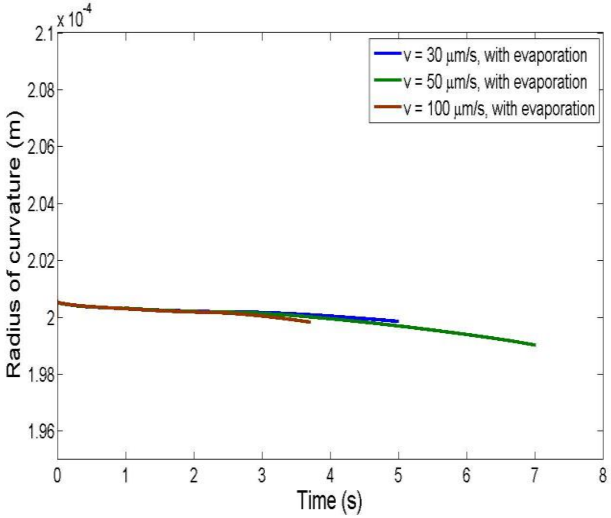
- Strongest evaporation flux at contact line
- Evaporation is stronger at right free surface
- Evaporation flux is dependant on substrate temperature

Results – Radius of Curvature

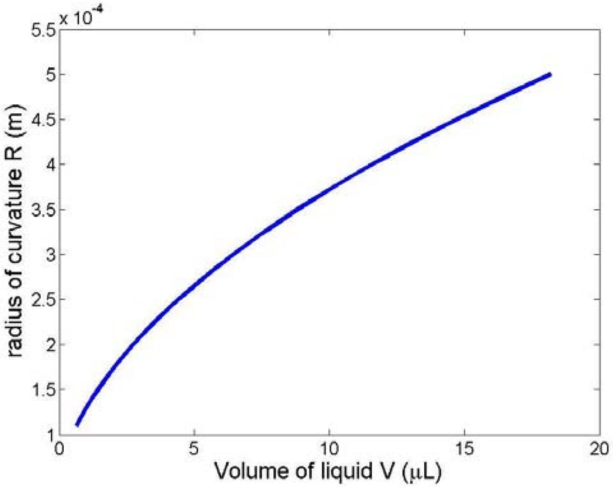


Evaporative flux around free surface

substrate temperature 50°C, V_blade = 50 μm/s, t = 3 s



Radius of curvature at free surface



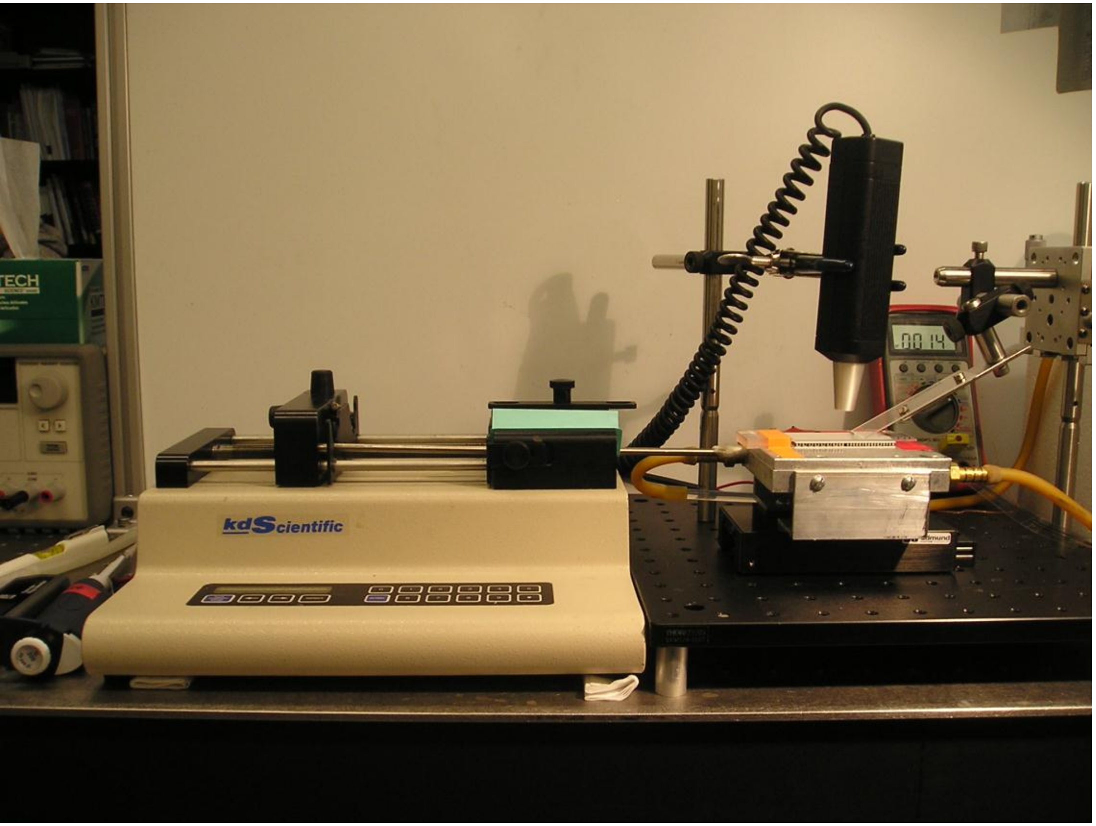
Radius of curvature changes with volume of liquid

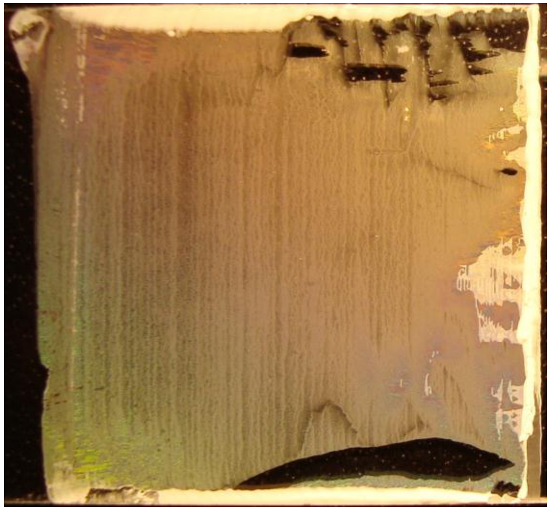
- Radius of curvature at free surface is decreasing as liquid domain is shrinking

Conclusion

- Solve coupled fluid dynamics, heat transfer and mass transfer in a changing geometry for convective deposition using moving mesh (ALE) method
- Special focus has been put on the free surface, such as mesh movement at free surface and evaporation at free surface
- Show flow pattern in the liquid domain with moving and deforming boundaries
- Predict the evaporation rate along the free surface
- Predict the evolution of radius of curvature at free surface

Future Work





Reference

1. Malaquin, L., et al., Controlled Particle Placement through Convective and Capillary Assembly, *Langmuir*, **23**(23): p. 11513-11521, (2007).
2. Deegan, R.D., et al., Capillary flow as the cause of ring stains from dried liquid drops, *Nature*, **389**(6653): p. 827-829, (1997).

Thanks for your attention!

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