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Modeling Encapsulation Processes

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

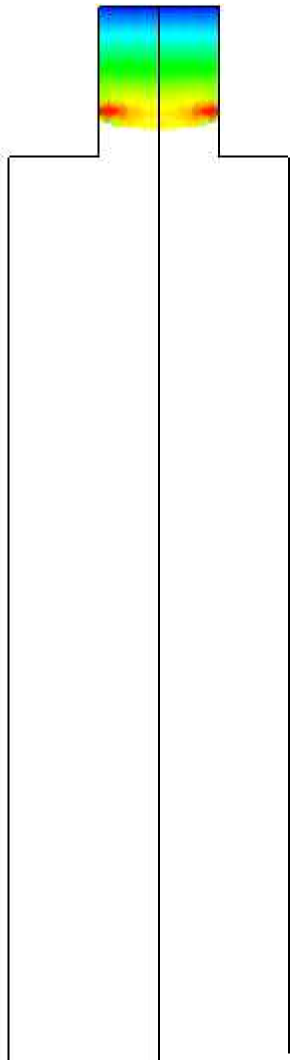
Motivation: Modeling Manufacturing Flows such as Injection Molding and Potting Processes

- Computational modeling provides insight into process improvements without expensive build-and-test cycles.

- Critical to develop "engineered processes" that are repeatable and minimize defects.
  - Improper filling or voids difficult to detect without expensive tear-down procedures.
  - Nondestructive evaluation often difficult because of geometry & materials involved.

GOMA and ARIA MULTIPHYSICS CODES

Massively parallel finite element codes for multiphysics free and moving boundary problems



- Coupled or separate heat, n-species, momentum (solid and fluid) transport
- Fully-coupled free and moving boundary parameterization
- Solidifcation, phase-change, consolidation, reaction of pure and blended materials
- Host of material models for complex rheological fluids and solids

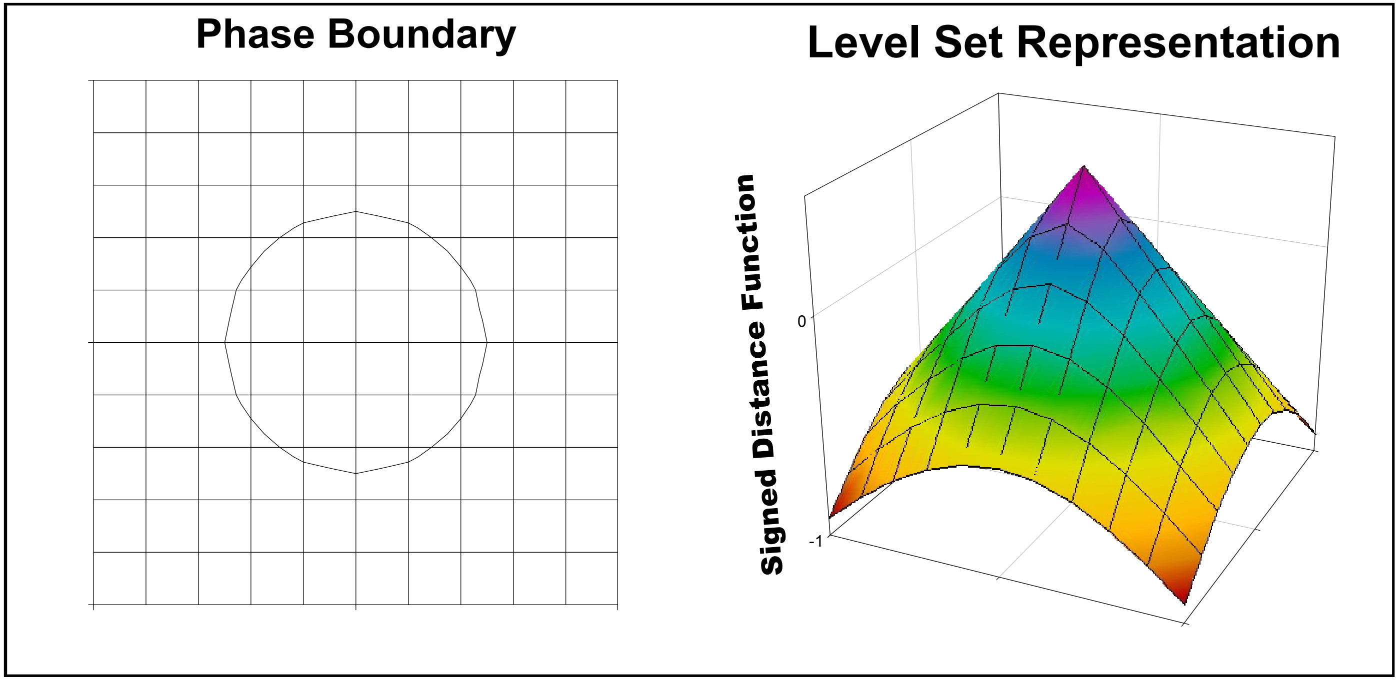
Unique features make GOMA/ARIA ideal for manufacturing processes in which:

- Free surfaces are ubiquitous
- Coupled fluid-solid mechanics
- Complex material rheology/low speed

Basics of Level Set Method

The level set function, $\phi(x,y,z)$ is the representing function

- Signed minimum distance to the interfacial curve
- Sign of ϕ distinguishes phase physics.
- The contour $\phi(x,y,z) = 0$ “represents” the interface <u>when needed</u>
- Evolution of $\phi(x,y,z)$ such that $\phi(x,y,z) = 0$ remains on the interface



Level Set Tracking of Interface

The level set function, $\phi(x,y,z)$ is the representing function

Given fluid velocity field, u(x,y,z), evolution on a fixed mesh is according to:

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

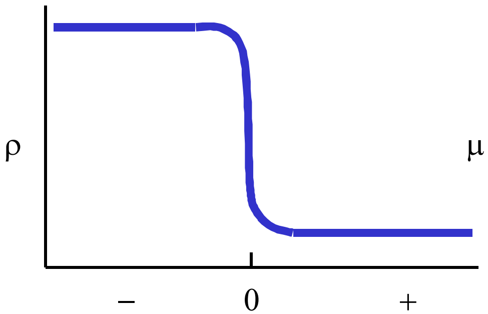
Purely hyperbolic equation … fluid particles on $\phi(x,y,z) = 0$ should stay on this contour indefinitely

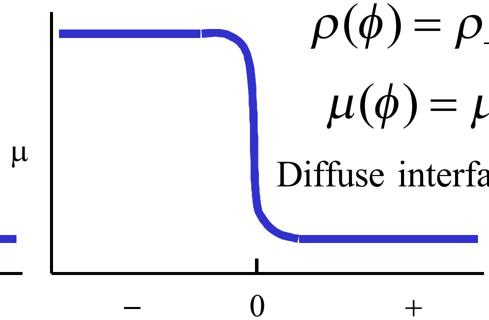
- Does not preserve $\phi(x,y,z)$ as a distance function
- Introduces renormalization step
- Derivatives useful for B.C.s: $n = \nabla \phi$ Normal

  $\zeta = \nabla \bullet \nabla \phi$ Curvature

Fluid velocity evolves as one-phase fluid with properties that depend on ϕ

$$\rho(\phi)\frac{Du}{Dt} = -\nabla P + \nabla \cdot (\mu(\phi)\dot{\gamma}) + \rho(\phi) g + I.T., \quad \nabla \cdot u = 0$$





$$\rho(\phi) = \rho_{-}(1 - H_{\alpha}(\phi)) + \rho_{+} H_{\alpha}(\phi)$$

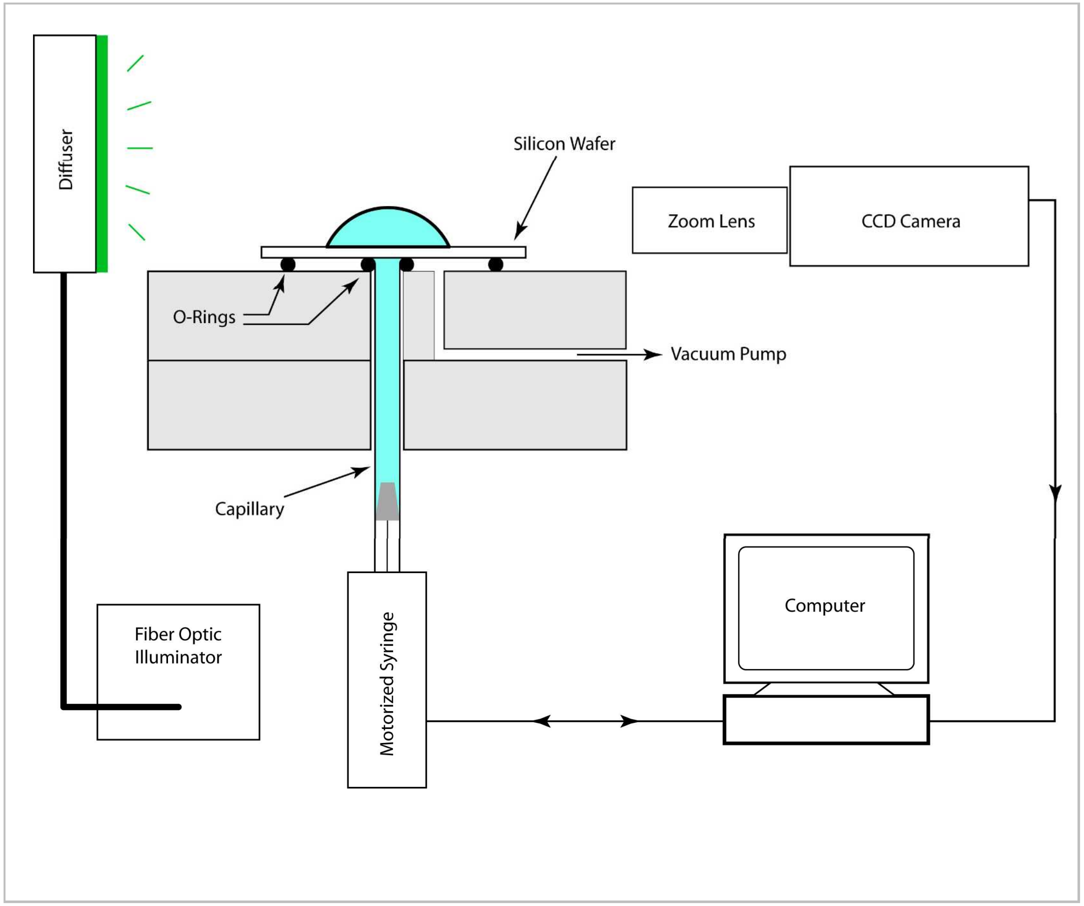
$$\mu(\phi) = \mu_{-}(1 - H_{\alpha}(\phi)) + \mu_{+} H_{\alpha}(\phi)$$

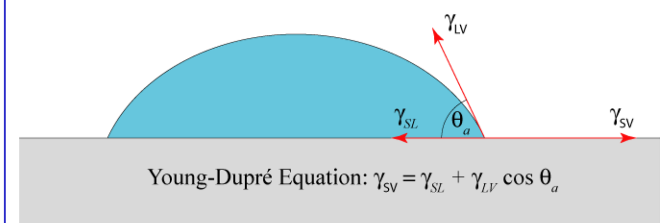
Diffuse interface with smooth Heaviside function

$$H_{\alpha}(\phi) = \frac{1}{2}\left(1 + \frac{\phi}{\alpha} + \frac{1}{\pi}\sin\left(\frac{\pi\phi}{\alpha}\right)\right)$$

Feed-Through Goniometer:

Apparatus to Measure Dependence of Contact Angle on Velocity

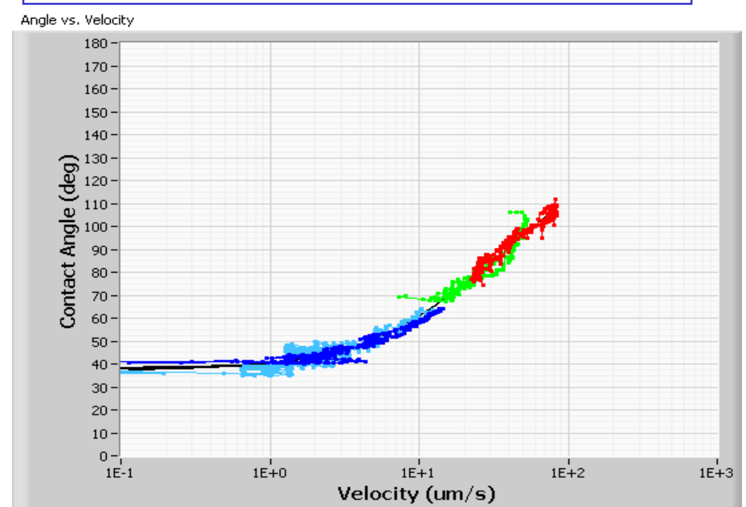




$$S \equiv \gamma_{SV} - \gamma_{SL} - \gamma_{LV}$$

$S > 0$ **Complete Wetting** $(\theta_a = 0^\circ)$

$S \leq 0$ **Partial Wetting** $(\theta_a > 0^\circ)$



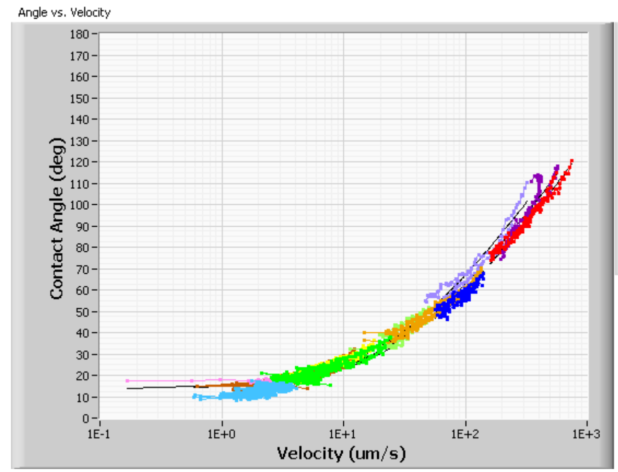
75-H-90000 Ucon Lubricant on Acrylic
T = 25°C

- Form a drop of desired volume (~ 370nL)
- Analyze dynamics of spontaneous spreading

Blake Wetting Line Model

- Molecular Kinetic Model

T.J. Blake, J. De Coninck *Adv. Colloid Int. Sci.* **2002**, *96*, 21-36.



Goniometer wetting data

Adhesion to Substrate

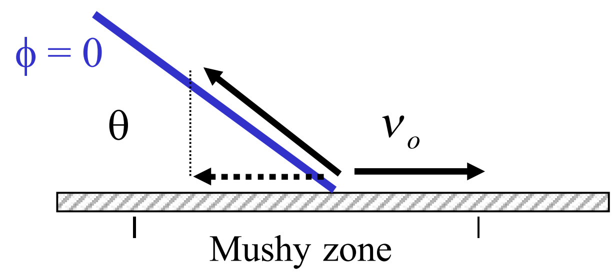
$$U = \frac{2kT\lambda}{\eta v_L} \exp\left[\frac{-\gamma_{LV}(1+\cos\theta_\infty)}{nkT}\right] \sinh\left[\frac{\gamma_{LV}(\cos\theta_\infty - \cos\theta)}{2nkT}\right]$$

Viscosity

Molecular-Kinetic

Lump terms

$$U = v_o \sinh[\gamma(\cos\theta_\infty - \cos\theta)]$$

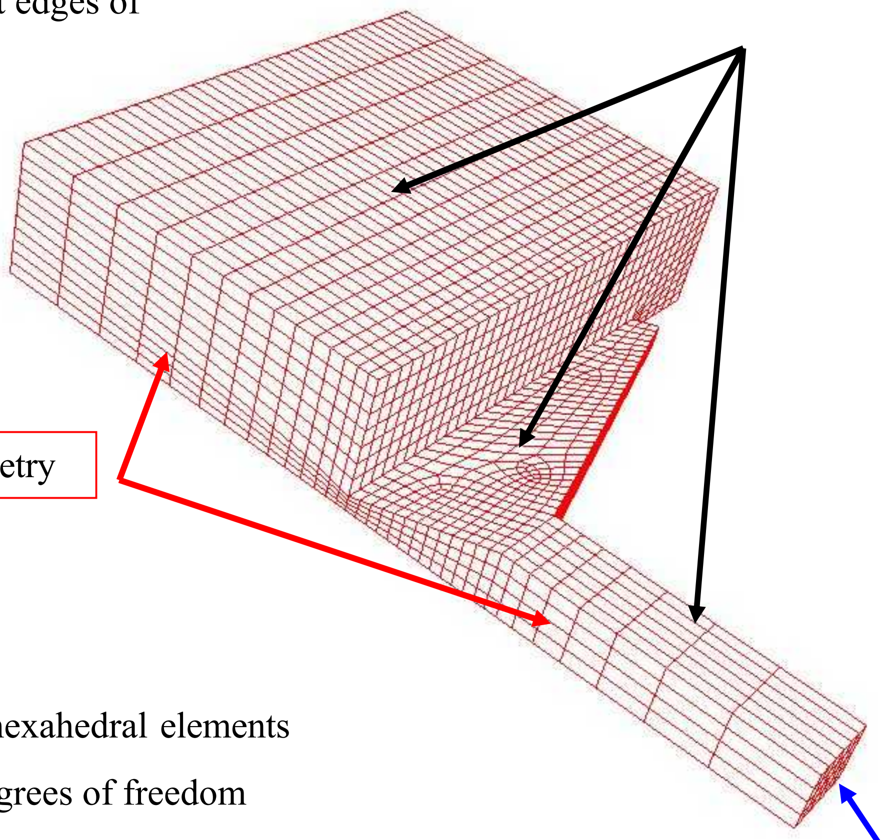


Three unknowns $\left\{ \begin{array}{l} v_o \\ \cos\theta_\infty \\ \gamma \end{array} \right.$ which can be functions of the can be fit to goniometer wetting experiments

3D Computational Model of Injection Molding

No penetration / no slip, except near contact region

Outflow occurs at edges of mold chamber



Centerline Symmetry

Flow In

- 6744 8-Node hexahedral elements
- 41300 total degrees of freedom

Parameters:

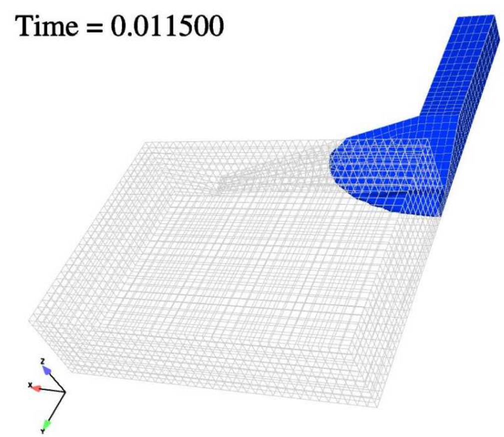
Newtonian

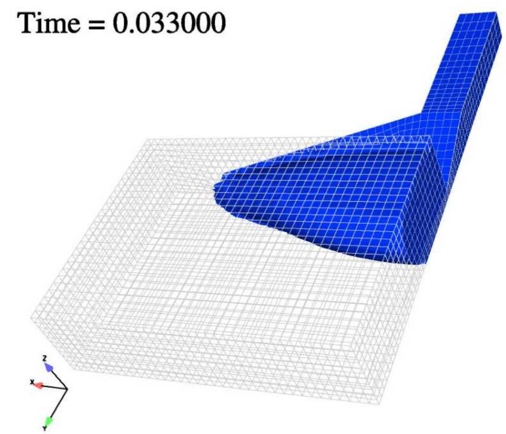
$\rho_{gas} = \rho_{liq} / 1000$

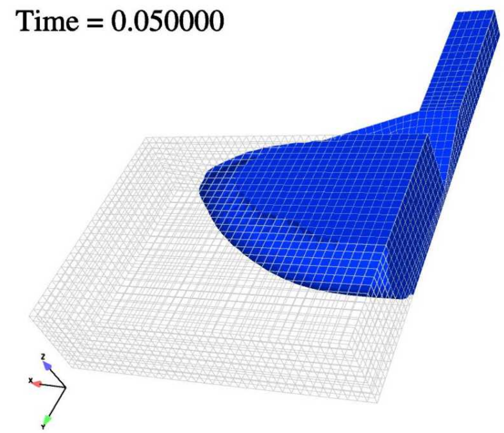
$\mu_{gas} = \mu_{liq} / 100$

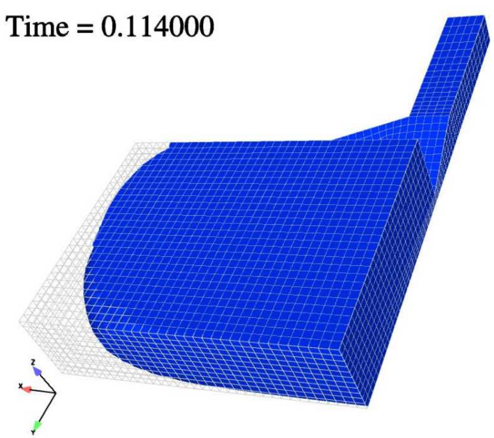
Wetting parameters same in both phases

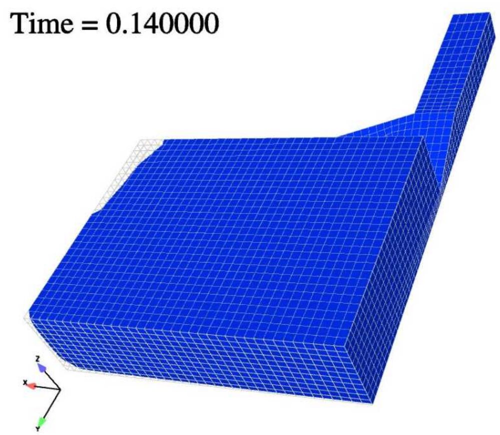
Original Distributor Design by Injection Loading Company





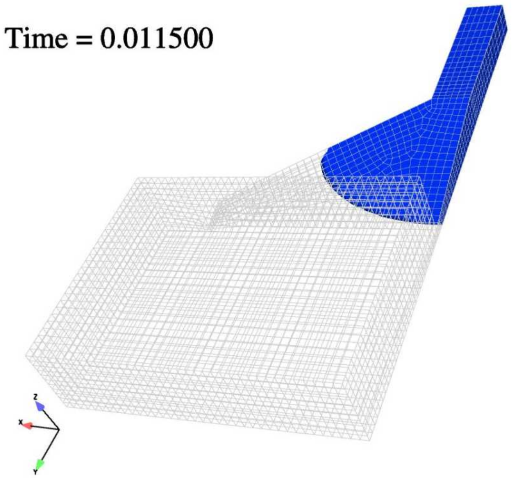


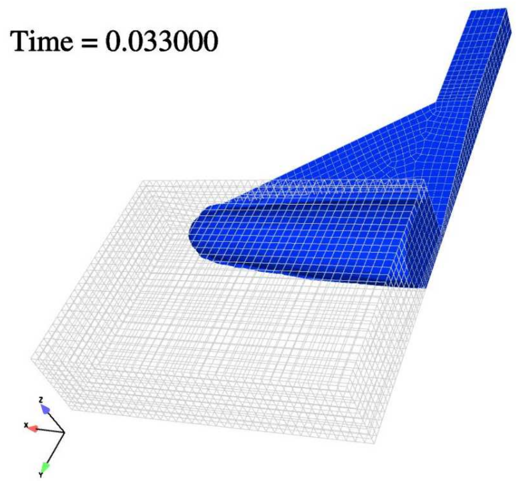


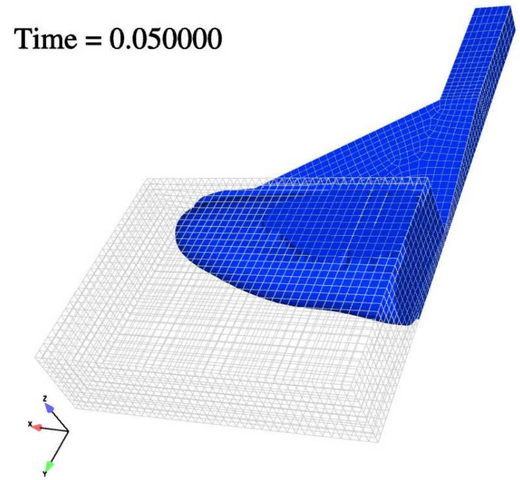


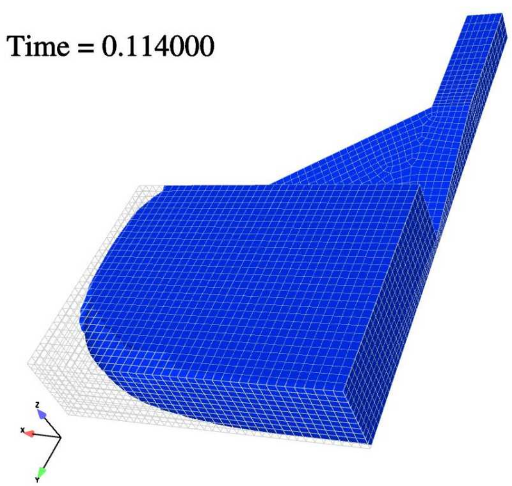
- Fluid enters main cavity before completely filling the distributor
- Fluid pools in center of the cavity before wetting top surface
- Top surface wetting front catches up to the bulk flow
- Void is left in corner after filling is complete

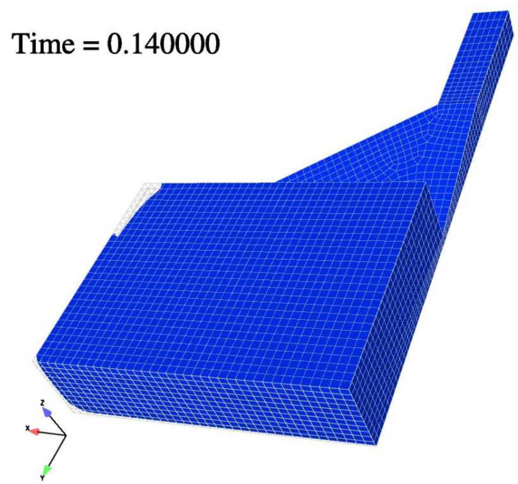
Second Geometry has Longer Distributor





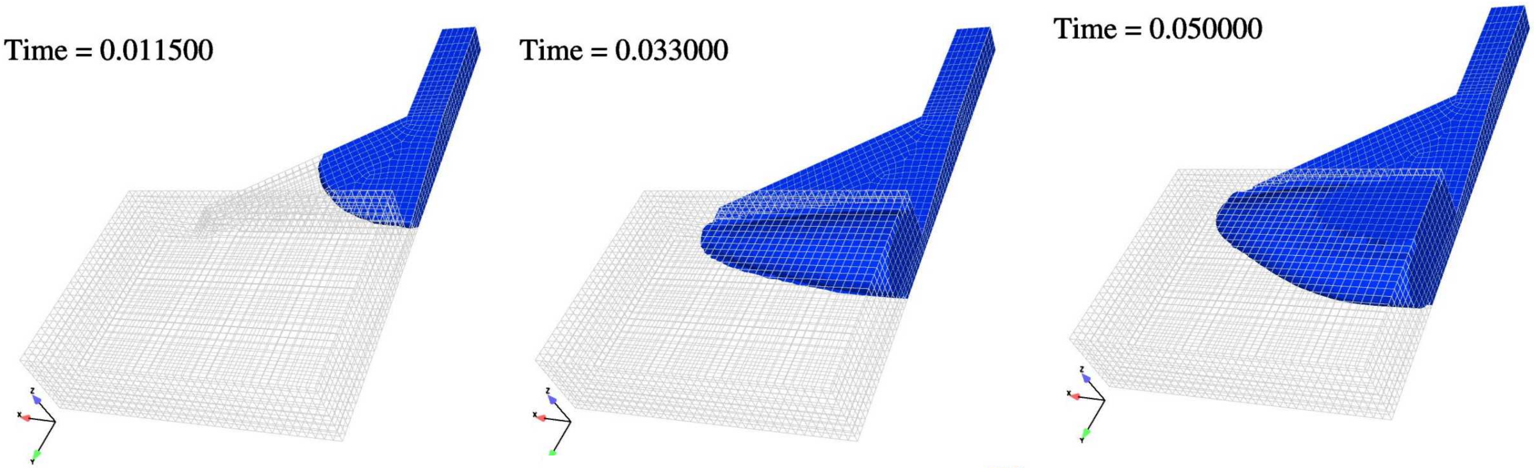


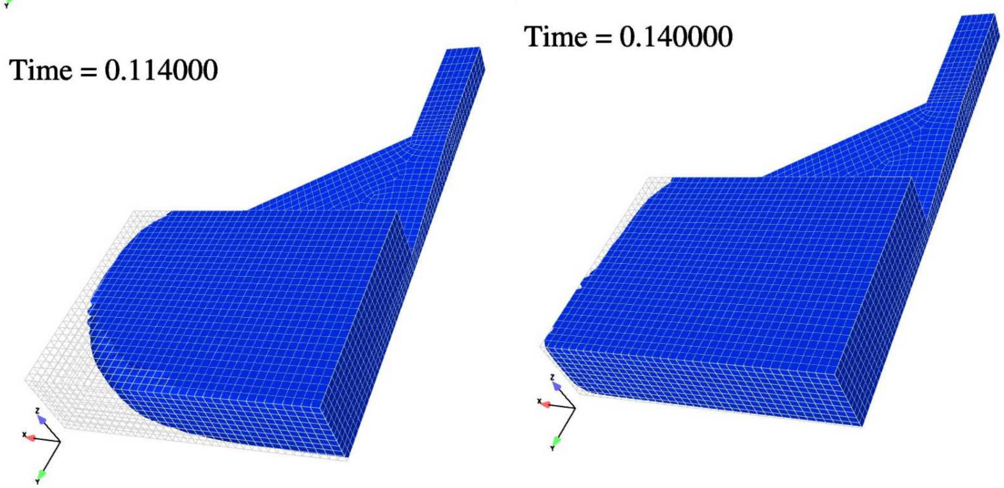




- Longer distributor leads to a flow front that is more evenly distributed and monotonic
- Void is still left in corner after filling is complete, but it is smaller than for the original geometry

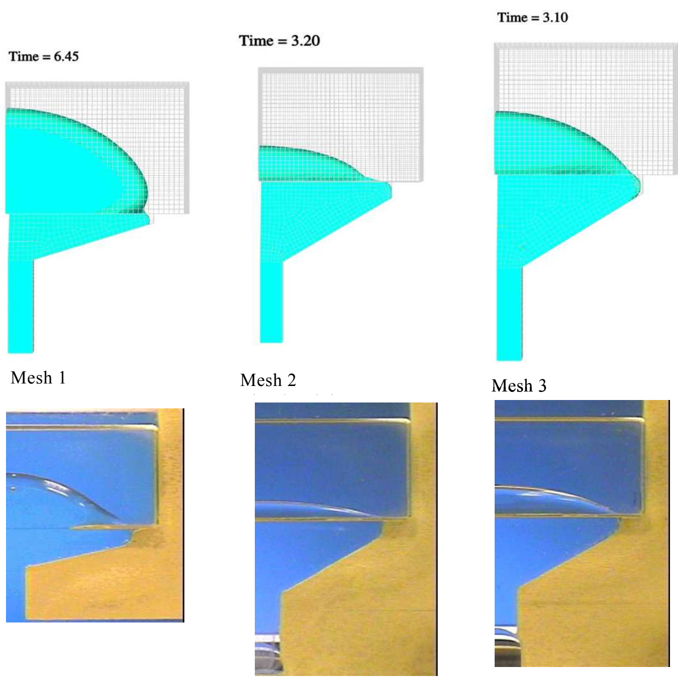
Third Geometry has both a Longer and Taller Distributor

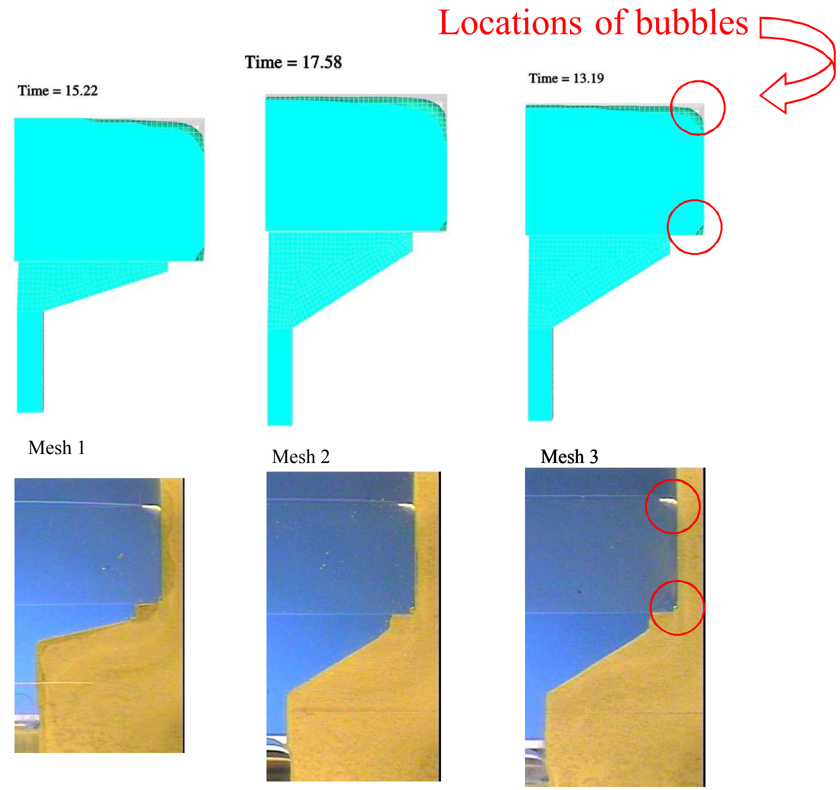




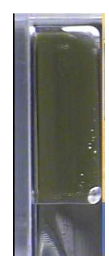
- Longer-Taller is slight improvement over original geometry, though not as good as second geometry
- Void is still left in corner after filling is complete, but it is smaller than for the original geometry

Comparison to Experiment





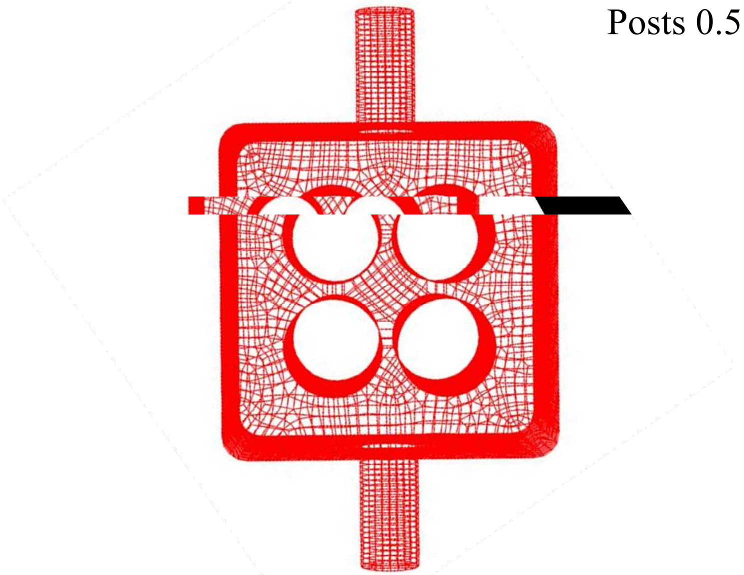
- Qualitative aspects captured – improvements in distributor and number and location of bubbles
- Increasing wetting speed from that measured improves shape of front



Encapsulation Sensitivity and Validation Studies

Simple geometries that are representative of the pressure injection process

Out flow



In flow

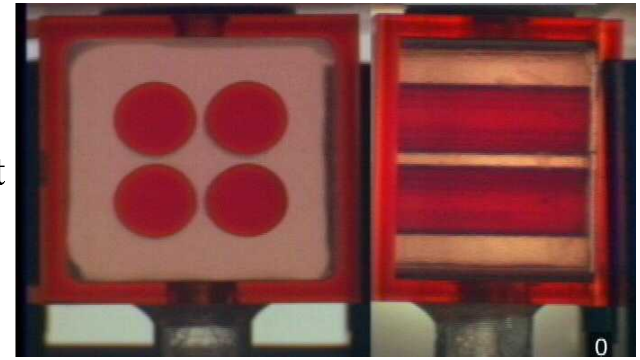
1.7 cm X 1.7 cm X 1.3 cm

Posts 0.5 cm diameter

- 3D mesh geometry with posts to represent components in real part
- In-flow velocity has a parabolic profile
- Blake wetting boundary condition is specified at all solid surfaces

Outlet Outlet

Front view

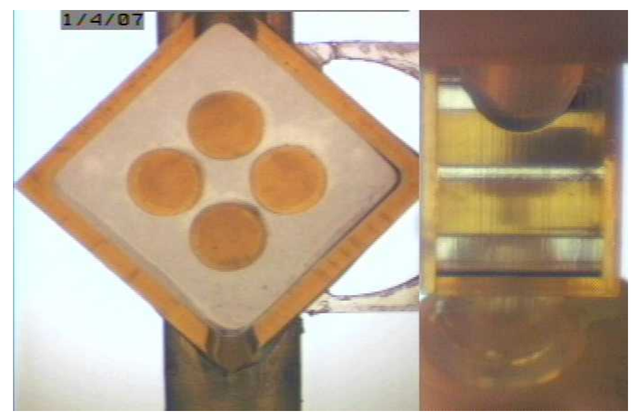


Side view

Inlet Inlet

Outlet

Front view



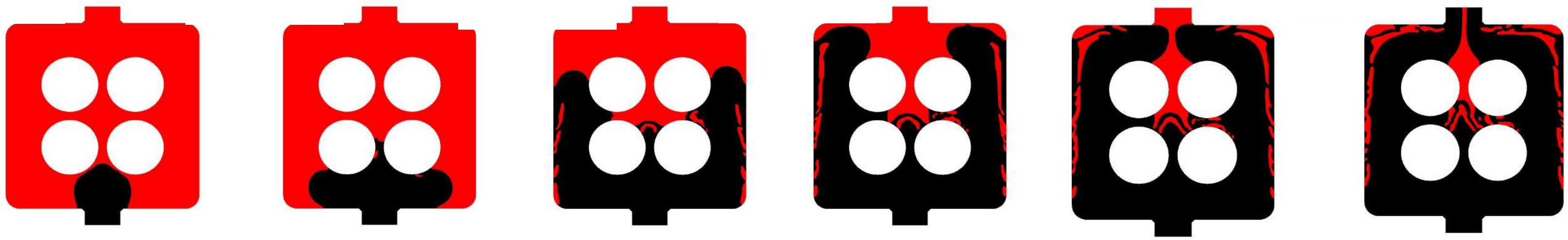
45° from top

Inlet

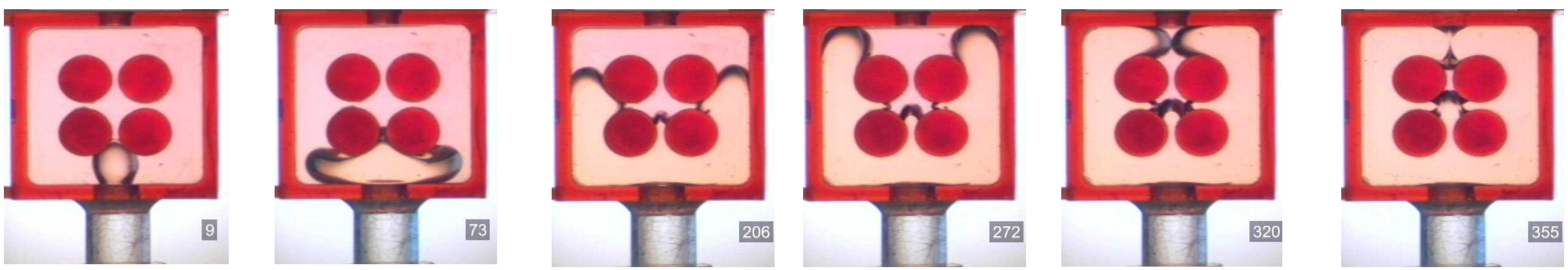
- Video flow for validation

2D Model Matches Experiment Well Even with Approximate Parameters

Model parameters: μ = 300 Poise, θ^{eq} = 45^o, v_o = 1 cm/s, σ = 12 dyne/cm, fill time=5 s



Time*=0.03 Time*=0.2 Time*=0.6 Time*=0.8 Time*=0.9 Time*=1.0



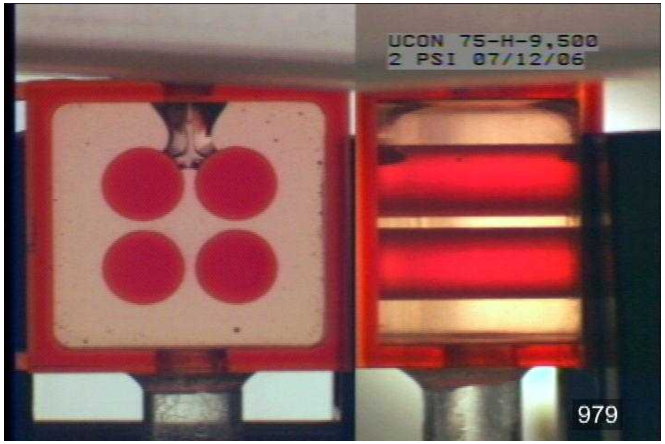
Real parameters: μ = 390 Poise, θ^{eq} = 37.8^o, v_o = 0.00193 cm/s, σ = 42.4 dyne/cm (Ucon 95-H-90000 measured parameters); fill time=12 s

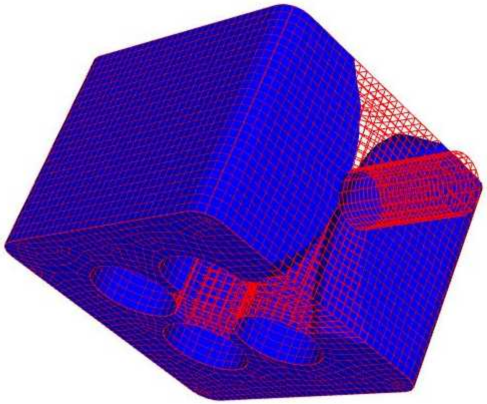
Both: Ca ≅ 20; Re ≅ 0.001

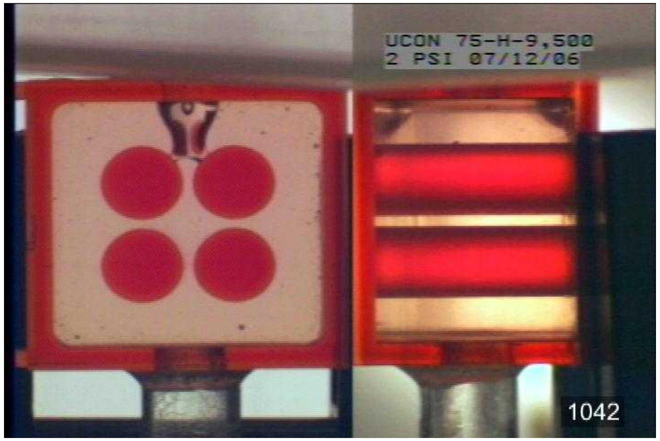
Time*=time/total time

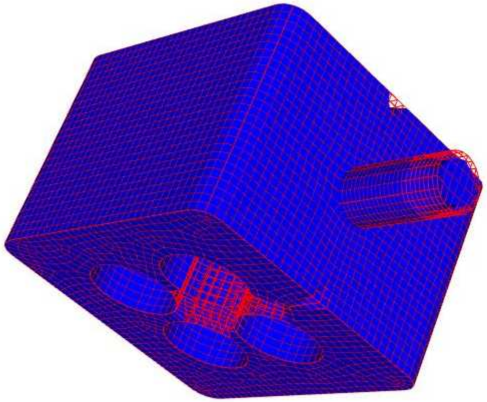
3D Effects

- Some air escapes as it continues to rise after flow stops
- Bubbles remain on back and front walls near outflow





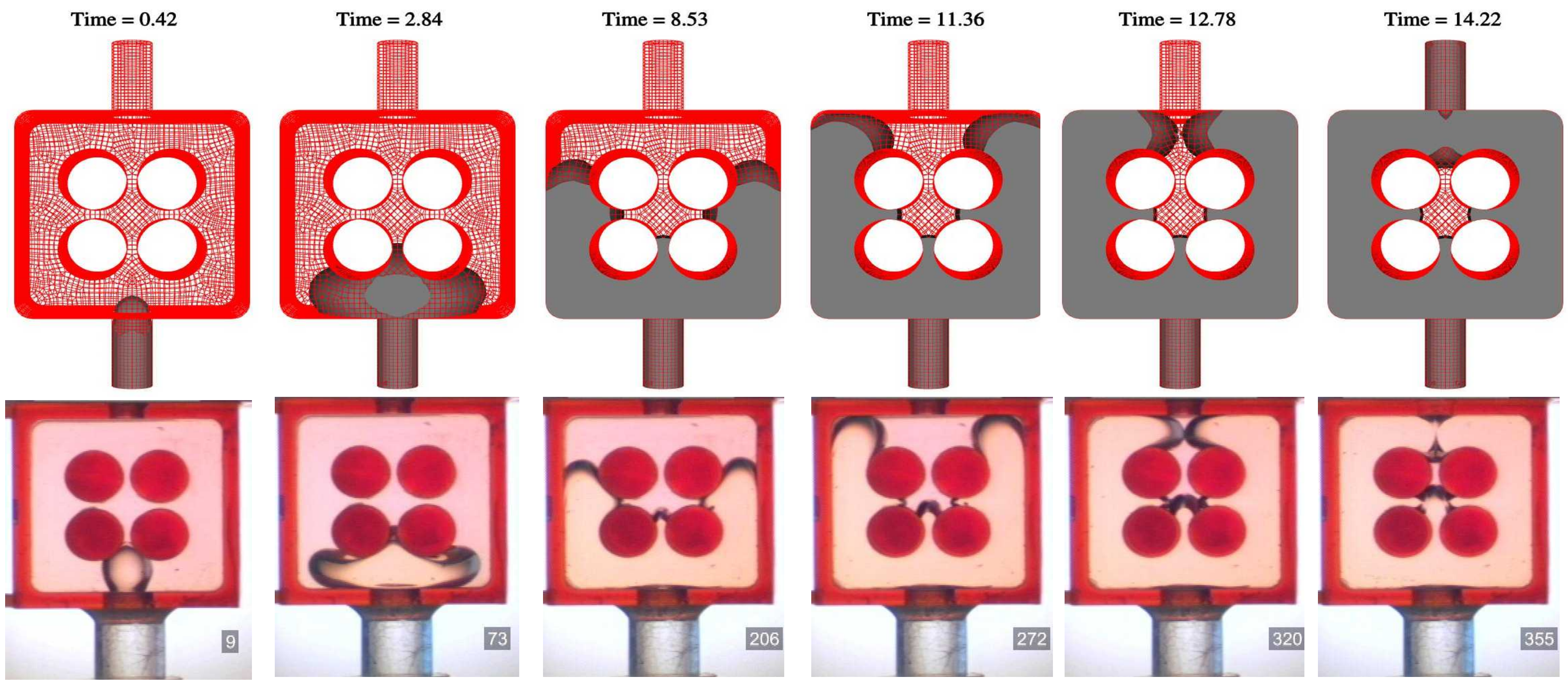




3D Model Compared to Experiment

Wetting speed in model doubled over measured value

Model parameters: m = 390 Poise, q^{eq} = 39.8°, v_o = 0.0026 cm/s, s = 42.4 dyne/cm, fill time=14 s

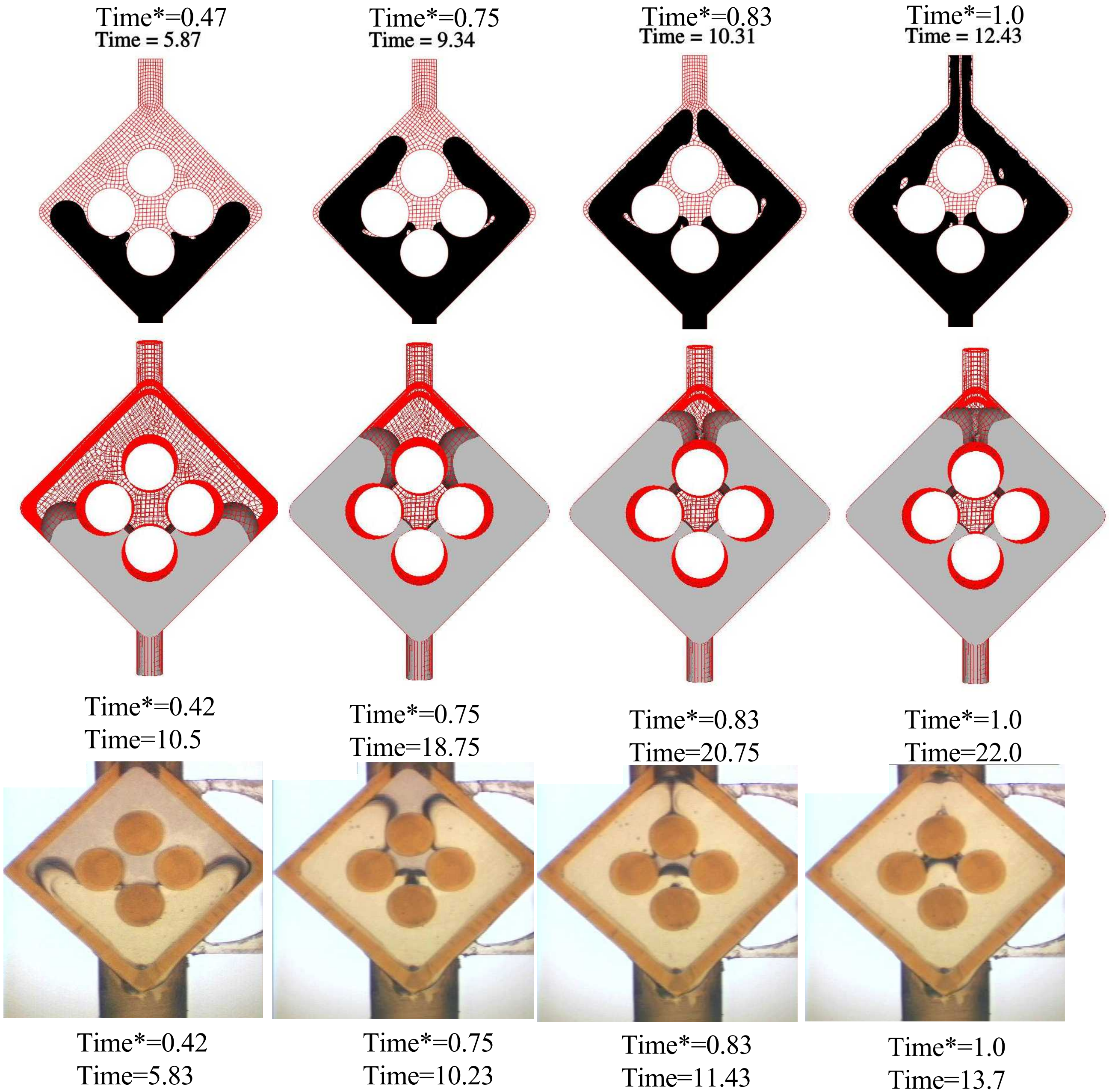


Real parameters: m = 390 Poise, q^{eq} = 39.8°, v_o = 0.0013 cm/s, s = 42.4 dyne/cm (Ucon 95-H-90000), fill time=12 s

Both: Ca ≅ 20; Re ≅ 0.001

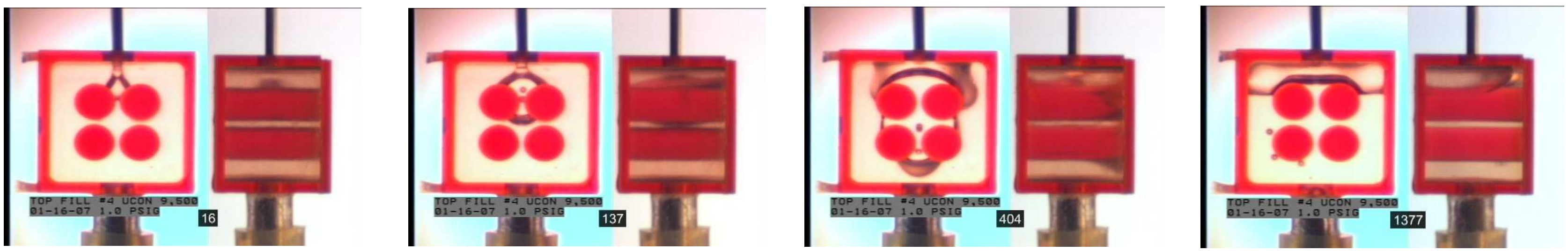
Time*=time/total time

Change of Injection Point: 2D vs. 3D Model



- Models use same materials as experiment: UCON 95-H-90000
- 2D (top) with same fill rate as experiment (bottom)
- 2D captures salient features –conservative in that area fraction of bubble larger than volume fraction in 3D
- 3D shown here at half the fill rate (middle) – little effect of fill rate in this range

Process/Material Change to Allow Much Slower Flow Rate Could Minimize Voids



UCON 95-H-90000 dripping slowly from the top simulates new KC process.

Top fill usually not ideal but it is done slowly enough to allow area between posts to wet.

ARIA model results

Conclusions and Lessons Learned

- Level Set scheme is successful in capturing dynamic wetting around geometric features.
- Feed-through Goniometer allows dynamic wetting measurements.
- Geometry (and orientation), Ca, and wetting properties affect the degree of air entrapment.
- Modeling can provide insight into die design and location of possible voids.
- Trapping of gas during flow around obstacles is relatively insensitive to Ca over the range expected in the application of interest (viscosities set, flow rate determined from pot life).
- Suggested to customer that process or material be changed
  - Vacuum potting
  - Increase pot life and drastically reduce the flow rate, fewer bubbles are trapped.