SAND2007-0266P

Computational Results

Gate 3 Review – January 18, 2007

Lisa Mondy for

Computations: **Rekha Rao,David Noble, Richard Givler, Amy Sun, Andy Kraynik, Ed Wilkes, Pat Notz, Randy Schunk, Jim Mahoney**

Rheology/Kinetic Modeling: **Doug Adolf**

Experiments: **Carlton Brooks, Ray Cote, Jaime Castañeda, Anne Grillet**

Statistics: **Brian Rutherford**

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

Readiness Technology Initiative Project: "Defect-Free Manufacturing and Assembly"

- Computational modeling provides insight into process improvements without expensive build-and-test cycles.
  - Modeling provides guidance to producing physical models for flow visualization studies.
  - Physical models can be another cost-effective way to improve understanding of sensitivities of process parameters, especially in complex geometries.

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

- Complex materials
  - KC hard encapsulants → viscosity depends exponentially on particle concentration, which can change locally.
  - Wetting depends on geometry, material properties, temperature, time, extent of reaction, and flow rate. Competing effects of viscous and surface forces.

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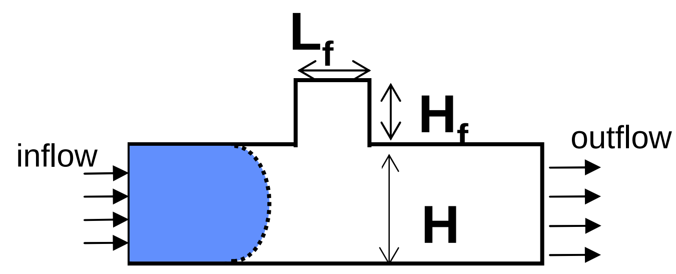
Overview

- Do computer simulations adequately predict results of the TIP validation studies?
  - Simple geometries that are representative of the processes at Pantex and at Kansas City
  - Compare predicted flows to observations in flow in transparent fixtures
  - Compare viscosity/cure model to data
- Use results to complement processing experiments (lessons learned)

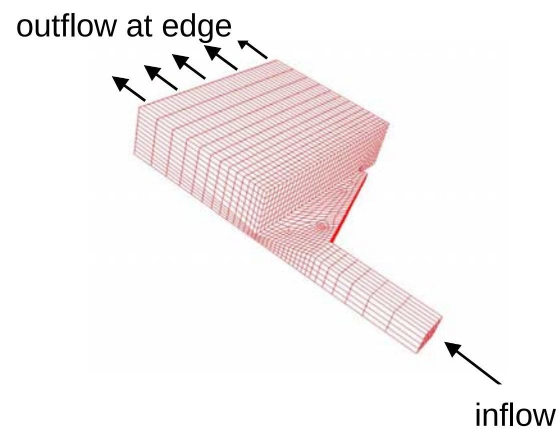
Pantex models for validation

Simple geometries that are representative of the process

- **Notch**: filling into joints



- Injection into a box



- Previous tests for heat calculations with curing material

Sensitivities for Notch Problem

- Estimated linear effects model (oversimplification to get initial estimates) – believe trends not absolute values of effect
- Nonlinearities noted especially in H_f/H
- "Estimated effect" is absolute change in % fill as change parameter from its lowest value to highest value

PARAMETER	LOW	HIGH	RANGE	ESTIMATED EFFECT
Hf/H	0.5	2	1.5	-8.73
F_in (cm/s)	0.001	1	0.999	-62.31
Top_ang.	15	60	45	-90
Bot_ang.	15	60	45	-45
Capillary	0.001	10	9.999	-18.6
Linear wetting model v0	0.1	5	4.9	-17.7
Wetting changing from linear to Blake (equivalent coefficients)				-13

Wetting angle by far most important in this geometry

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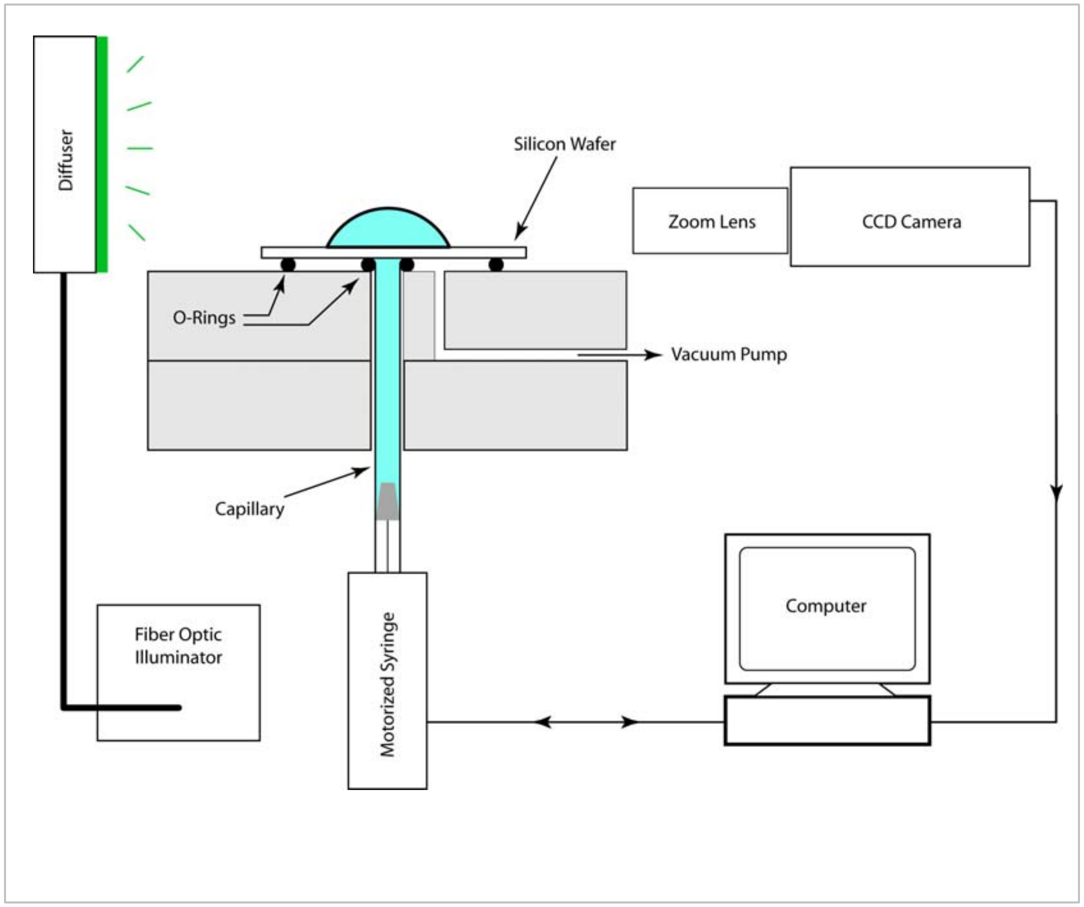
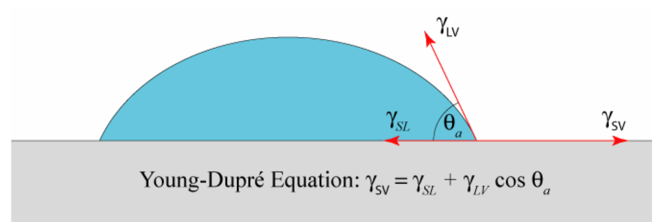
Feed-Through Goniometer

Apparatus to Measure Dependence of Contact Angle on Velocity

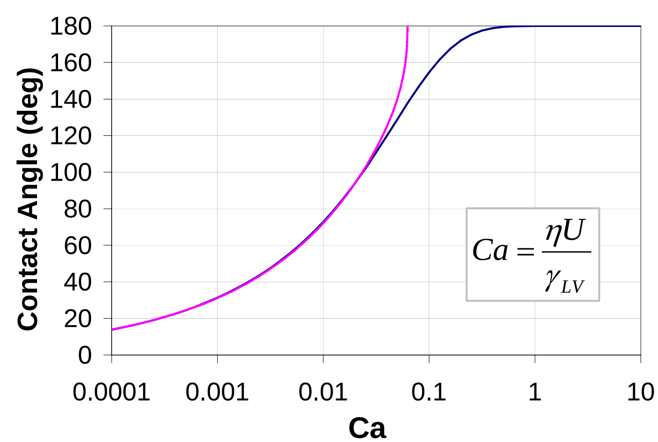




$S \equiv \gamma_{SV} - \gamma_{SL} - \gamma_{LV}$

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

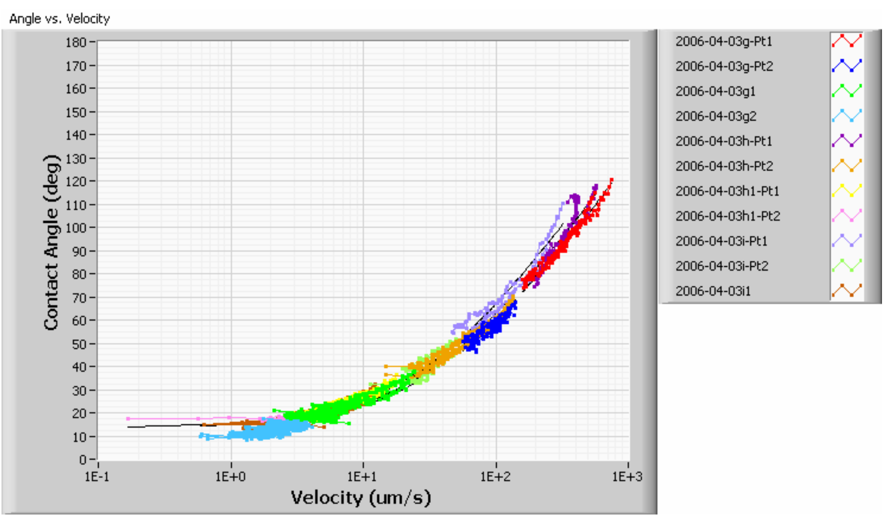
$S \leq 0$ **Partial Wetting** $(\theta_a > 0^\circ)$



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

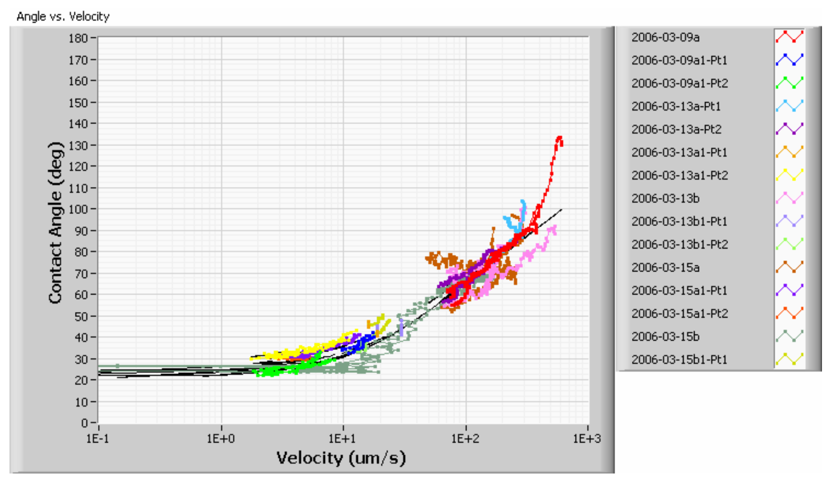
Examples of Pantex and KC Materials

Sylgard 184 on Aluminum with Mirror Finish
5 wt.% Accelerator in Part A
T = 25°C
Tested over ~ 40 minutes



RMS error = 3.1°
3.5° with "no cure model"

RSF200A Wetting on PC-Smooth at 80°C
Tested over ~10 minutes



RMS error = 6.2°
6.4° with "no cure model"

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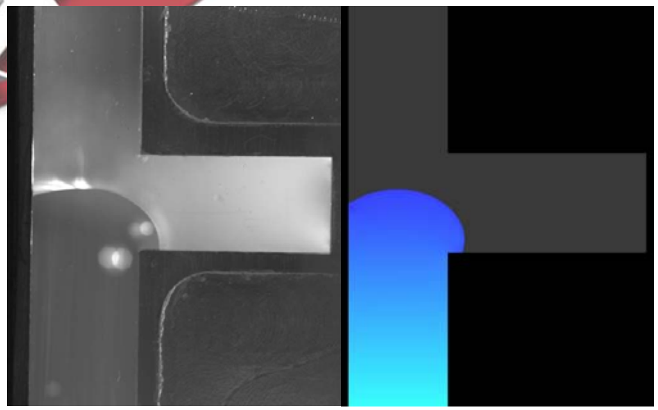
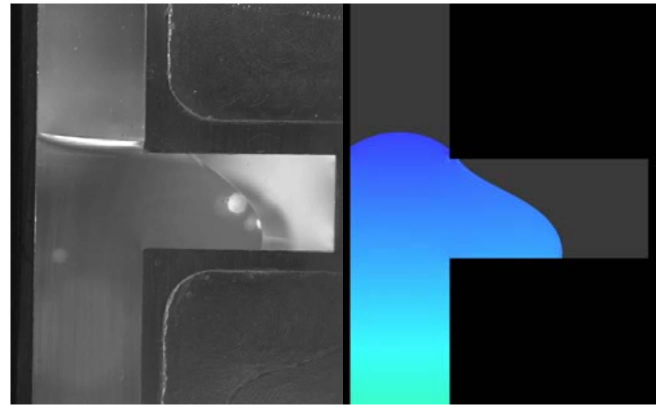
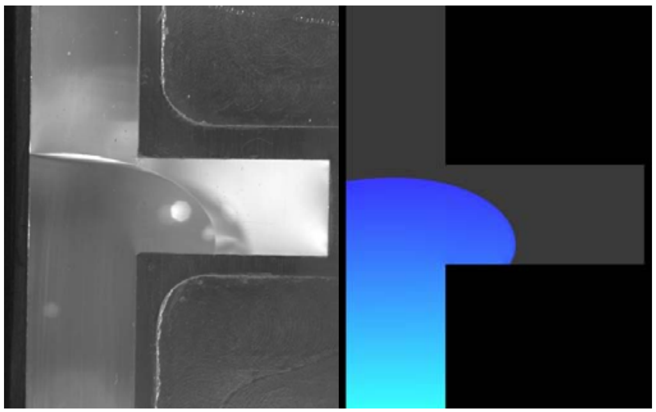
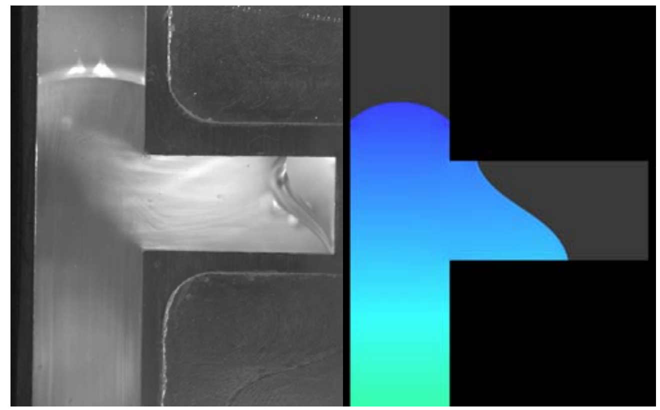
Simulation with measured parameter compared to experimental results

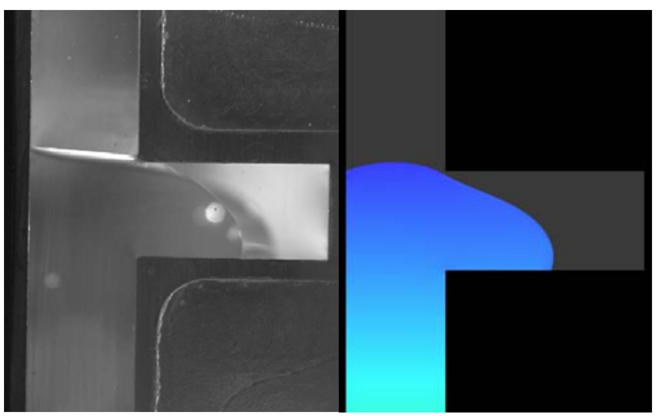
2D vs. 3D effects in next 3 slides

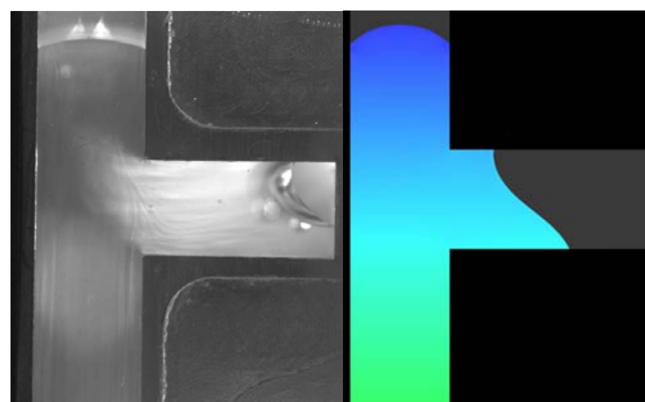


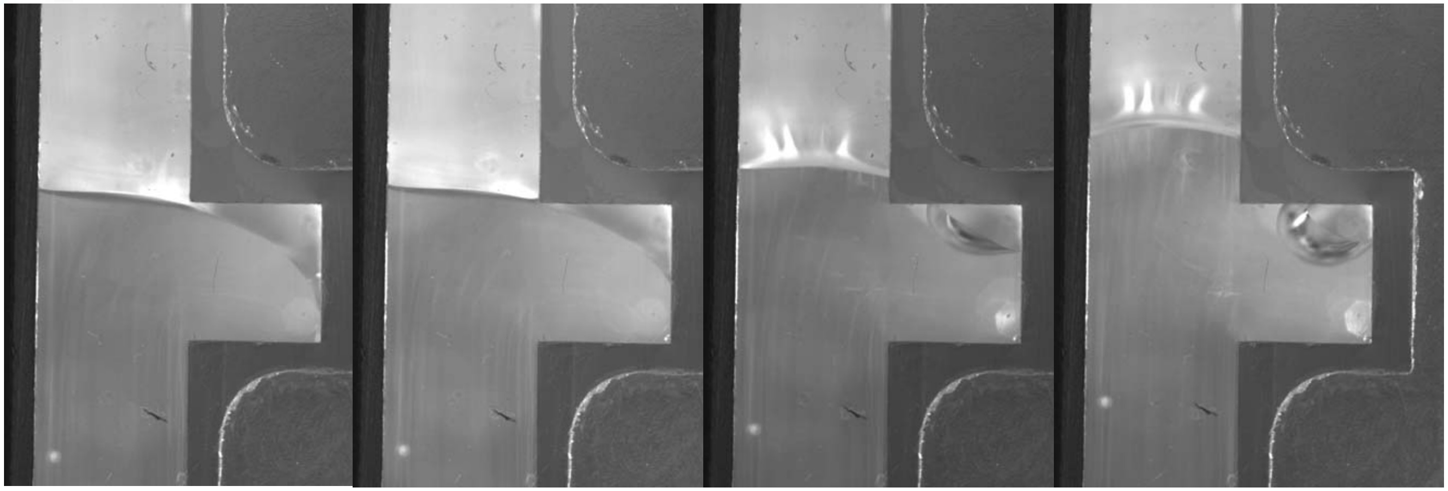


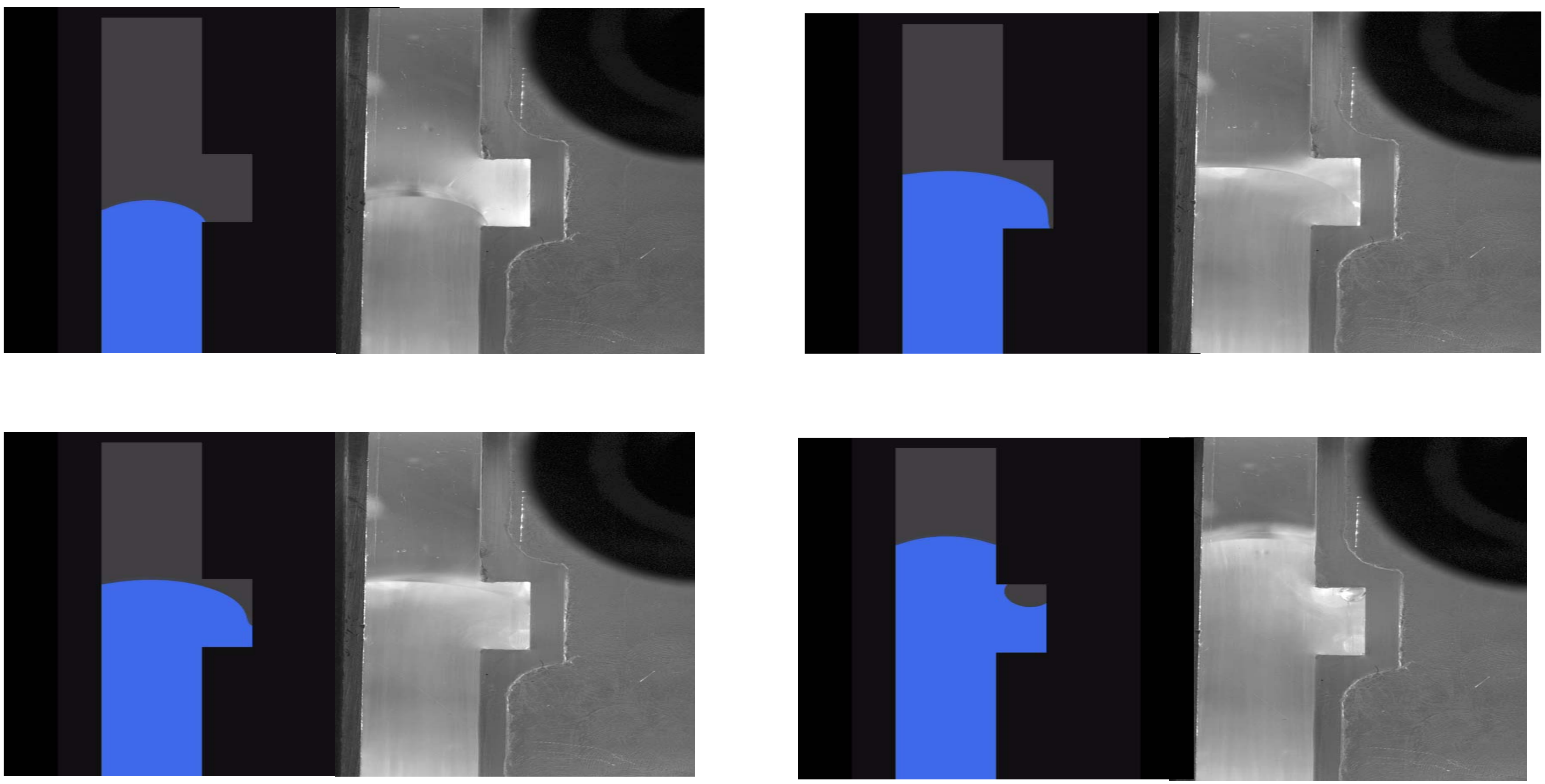




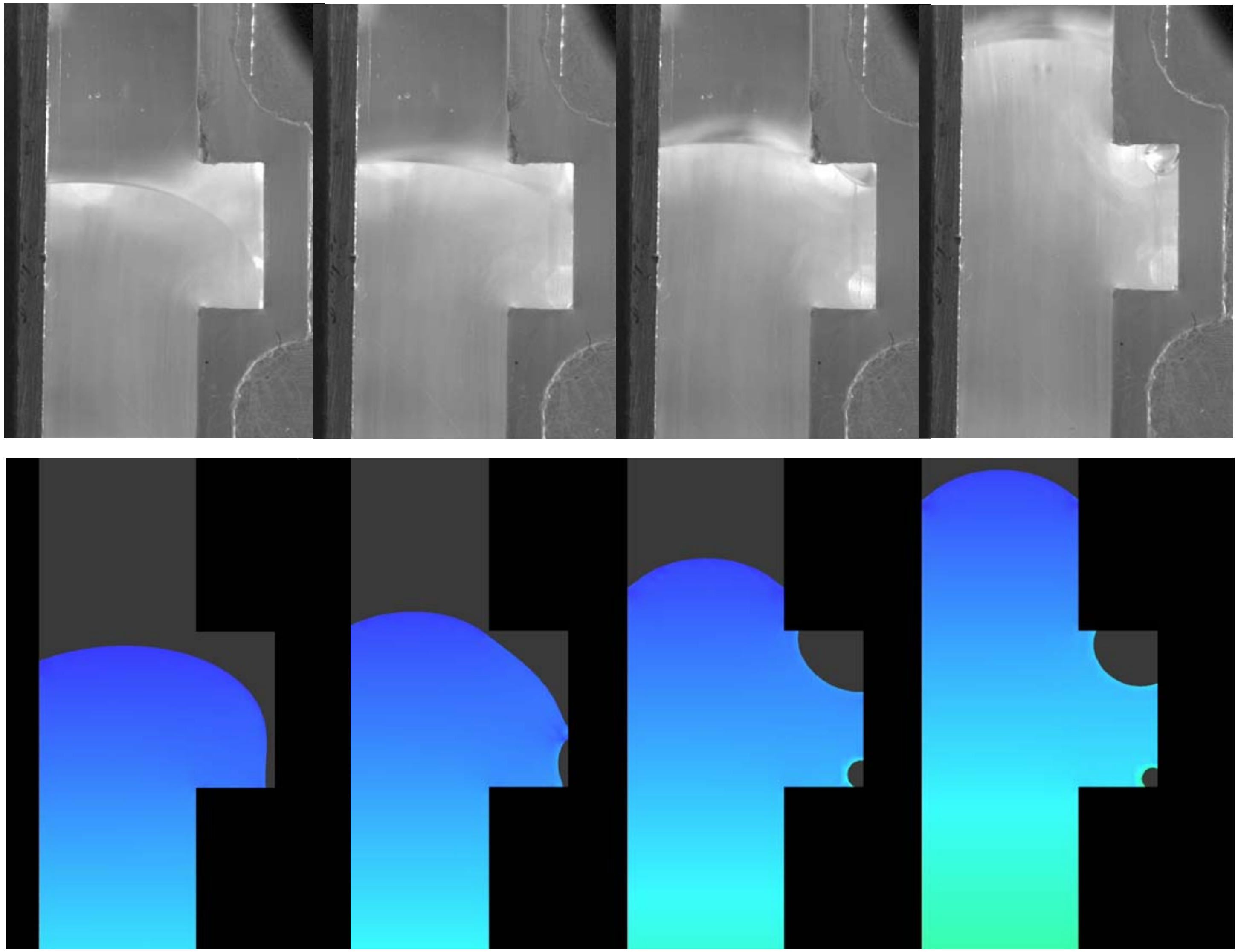








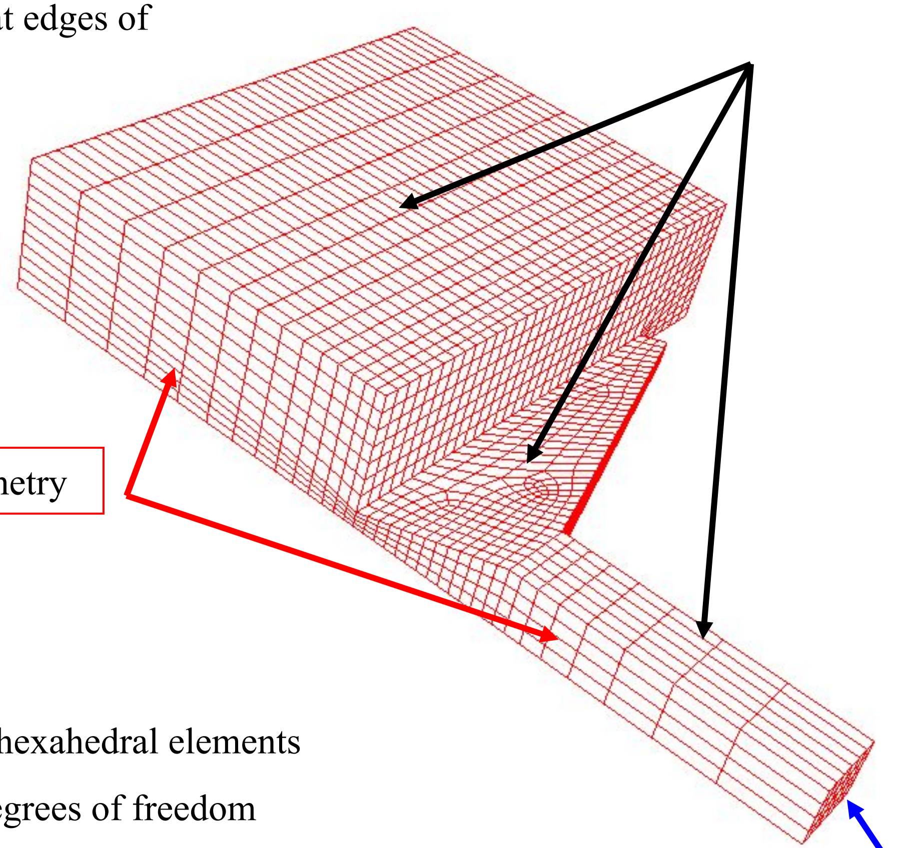
Increased wetting angle on notch side changes bubble locations



3D Computational Model of Injection Molding

Outflow occurs at edges of mold chamber

No penetration / no slip, except near contact region



Centerline Symmetry

Flow In

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

Parameters:

ρ_{liq} = 4.5 g/cm^3
ρ_{gas} = 0.0045 g/cm^3

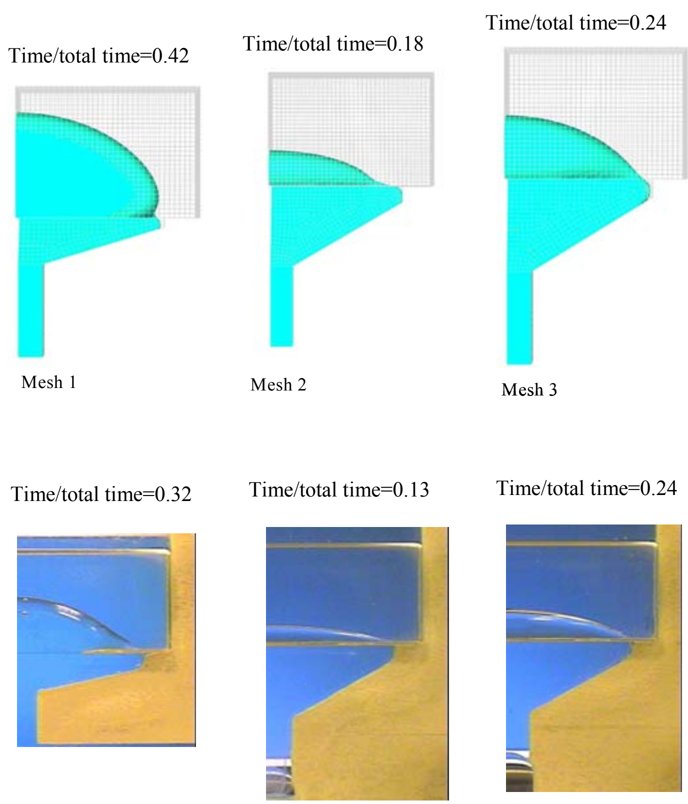
Newtonian

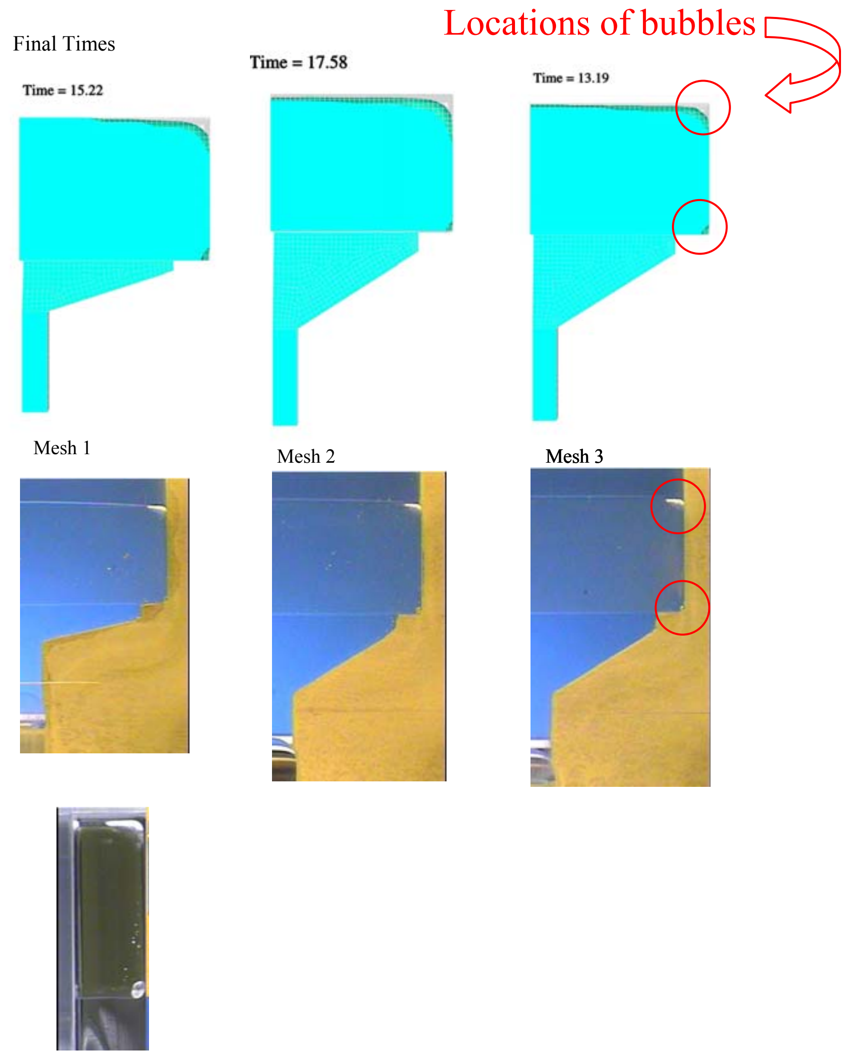
μ_{liq} = 1000 P
μ_{gas}= 12.5 P

σ = 1.0 dyne/cm

Comparison to Experiment

Vertical Alignment





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

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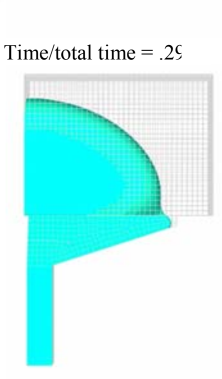
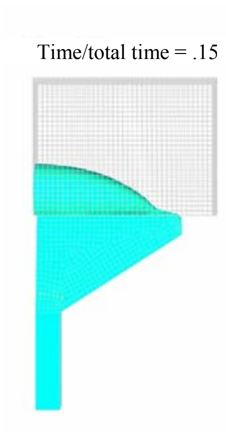
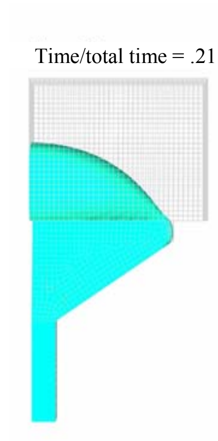
Comparison to Experiment

Horizontal Alignment







A

B

C

Time/total time=0.26

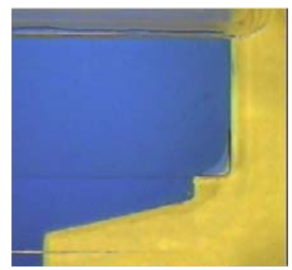
Time/total time=0.13

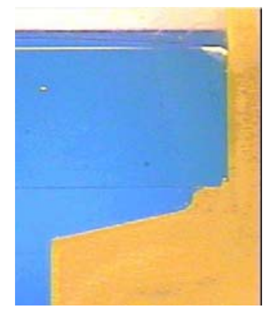
Time/total time=0.22

Horizontal

Vertical

Final times A





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

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Wetting Bottom Line

- Showed Sylgard wetting dependent on material
- Found mocks for case and high explosive
- Showed KC encapsulant wets basically all relevant materials in similar fashion

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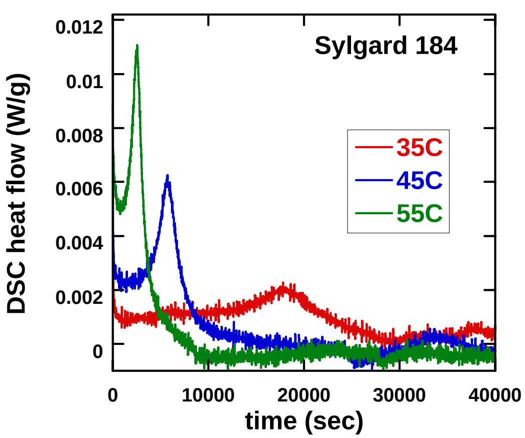
Fluid Material Models for Potting

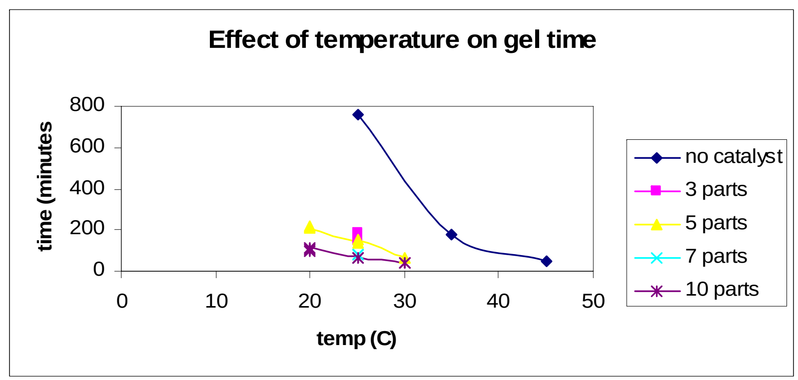
Need

- Viscosity (affected by cure time, temperature, shear, composition, etc)
- heat generated by reaction

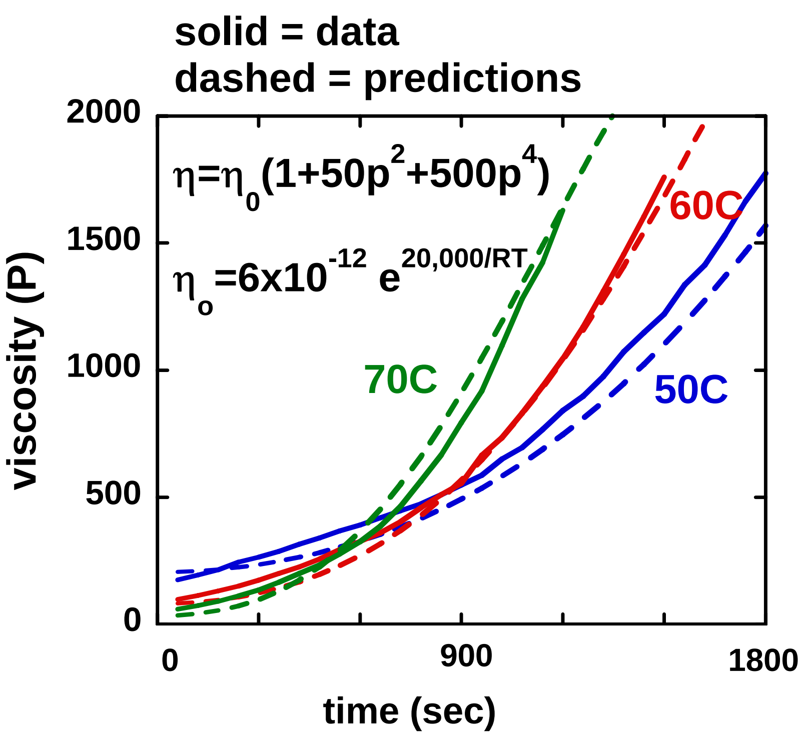
Tests:

1. DSC for reaction rate
2. Parallel plate steady shear for viscosity increase during cure
3. Oscillatory for gel time as function of composition and temperature

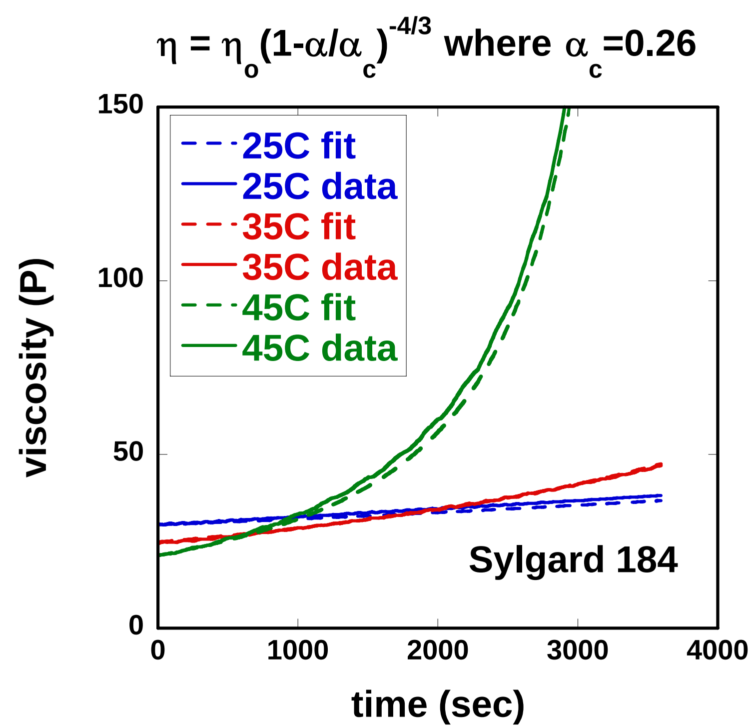




Yields estimate of viscosity coupled to time and temperature history



KC's RSF200 - very high viscosity and fast reaction



PX's Sylgard 184 with no additional catalyst

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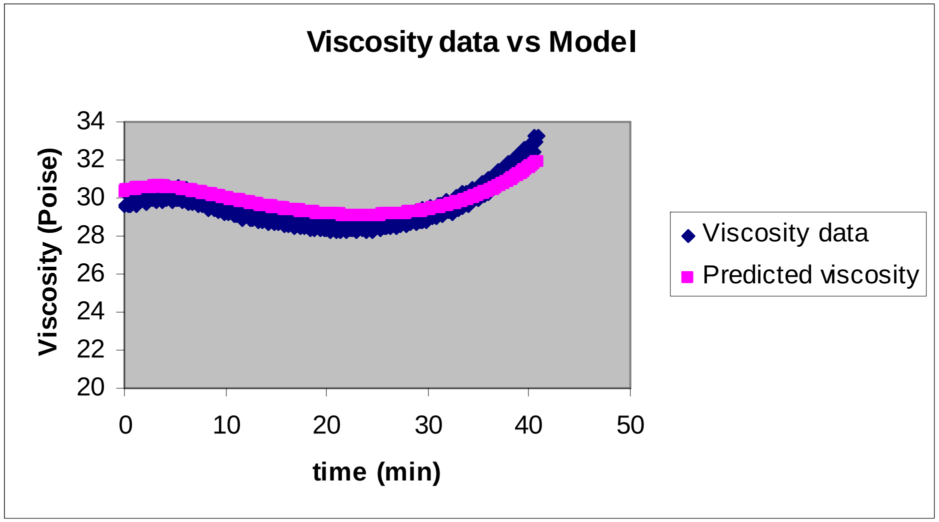
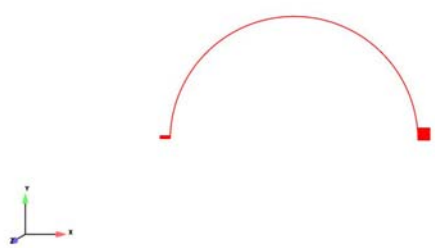
Test viscosity model in nonisothermal experiment for validation

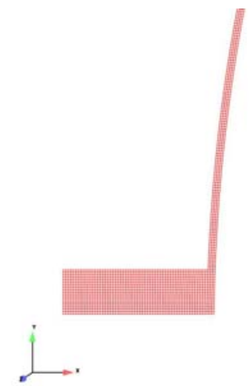


GOMA mold filling implementation

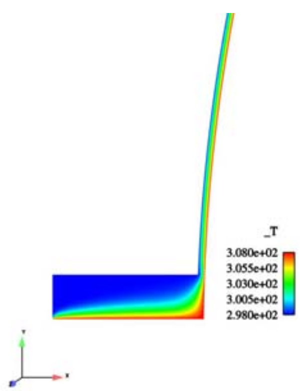
Axisymmetric FE mesh



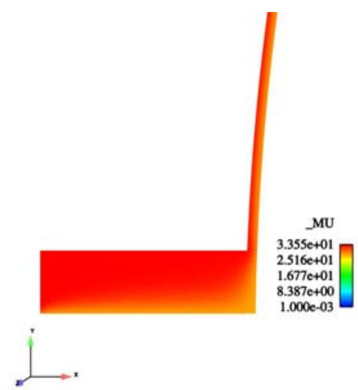
Mesh detail near inlet



Temperature after 5 min



Viscosity after 5 min



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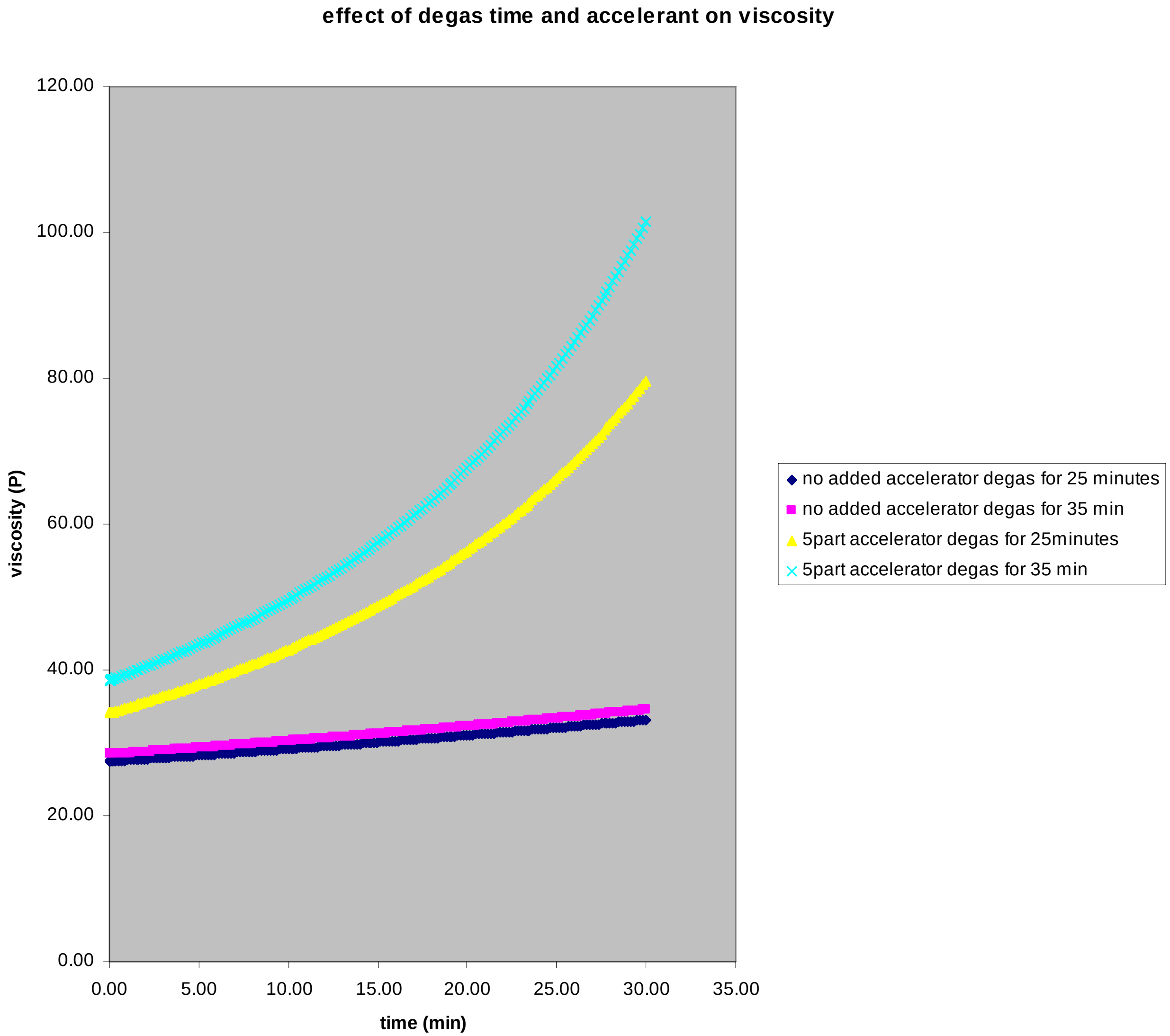
Viscosity in calculated with GOMA code in sphere problem



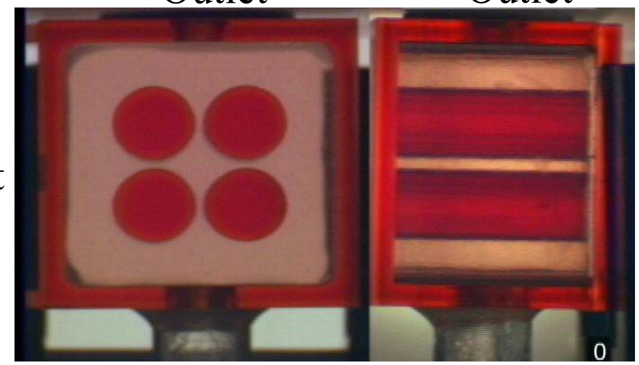
Kansas City models

Simple geometries that are representative of the pressure injection process

- Injection into a box and filling around obstacles
  - 1.7 cm X 1.7 cm X 1.3 cm
  - Posts 0.5 cm diameter

Outlet Outlet

Front view



Side view

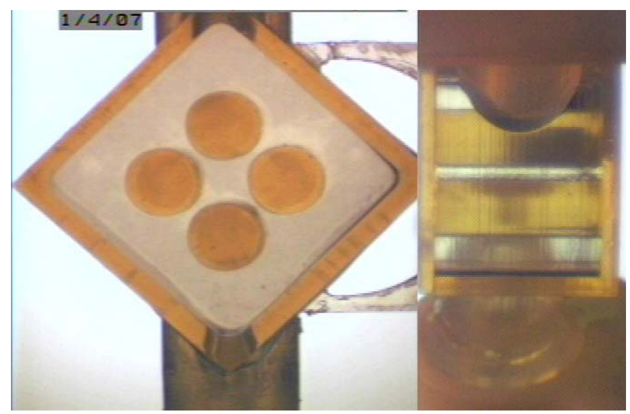
Inlet Inlet

- Injection site changed

- Previous tests for heat calculations with curing material

Outlet

Front view



45^{o} from top

Inlet

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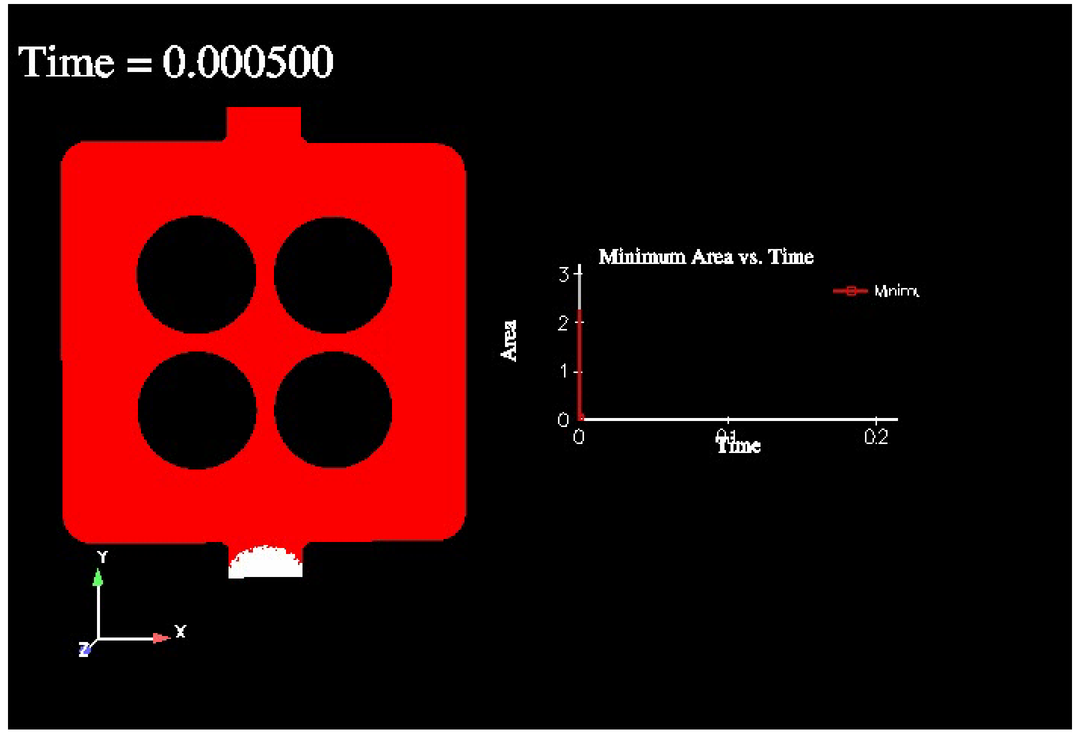
Earlier Sensitivity Study
Large flow rate in 4-post geometry never completely fills

- 2D approximation with approximations for surface tension, wetting, etc. (before measurements available)

- Fairly rapid injection rate assumed (very limited pot life)

- Factor of 10 change in flow rate
  - slight change in shape of interface
  - Maximum fill hovers around 90%

- Movie shows bubbles remaining after overfill by a factor of 5 times the box volume



Suggests that pressure filling will never be void-free

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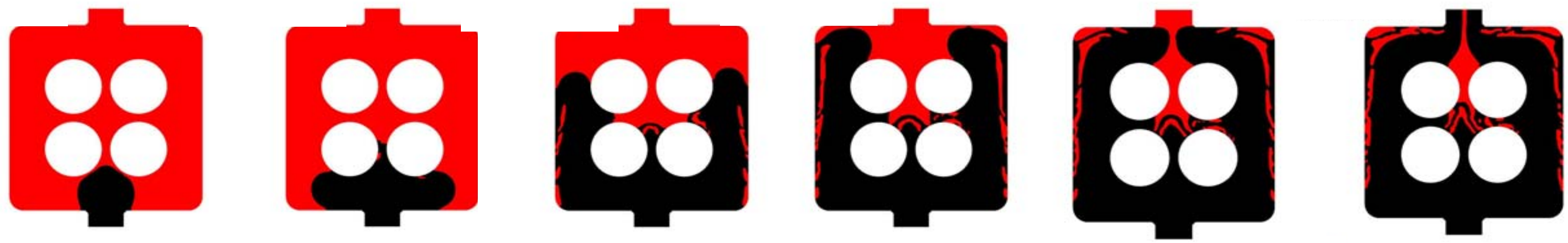
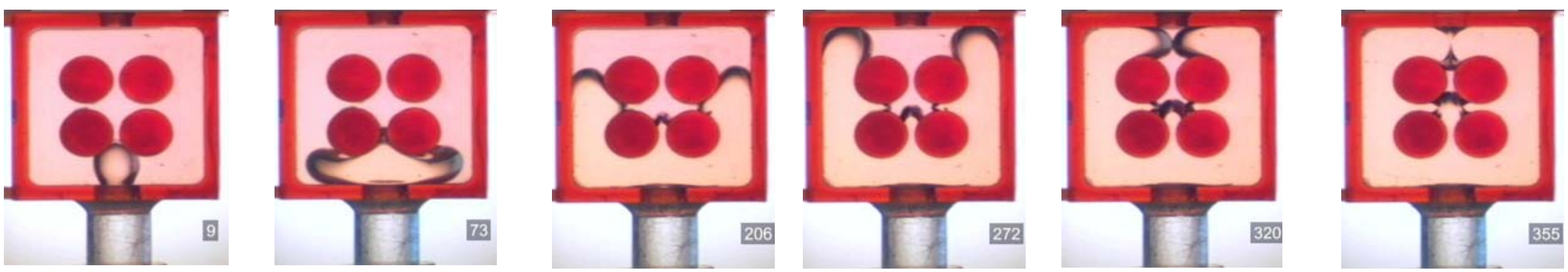
2D Model Matches Experiment Well Even with Approximate Parameters

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



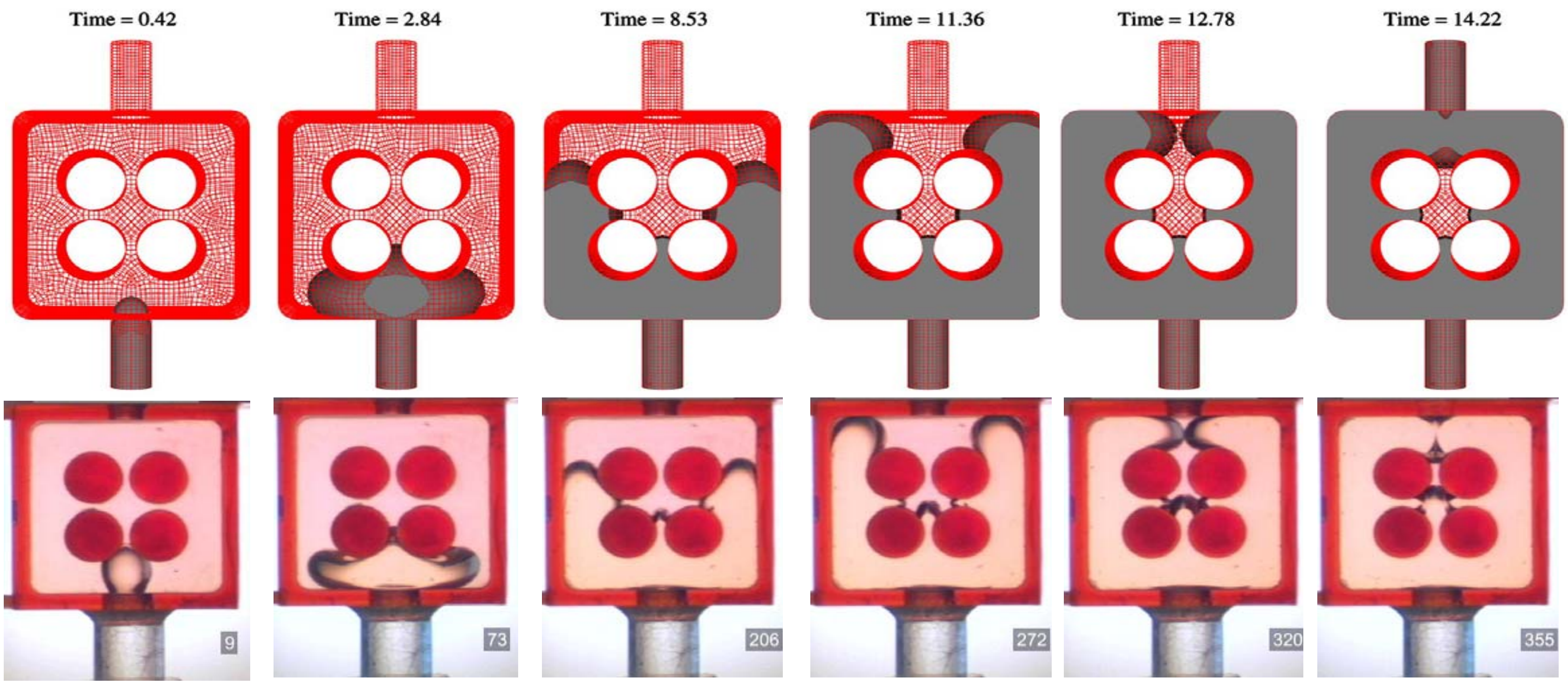
Real parameters: μ = 390 Poise, θ^{eq} = 37.8^o, v_o = 0.00193 cm/s, σ = 42.4 dyne/cm (Ucon 95-H-90000 measured parameters); fill time=12 s

Both: $Ca \cong 20$; $Re \cong 0.001$

Time*=time/total time

3D Model Matches Experiment Well with Faster Wetting Speed

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



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

Both: Ca $\cong$ 20; Re $\cong$ 0.001

Time*=time/total time

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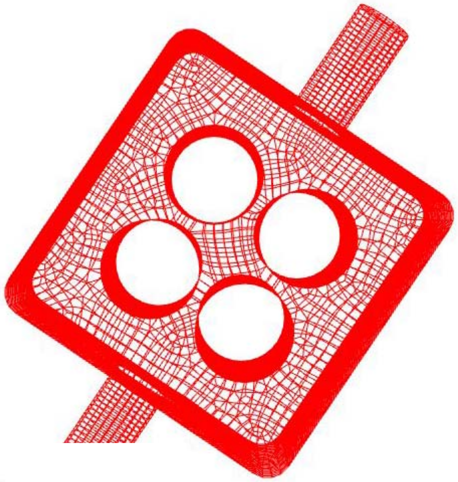
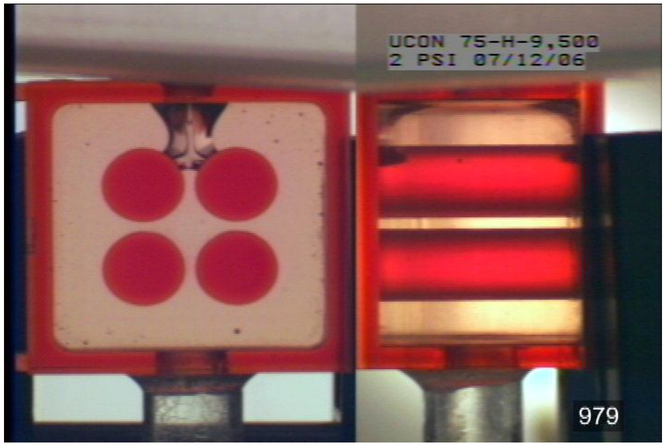
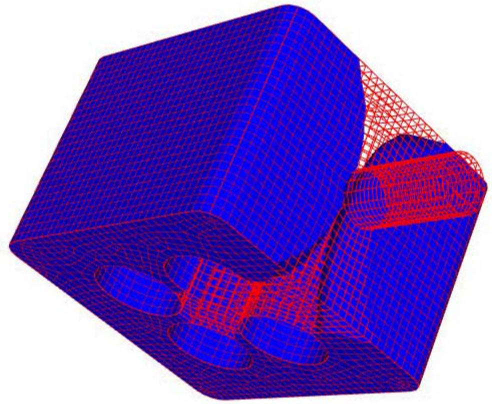
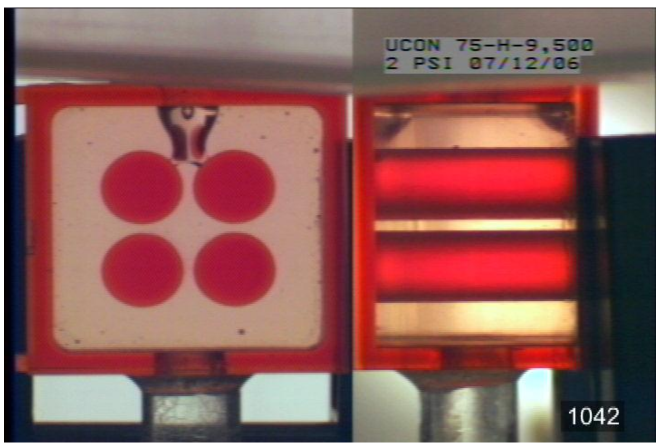
3D Effects

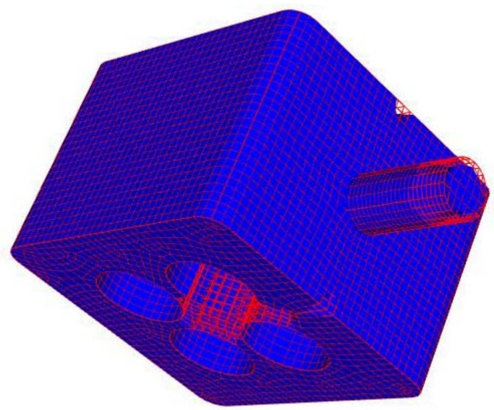
- Some air escapes as it continues to rise after flow stops
- Bubbles remain on back and front walls near outflow











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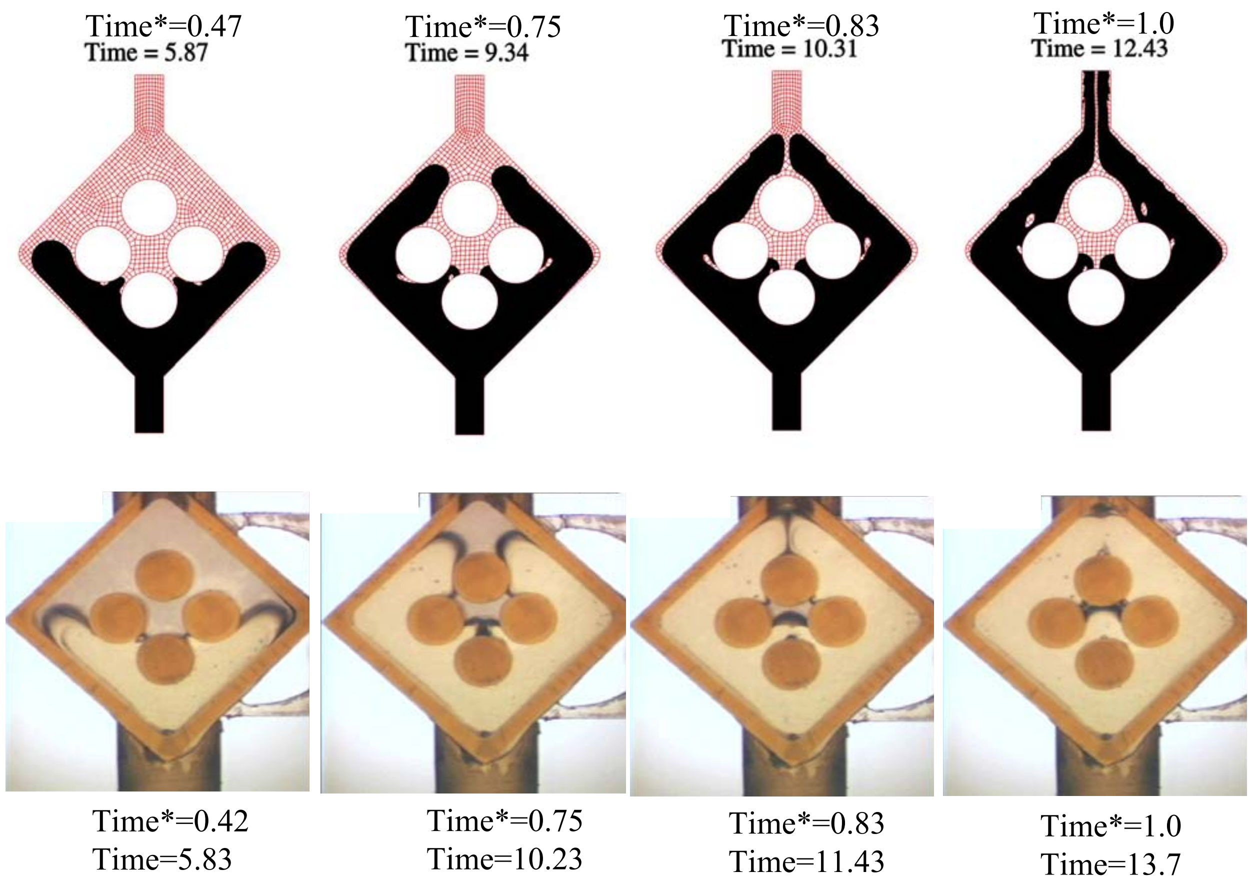
Change of Injection Point: 2D Model With Same Parameters as Experiment

2D model "conservative" in that it predicts larger volume of trapped air



Ucon 95-H-90000 – correct parameters in model

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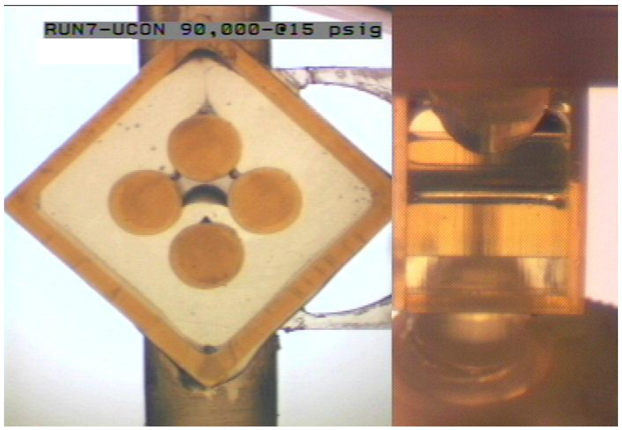
Change of Injection Point: Still Traps Air

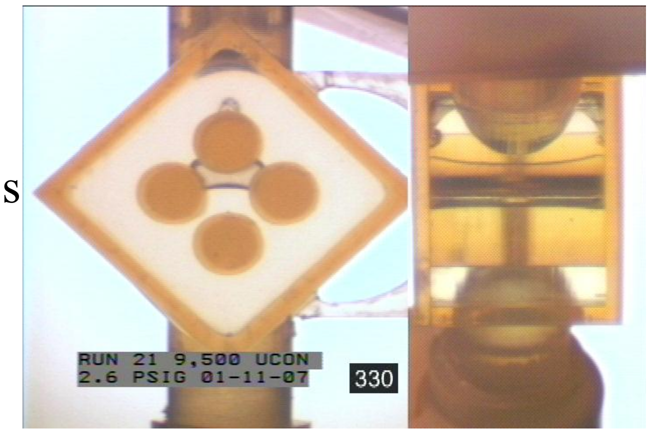
Not much change if fill rate is 12s or 25s

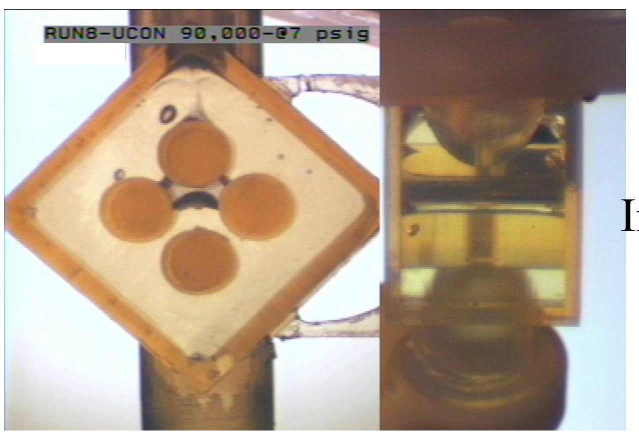
- Bubble across complete height of box

May help to inject slower with a less viscous liquid (here 1/10th viscosity)



Injection time ≅ 12s





Injection time ≅ 25s

(small bubbles are from injection process)

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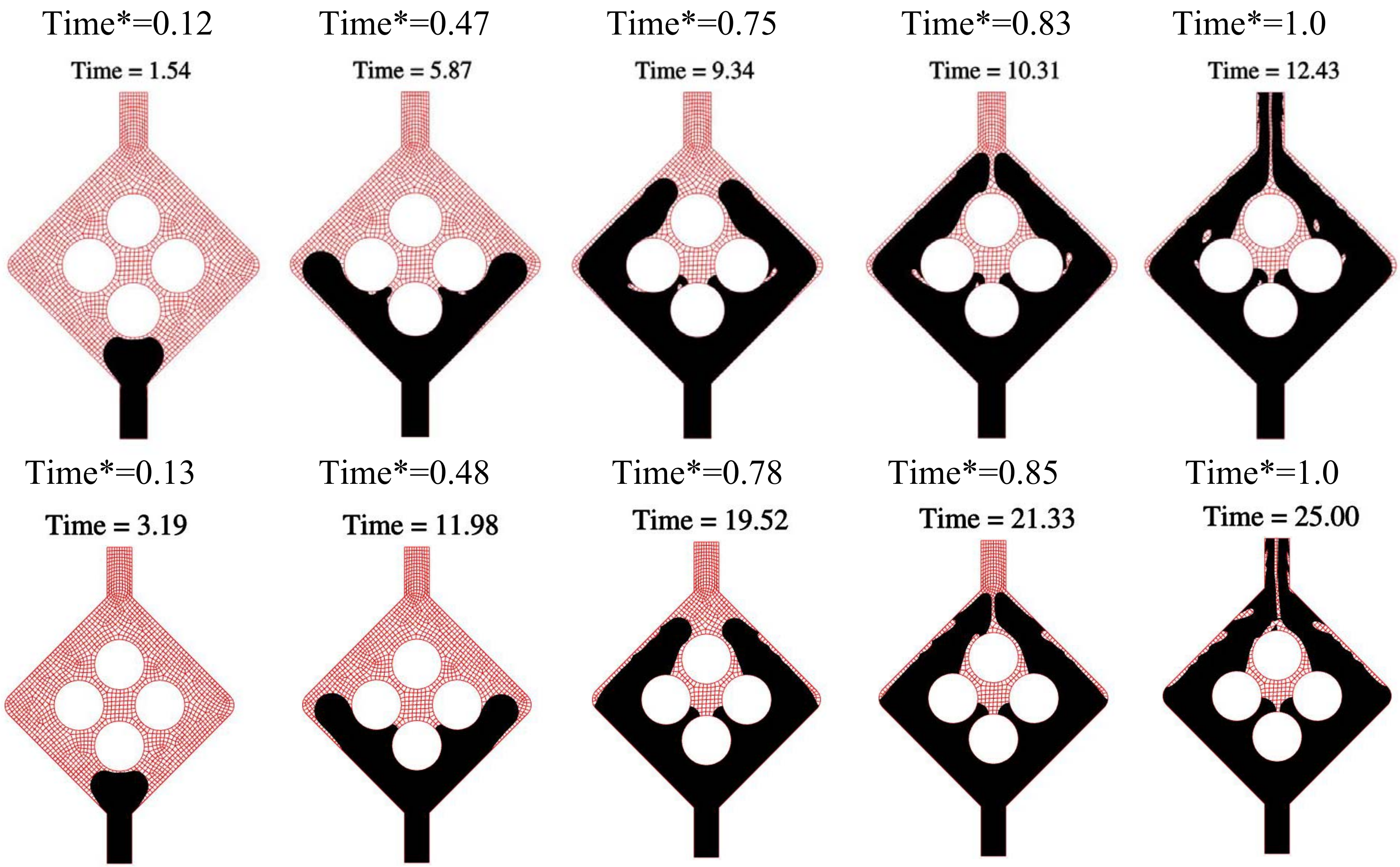
Model Correctly Predicts that Doubling Flow Rate Affects Results Little for High Viscosity



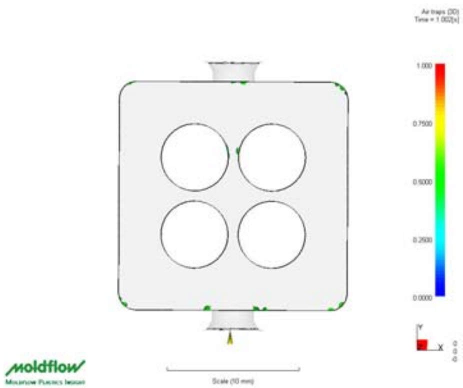
2D Corner Fill of KC Box at Two Different Flow Rates for UCON 90000

Simpler models still yield valuable information

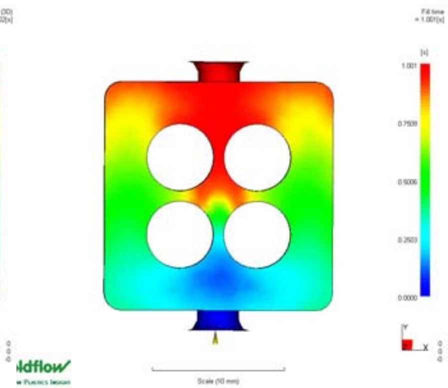
Box L filling evaluations – effect of fill time

1 sec fill ← | → **100 sec fill**

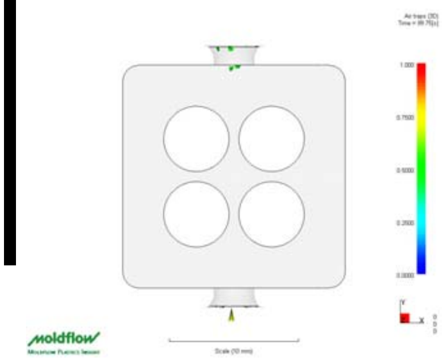
Voids/gas traps



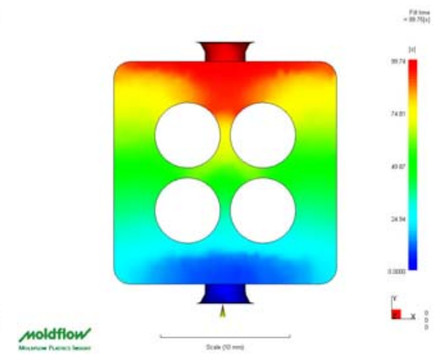
Time to fill



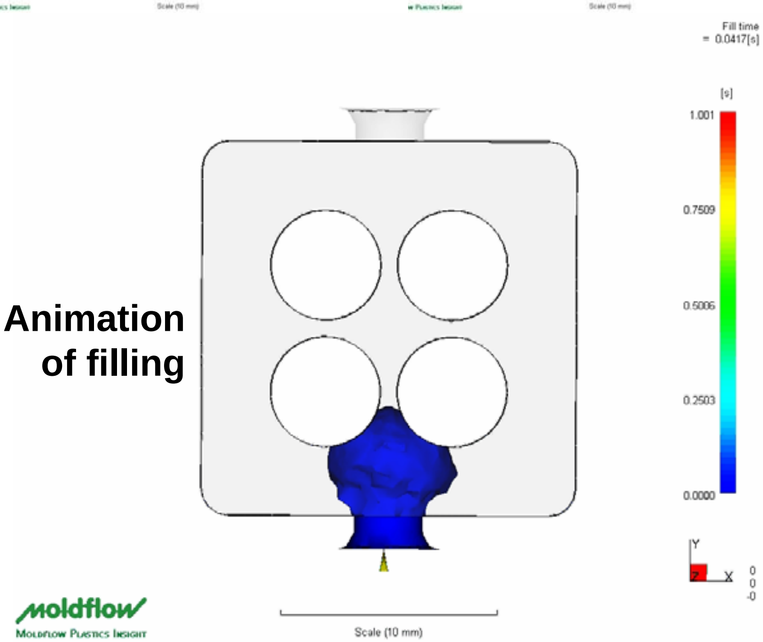
Voids/gas traps



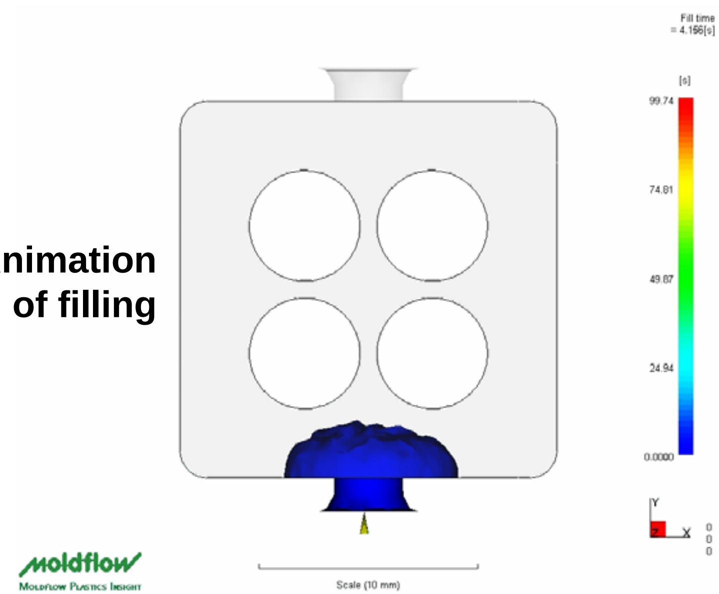
Time to fill



Animation of filling



Animation of filling



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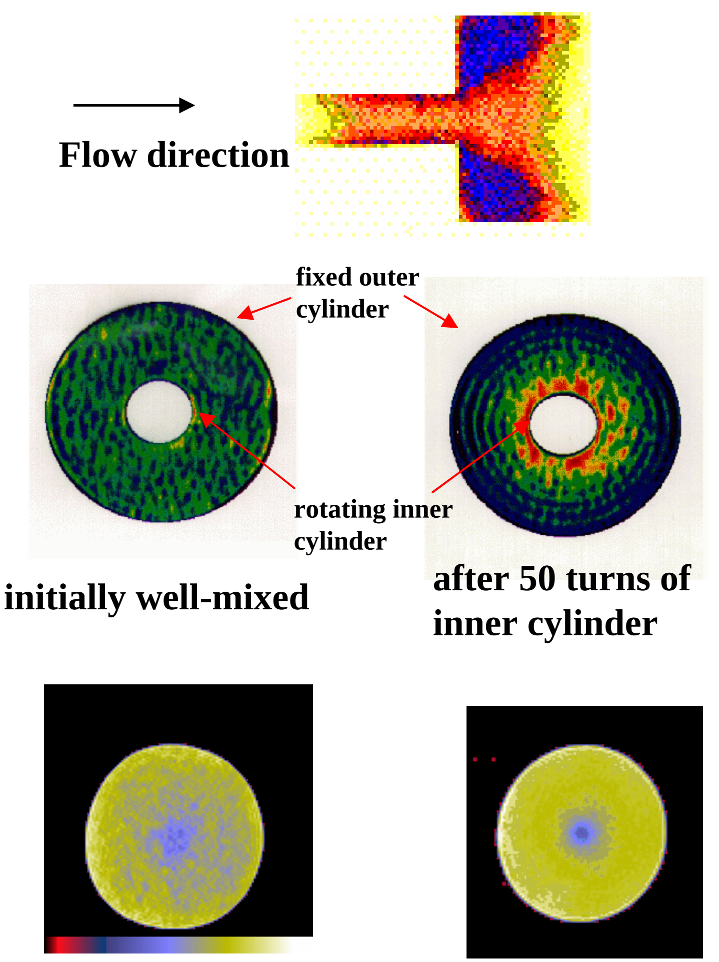
In Syntactic Foams Rheology Could be Complicated By Particle Migration

NMR IMAGING EXPERIMENTS



near inline mixer

steady state profile

During flow, migration of particles creates inhomogeneities that cannot be described by a constant Newtonian viscosity

Expansion Flow

Fluid rich region appears at corners of large pipe as particles are swept out (Mondy et al., 1995)

Concentric Couette

Particles move away from inner cylinder (Graham et al., 1991)

Pipe Flow

Particles migrate toward the center of the pipe (Hampton et al., 1997)

Particles migrate from regions of high shear-rate to low, from high concentration to low and from high relative viscosity to low (Leighton and Acrivos, 1987)

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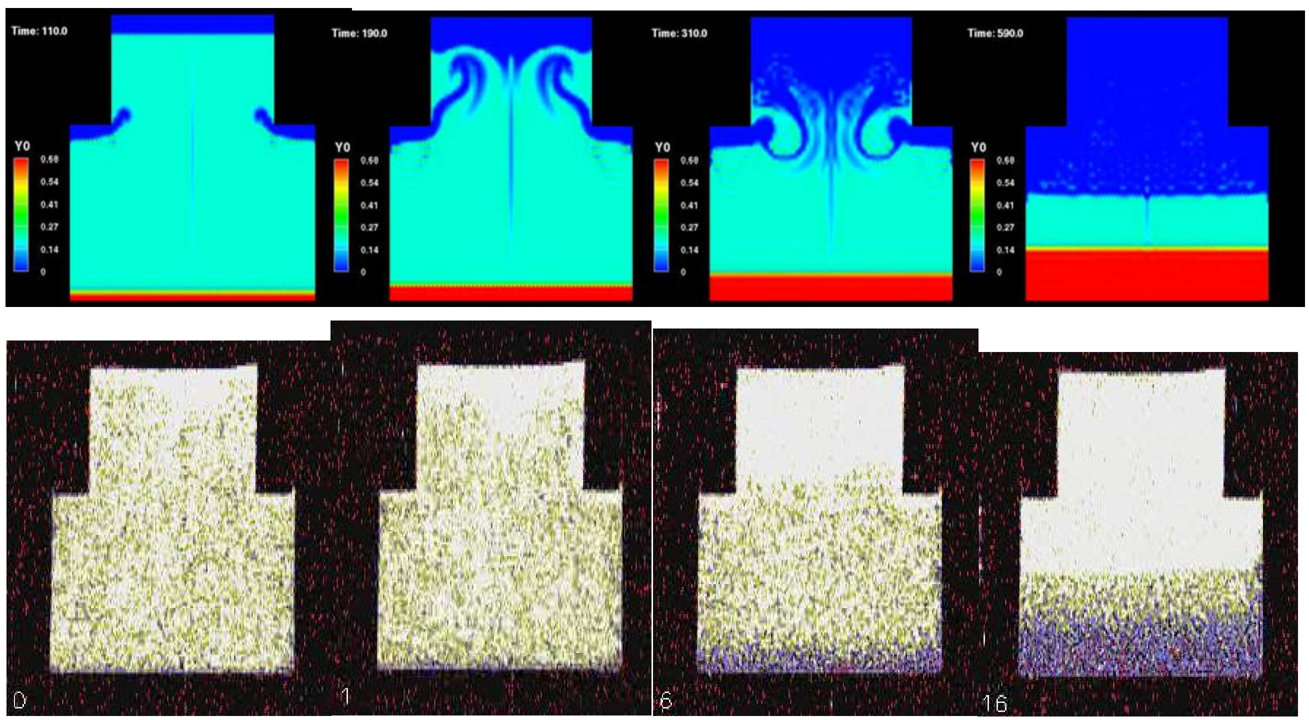
GOMA/ARIA Suspension Models Have Been Validated through ASC/C6 Programs

- Syntactic foams are epoxies filled with glass microballoons
- Under certain circumstances the particles can settle and migrate

Instabilities can form during quiescent settling

GOMA prediction

NMR imaging



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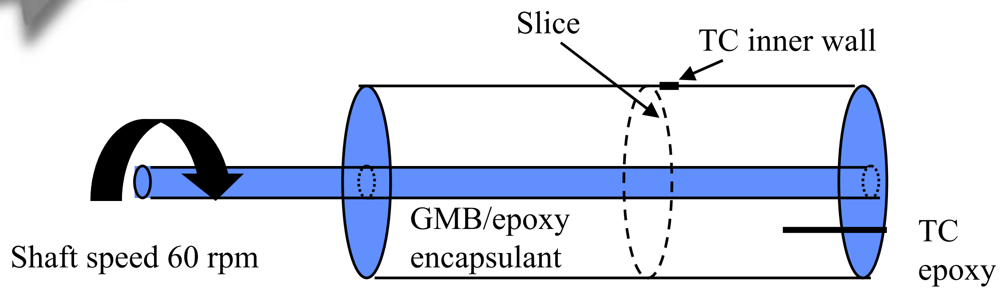
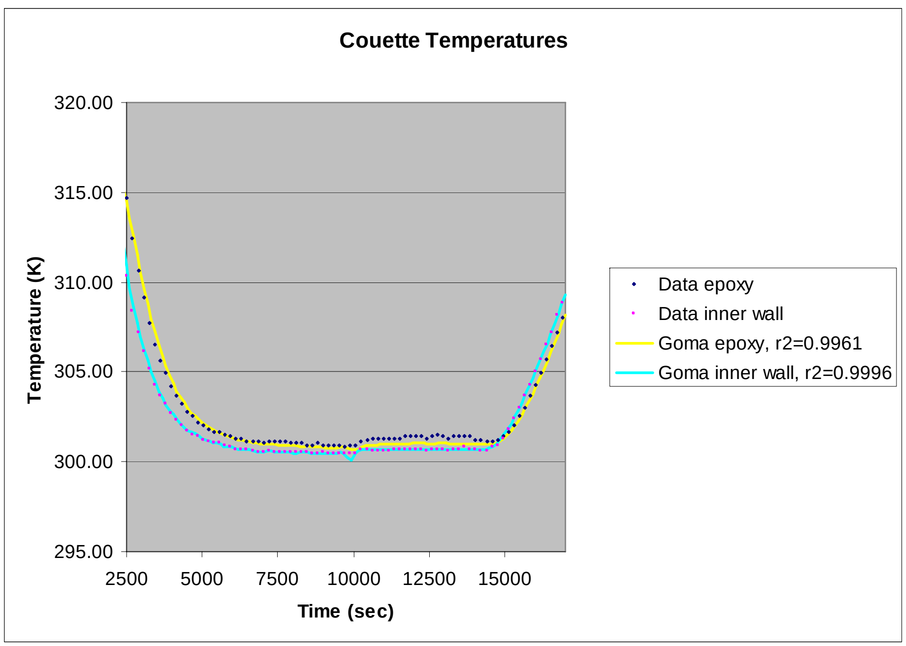
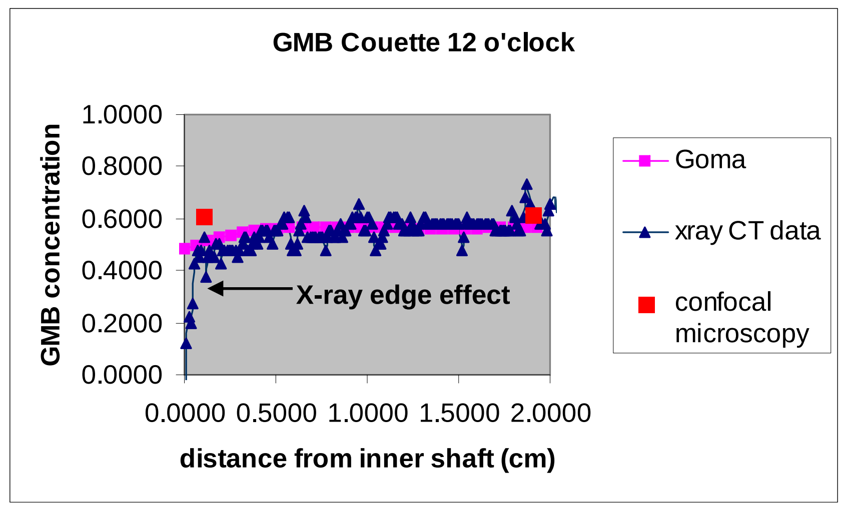
Particle migration in curing syntactic foam



Shaft turned until vitrification of epoxy

- **Experiment provides severe test of flow-induced particle migration/cure computational models**
- **Viscosity can change 3 orders of magnitude**
- ***Includes effects of heat of reaction and oven temperature***
- **Concentration prediction between two independent measurements**





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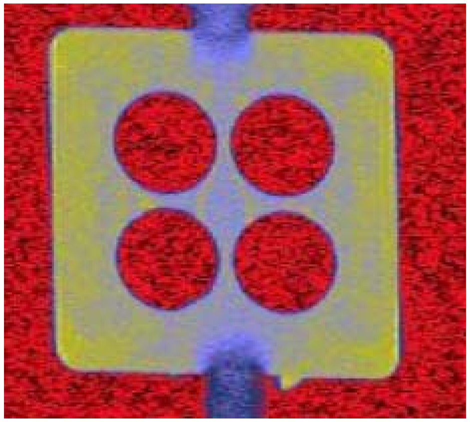
Flow Induced Particle Migration May Lead to Concentration Inhomogeneities

NMR images of box with four posts (two color scales)

- The NMR detects the liquid, so voids, the obstacles, and GMB particles reduce the signal in proportion to the liquid content.
- GMB suspended in unreacting liquid of roughly the expected epoxy viscosity
- Images were taken after flow has stopped.
- Slices taken in center away from bubbles remaining on the walls.
- Particle volume fraction varies from about 37 to 57 volume %.



- A liquid-rich region (yellow) appears around the outside of the posts.
- Particle-rich regions exist between the top and bottom posts outlined with liquid-rich streaks.
- A particle-rich region also appears at the injection entrance.

X-ray CT in more realistic geometry detected no concentration changes – resolution limitation or real?

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Lessons Learned: Syntactic Foam Encapsulants

- **Kansas City:**
  - 2D model captures salient features of 3D reality in simple box geometry
  - Geometry conducive to trapping air voids in pressure fill (vacuum fill suggested at Gate 2)
  - Improving wetting offers marginal improvement (Gate 2)
  - Changing injection point changed bubble but did not eliminate it
  - If *drastically* lower viscosity it might help (but these are filled systems and particles could segregate)
  - Particle concentration inhomogeneities might exist – if of interest we have validated suspension rheology models

Lessons Learned

- **Pantex:**
  - Sensitivity study in simple geometry shows flow rate, and wetting angles most important if must flow over indentations
  - Viscosity (Ca number) and dynamic wetting model also influences response
  - Preliminary modeling with more realistic parameters shows material heats quickly to pin temperature from room temperature
  - Flow in gap model will be used to assess effects of cure rate changing with % accelerator
- **Kansas City:**
  - 2D model captures salient features of 3D reality in simple box geometry
  - Geometry conducive to trapping air voids in pressure fill (vacuum fill suggested at Gate 2)
  - Improving wetting offers marginal improvement (Gate 2)
  - If *drastically* lower viscosity it might help (but these are filled systems and particles could segregate)
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