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Mold Filling Simulations Using The Level Set Method

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Goal: To Use Numerical Modeling To Help Optimize Mold Filling Process

Finite element models of mold filling

- –Complex free surface flow
- –Wetting line motion
- –3D geometry

Use experimental validation to increase confidence in numerical models to allow for design simulations

Modeling can be used to choose the best gate and vent location and to minimize void formation

Numerical Solution Methods for Interfacial Motion

Tracking motion of interface between two distinct phases appears often:

- Phase changes
- Film growth
- Fluid filling

Interface tracking:

- Explicit parameterization of location
- Interface physics more accurate
- Moving mesh
- Limits to interface deformation
- No topological changes

Examples:

Spine methods (*Scriven*)

ALE

Embedded Interface Capturing:

- Interface reconstructed from higher dimensional function
- Fixed mesh
- “Diffuse” interface physics
- Interface deformation theoretically unconstrained

Examples:

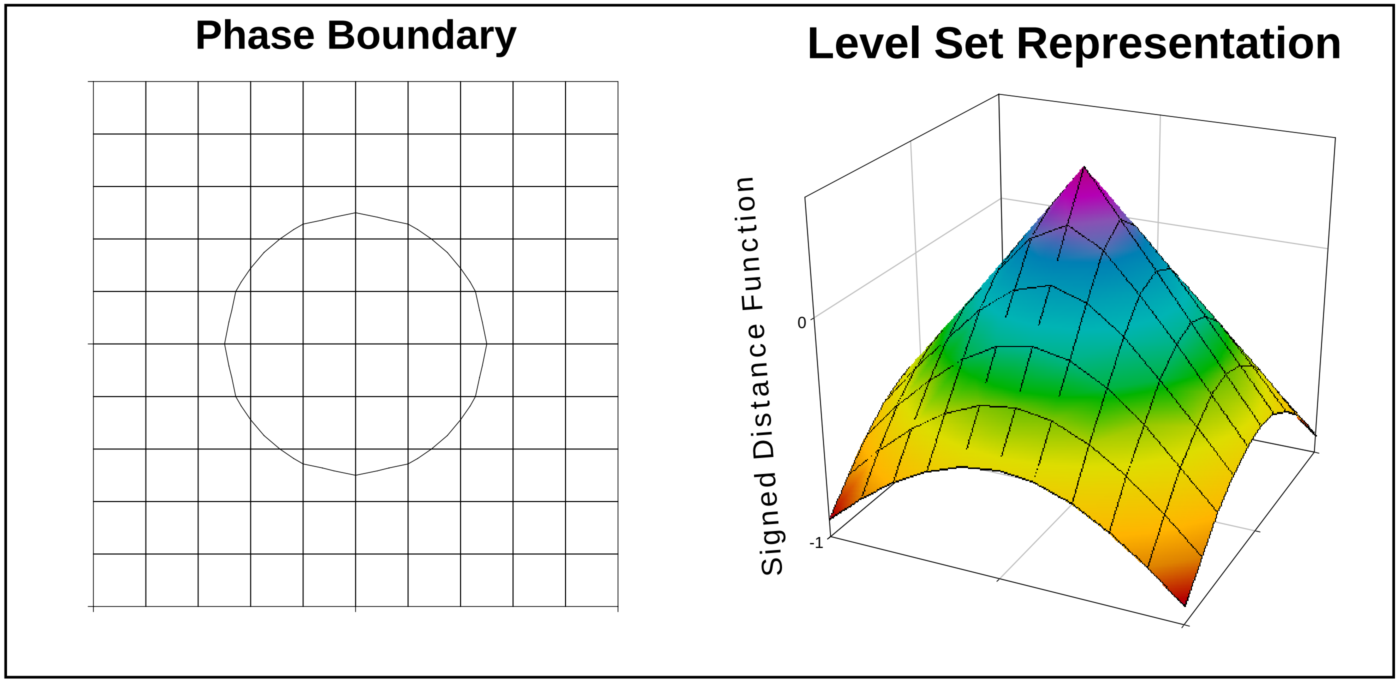
Volume-of-Fluid (*Hirt*)

Level Sets (*Sethian*)

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



Evolving ϕ for Fluid Filling

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

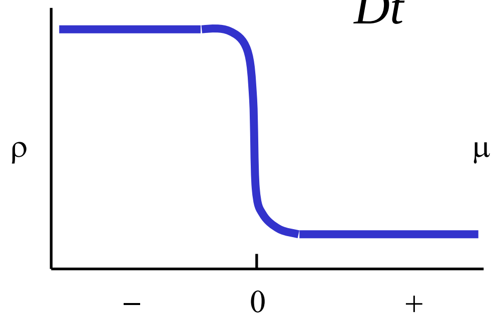
$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0$$

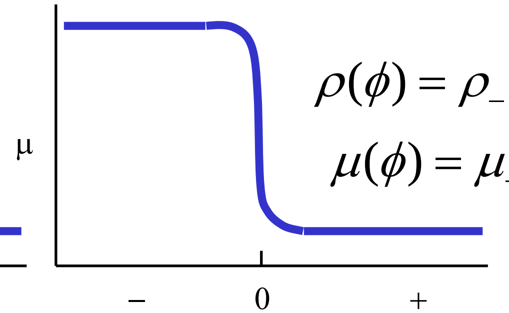
Purely hyperbolic equation … fluid particles on ϕ(x,y,z) = 0 should stay on this contour indefinitely

- Does not preserve ϕ(x,y,z) as a distance function
- Introduces renormalization step.

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

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





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

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

Surface Tension Level Sets

Distributed Surface Tension Terms:

1) Addition of following to fluid stress tensor (Jacqmin 1995)

$$\underline{T_\sigma} = \sigma\delta_\alpha(F)\left(\underline{I} - \vec{n}\vec{n}\right)$$

$$\delta_\alpha(F) = \left(1 + \cos\left(\frac{\pi F}{\alpha}\right)\right) / 2\alpha$$

$$\vec{n} = \nabla\phi, \kappa = \nabla \cdot \nabla\phi$$

2) Projection of normal based on grad phi circumvents integration by parts for this term and improves mass conservation

Blake Wetting Line Model

- Molecular Kinetic Model

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

Adhesion to Substrate

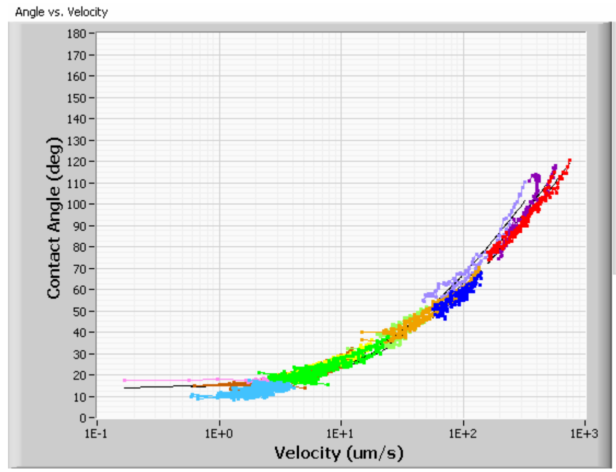
$$U = \frac{2kT\lambda}{\eta v_L} \exp\left[\frac{-\gamma_{LV}(1+\cos\theta_\infty)}{nkT}\right] \sinh\left[\frac{\gamma_{LV}(\cos\theta_\infty - \cos\theta)}{2nkT}\right]$$

Viscosity

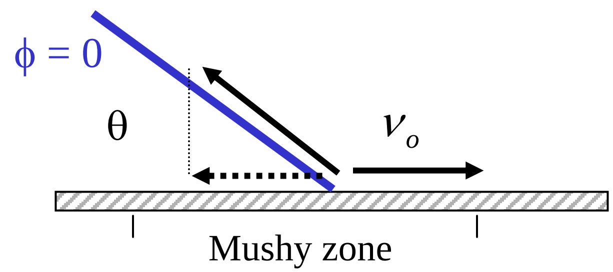
Molecular-Kinetic

Lump terms

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

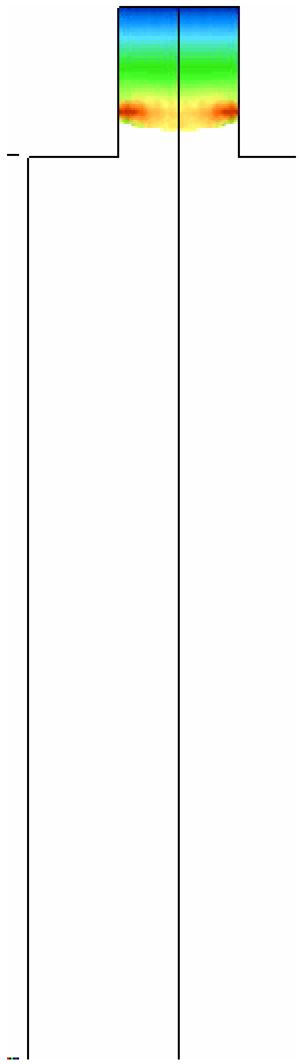


Goniometer wetting data

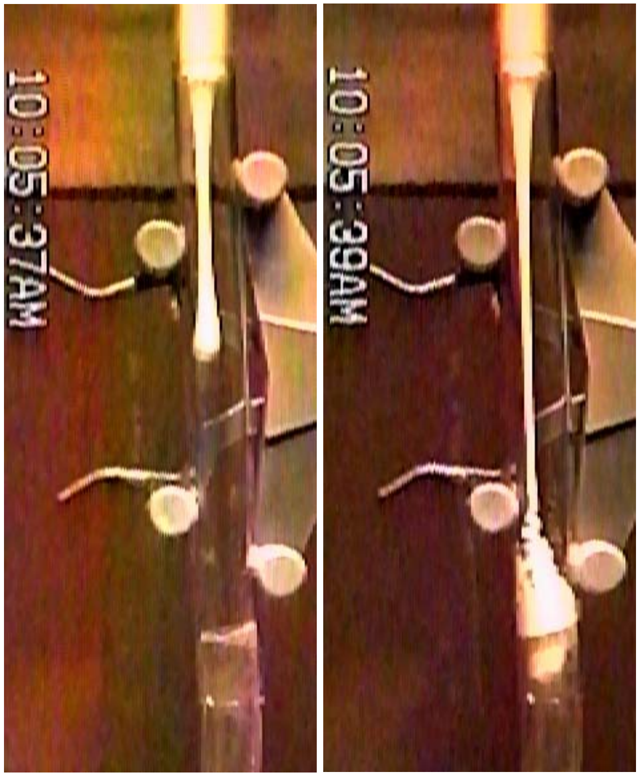


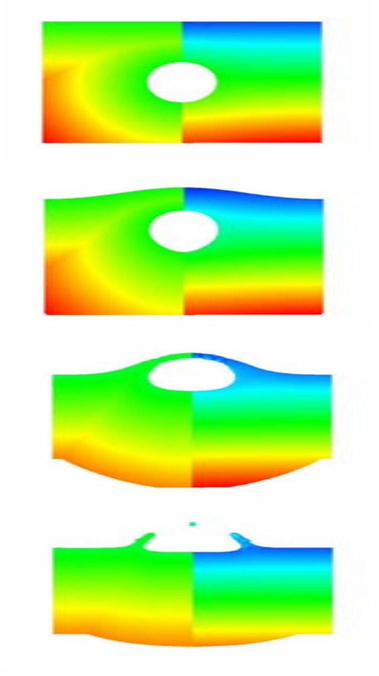
Three unknowns $\begin{cases} v_o \\ \cos\theta_\infty \\ \gamma \end{cases}$ which can be functions of the can be fit to goniometer wetting experiments

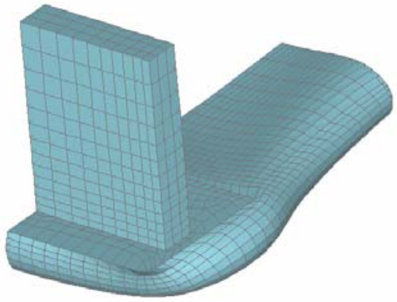
Embedded Interface Methods Can Capture Topological Changes

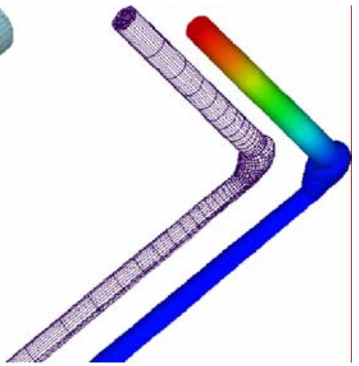


•Level set method has possibility of modeling "Dairy Queen" effect





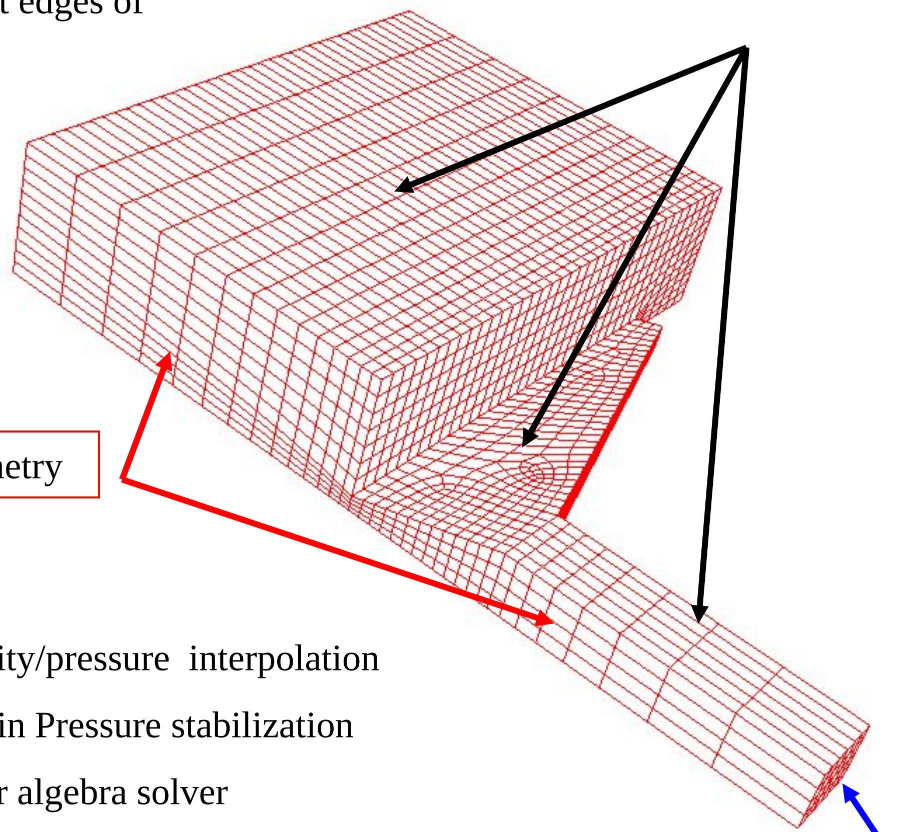




3D Computational Model

No penetration / no slip, except near contact region

Outflow occurs at edges of mold chamber



Centerline Symmetry

Flow In

Parameters:

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

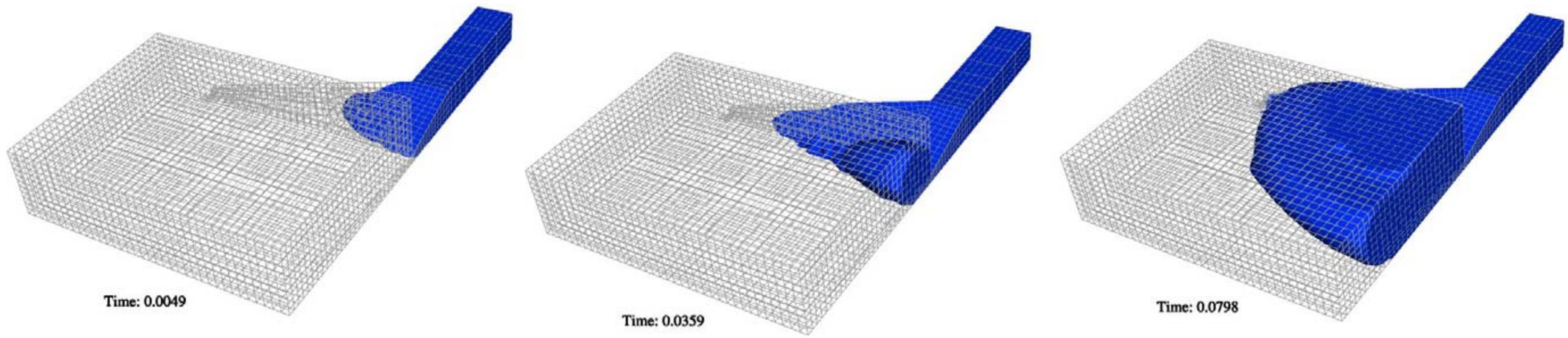
Newtonian

μ_{liq} = 1000 P
μ_{gas}= 12.5 P

σ = 10.0 dyne/cm

- Bilinear velocity/pressure interpolation
- Petrov-Galerkin Pressure stabilization
- GMRES linear algebra solver
- ILUT preconditioning
- 6744 8-Node hexahedral elements
- 41300 total degrees of freedom

3D Newtonian Model Gives Insights into Distributor Design



•To minimize mass loss, small amounts of pressure stabilization are used. Matrix is poorly conditioned, requiring GMRES with ILUT fill factors of 3

•Simulation ran for several months on four processors of a Linux HP workstation

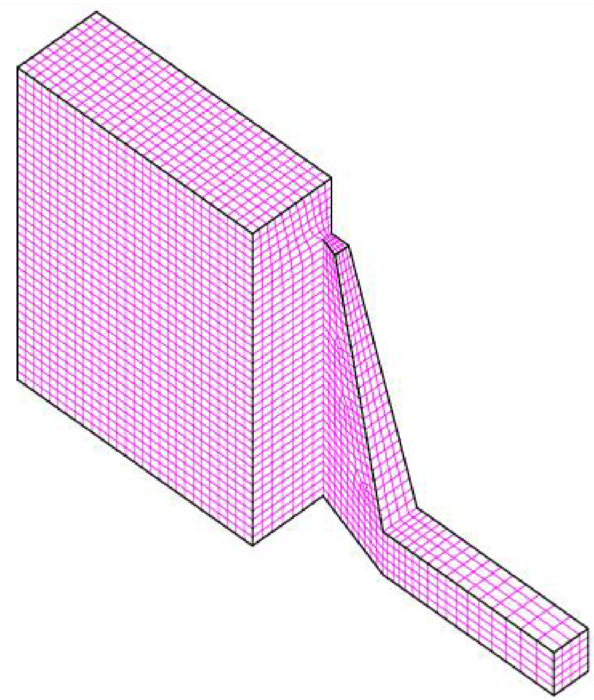
•Fluid enters main cavity before completely filling the distributor

•Fluid pools in center of the cavity

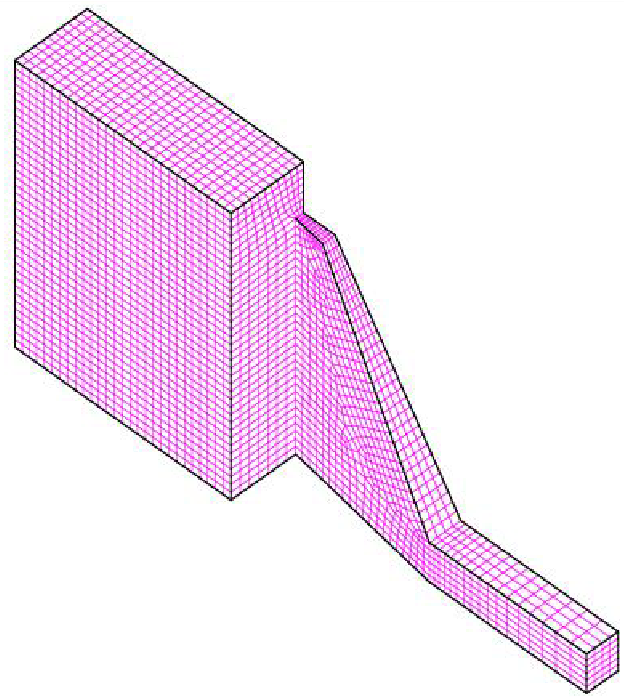
•Redesign of distributor may help flow be more uniform

Short shot at 140°C, 100% speed, 50% pressure, 75% fill

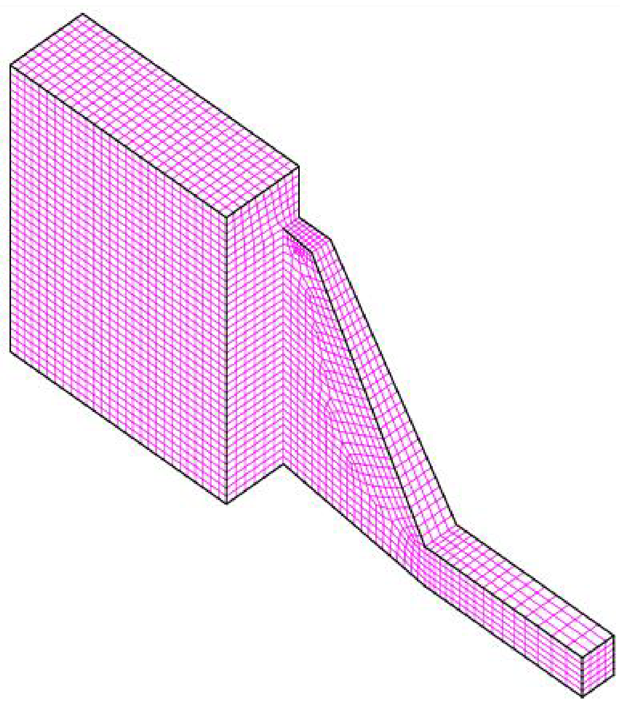
Geometry Evolution: Redesign of the Distributor



Original Geometry



Longer Distributor



Longer-Taller Distributor

Developments Regarding Element Selection for Level Set Simulations

Problems

- Q1Q1 – Unstable, requires large amounts of PSPG ⇒ mass loss
- Q2Q1 – Stable, prohibitively expensive for large 2-D, all 3-D problems, ill-behaved with iterative solvers
- Q1P0 – Unstable, requires edge based stabilization ⇒ cumbersome, possibly difficult to tune to avoid mass loss

Developments

- Confirmed Q1Q1 issues in Aria simulations of 3-D mold filling
  - Level of PSPG required for good convergence with Q1Q1 can produce 100% mass loss
- Q1P0 much more ill-behaved than previously thought, especially in Aria with adaptivity

Promising Directions

- Appears that relatively minor preconditioner work may alleviate problems with iterative solvers for Q2Q1 – ILUT with pivoting or Dohrmann's work
- Dohrmann and Bochev stabilization for Q1Q1 or Q1P0
  - Simple, "parameter-less," divergence-less non-residual based stabilization technique
- Consistent PSPG implementation
  - loosely coupled projection of diffusion terms for more accurate PSPG
  - Should dramatically lower magnitude of momentum residual while maintaining level of stabilization

Dohrmann and Bochev Stabilization

References

- Dohrmann, and Bochev, *IJNMF*, vol. 46, pp. 183-201, 2004.
- Bochev, Dohrmann, and Gunzberger, *SIAM J. Numer. Anal.,* vol. 44, pp. 82-101, 2006.

Description

- Penalize deviation from polynomial projection
  - Form for Q1Q1: $$\int_{\Omega_e} (p - \pi p)(N_i - \pi N_i)\, d\Omega \qquad \pi p = \int_{\Omega_e} p\, d\Omega \Big/ \int_{\Omega_e} d\Omega$$
- Resulting Matrix: $$\begin{bmatrix} A & B^T \\ B & -G \end{bmatrix}$$

Questions

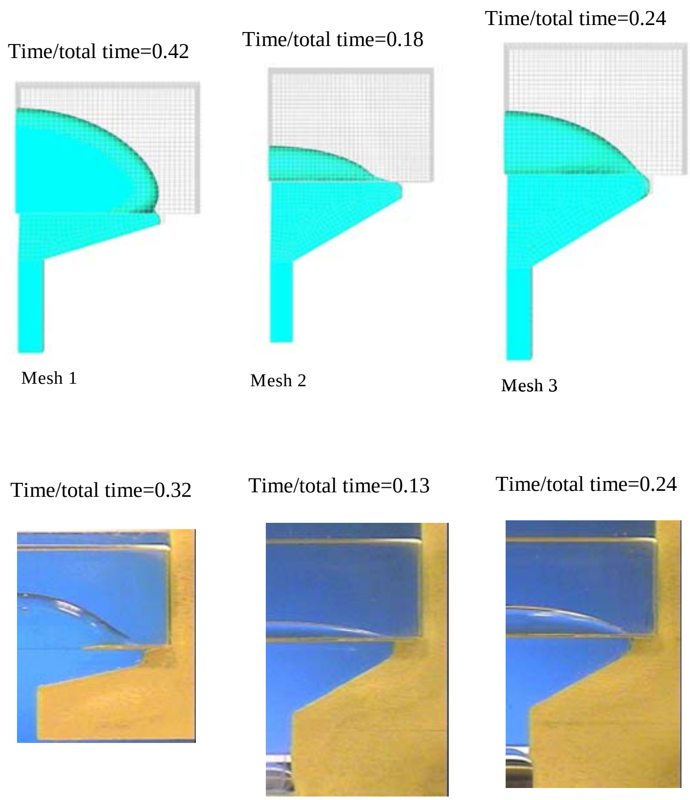
- Can a diagonal-only term stabilize without mass-loss?
- How will it behave for level set problems?
  - Unlike most single-phase problems has significant Laplacian of pressure
- Derived for Stokes equations, will it work for nonzero Reynold's number?

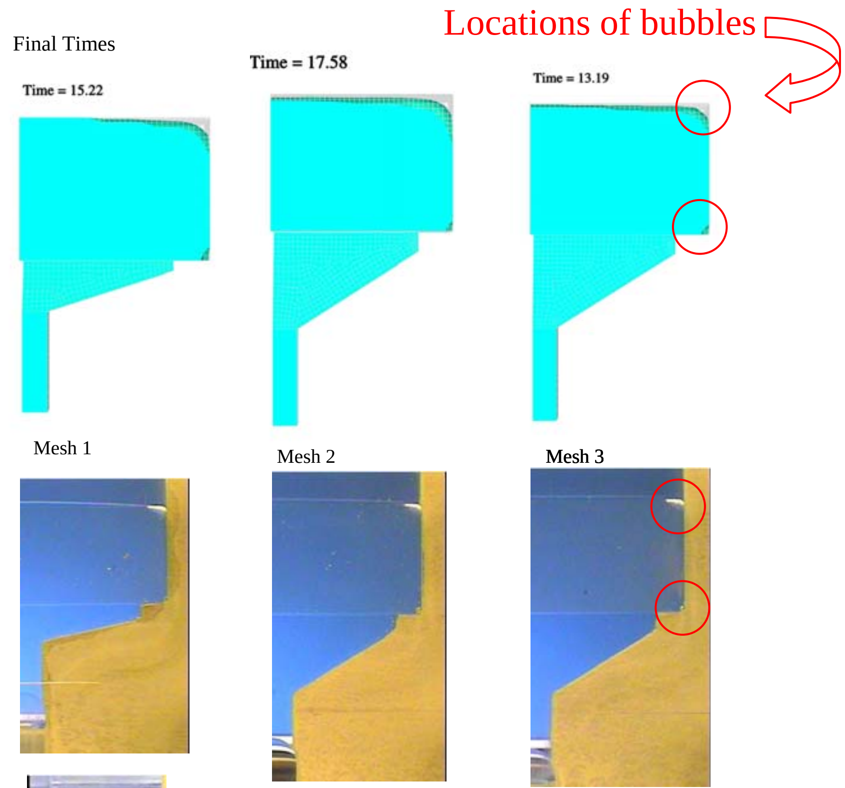
Answers

- Yes, mass loss is small and improved by introducing a coefficient
- Run times for simulations reduced by nearly a factor of 100 from PSPG/GMRES/ILUT to PSPP/BiCGStab/ILU

Comparison to Experiment

Vertical Alignment



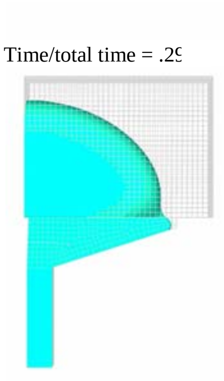


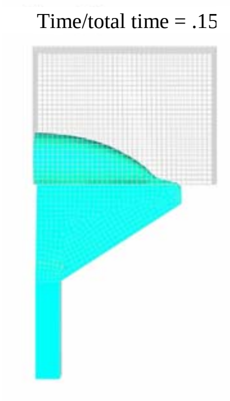
- Qualitative aspects captured – improvements in distributor and number and location of bubbles
- Increasing wetting speed from that measured improves shape of front
- Measured wetting line speed outside of range of goniometer data

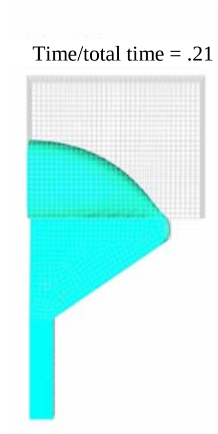
Side view shows two bubbles

Comparison to Experiment

Horizontal Alignment







A B C

Time/total time=0.26

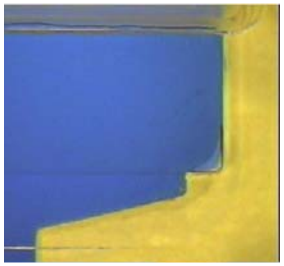
Time/total time=0.13

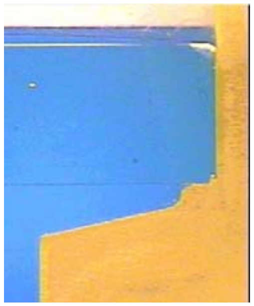
Time/total time=0.22

Horizontal

Vertical

Final times A



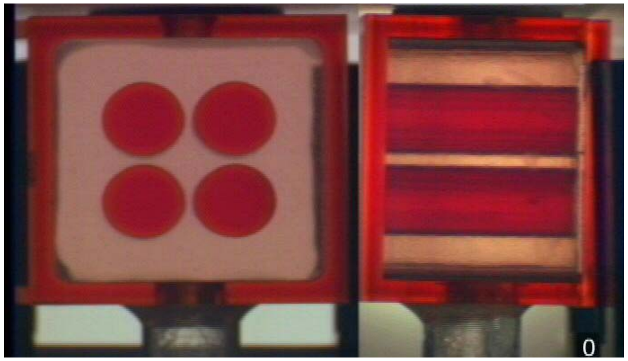


- Qualitative aspects captured – improvements in distributor and number and location of bubbles
- Increasing wetting speed from that measured improves shape of front

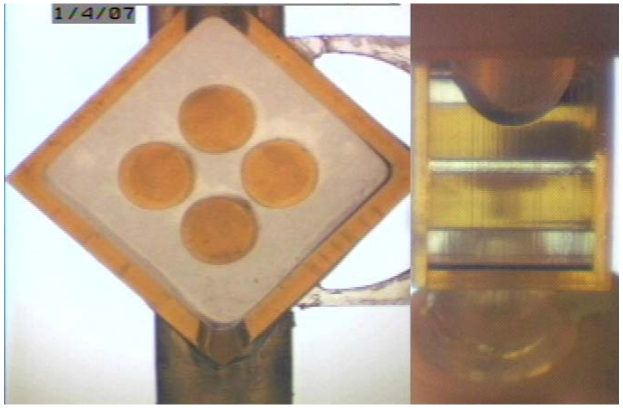
Validation Models II

Simple geometries that are representative of the pressure injection process

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

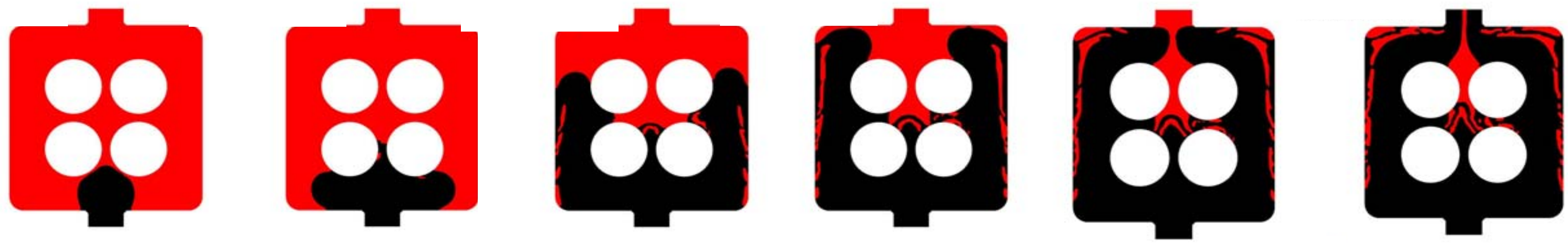


2. Injection site changed

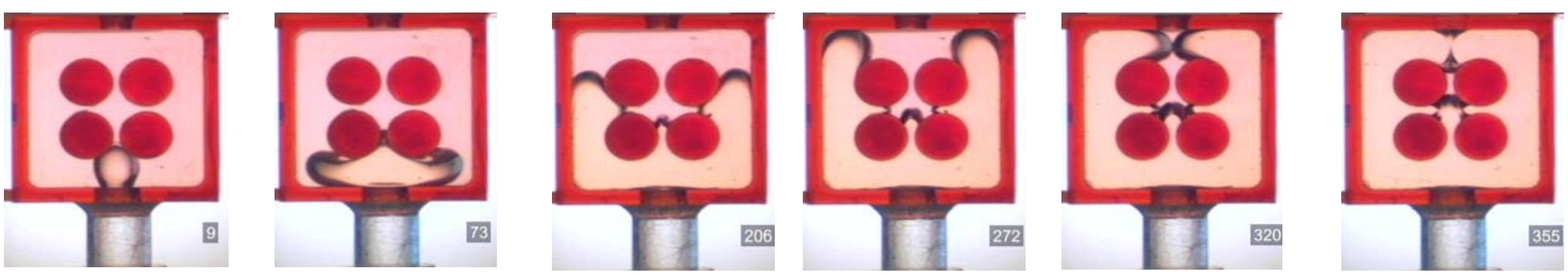


2D Model Matches Experiment Well Even with Approximate Parameters

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



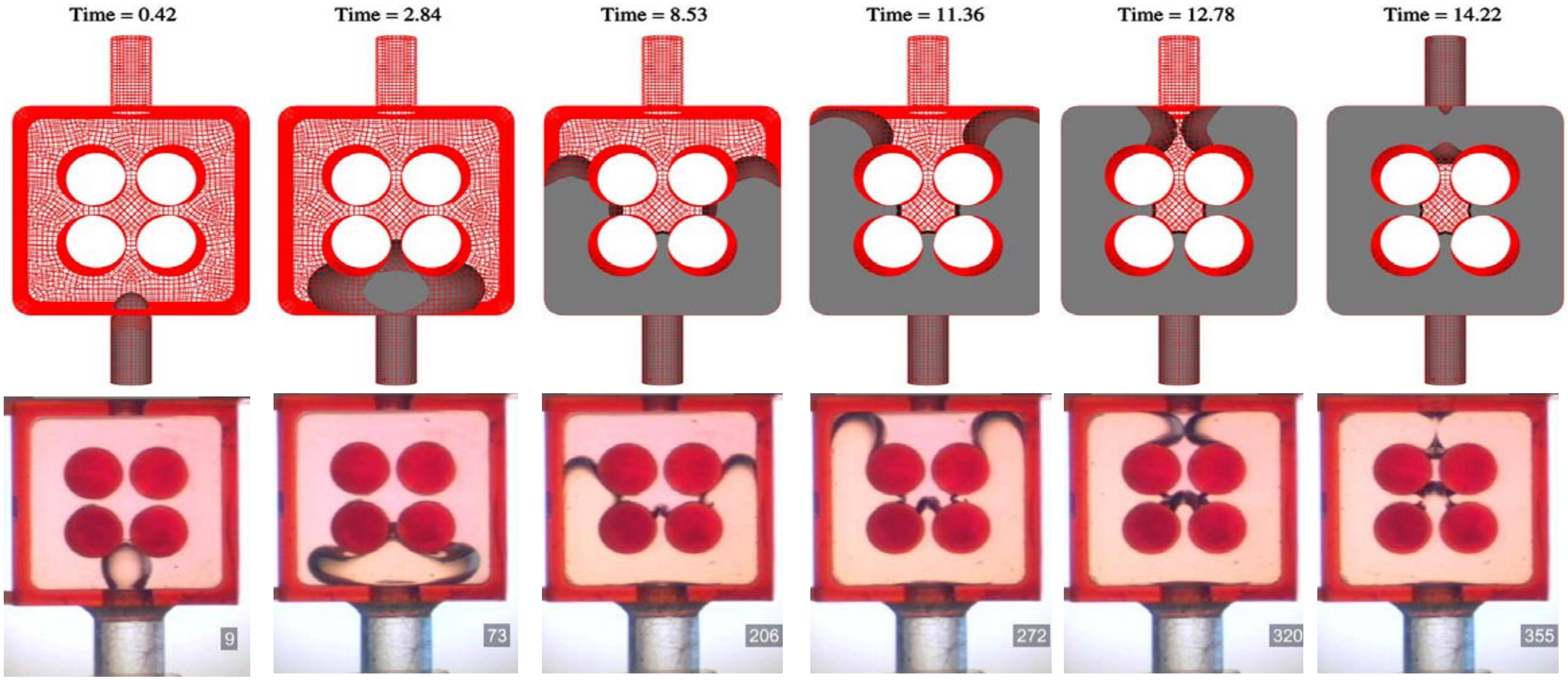
Real parameters: μ = 390 Poise, θ^{eq} = 37.8^o, v_o = 0.00193 cm/s, σ = 42.4 dyne/cm (Ucon 95-H-90000 measured parameters); fill time=12 s

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



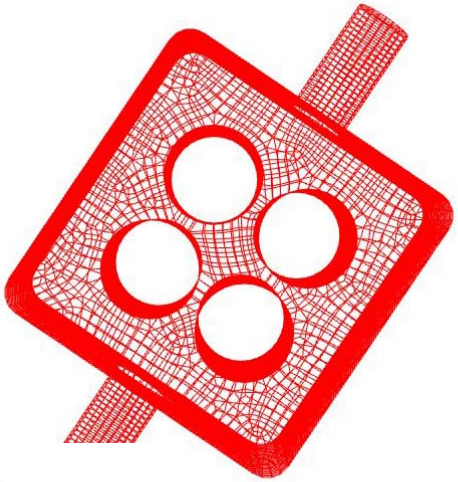
Real parameters: μ = 390 Poise, θ^{eq} = 39.8°, v_o = 0.0013 cm/s, σ = 42.4 dyne/cm
(Ucon 95-H-90000 measured parameters); fill time=12 s

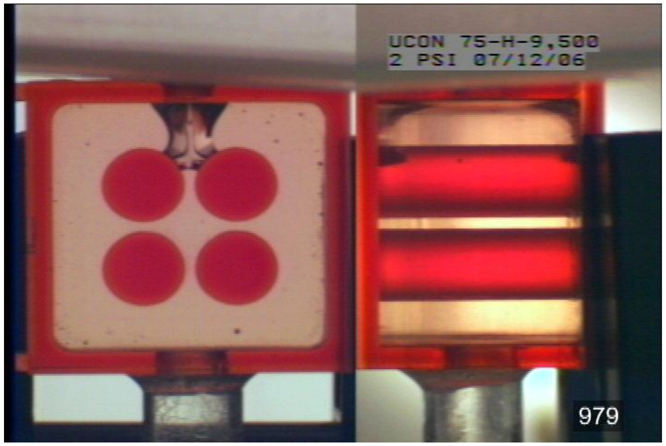
Both: Ca $\cong$ 20; Re $\cong$ 0.001

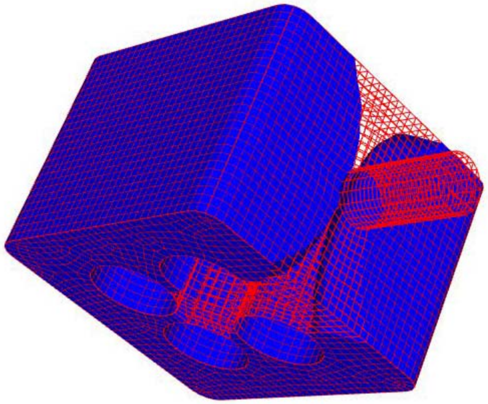
Time*=time/total time

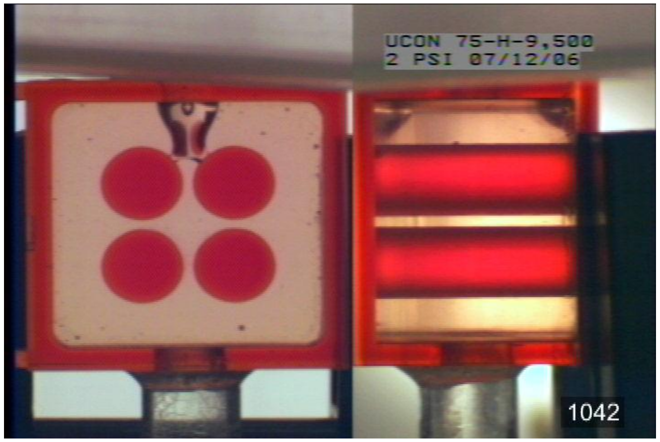
3D Effects

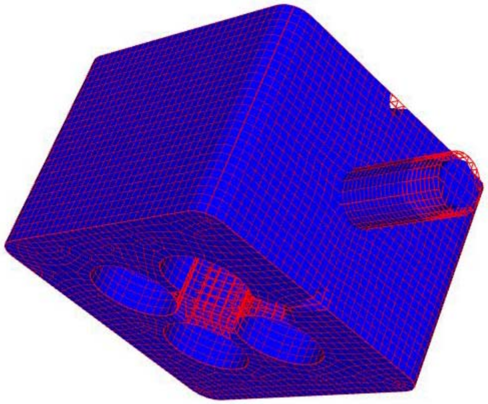
- **Some air escapes as it continues to rise after flow stops**
- **Bubbles remain on back and front walls near outflow**





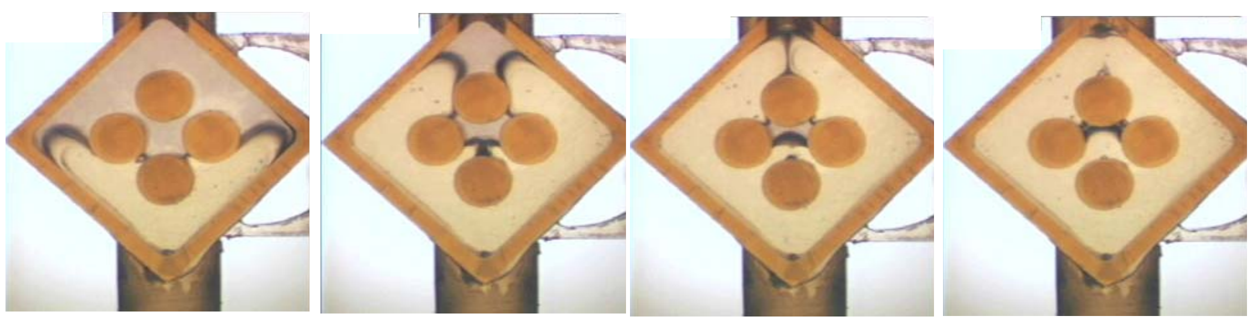






Change of Injection Point: 2D Model With Same Parameters as Experiment

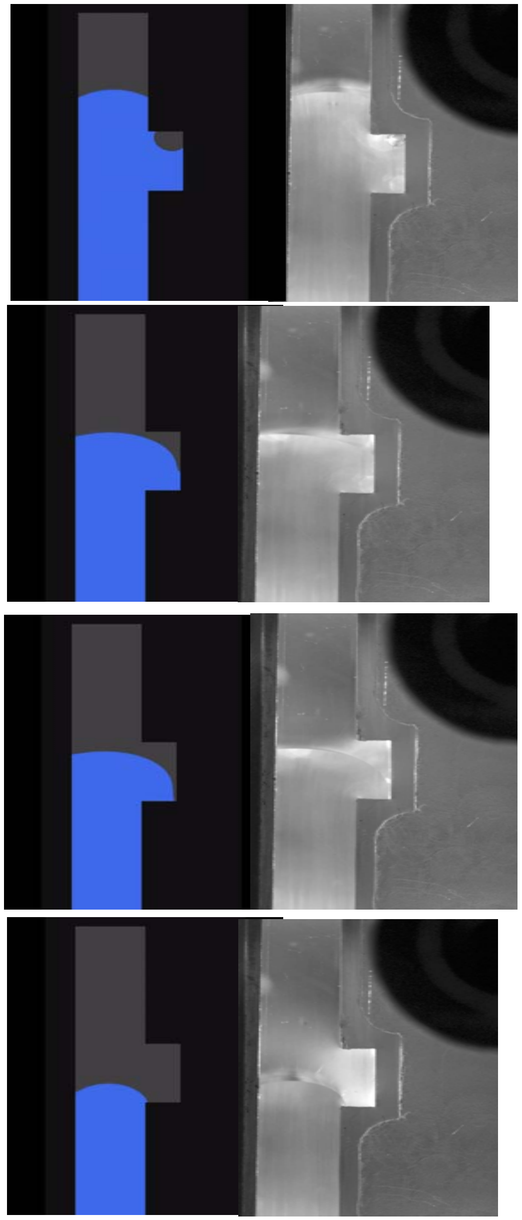
2D model “conservative” in that it predicts larger volume of trapped air



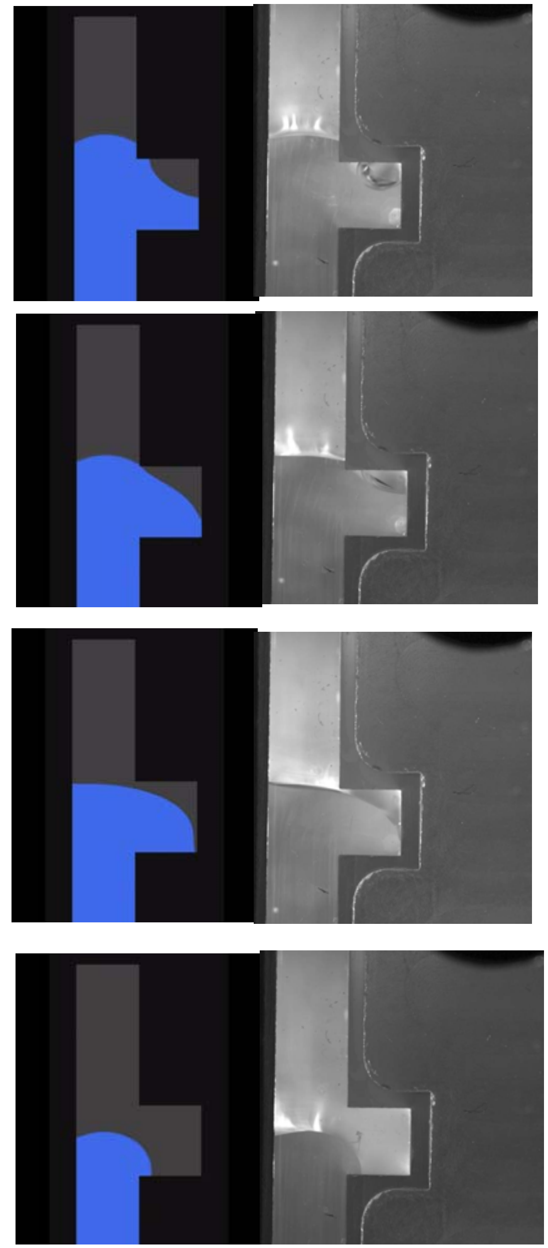
Ucon 95-H-90000 – correct parameters in model

Comparison of Simulation and Data

Side view of two notch sizes

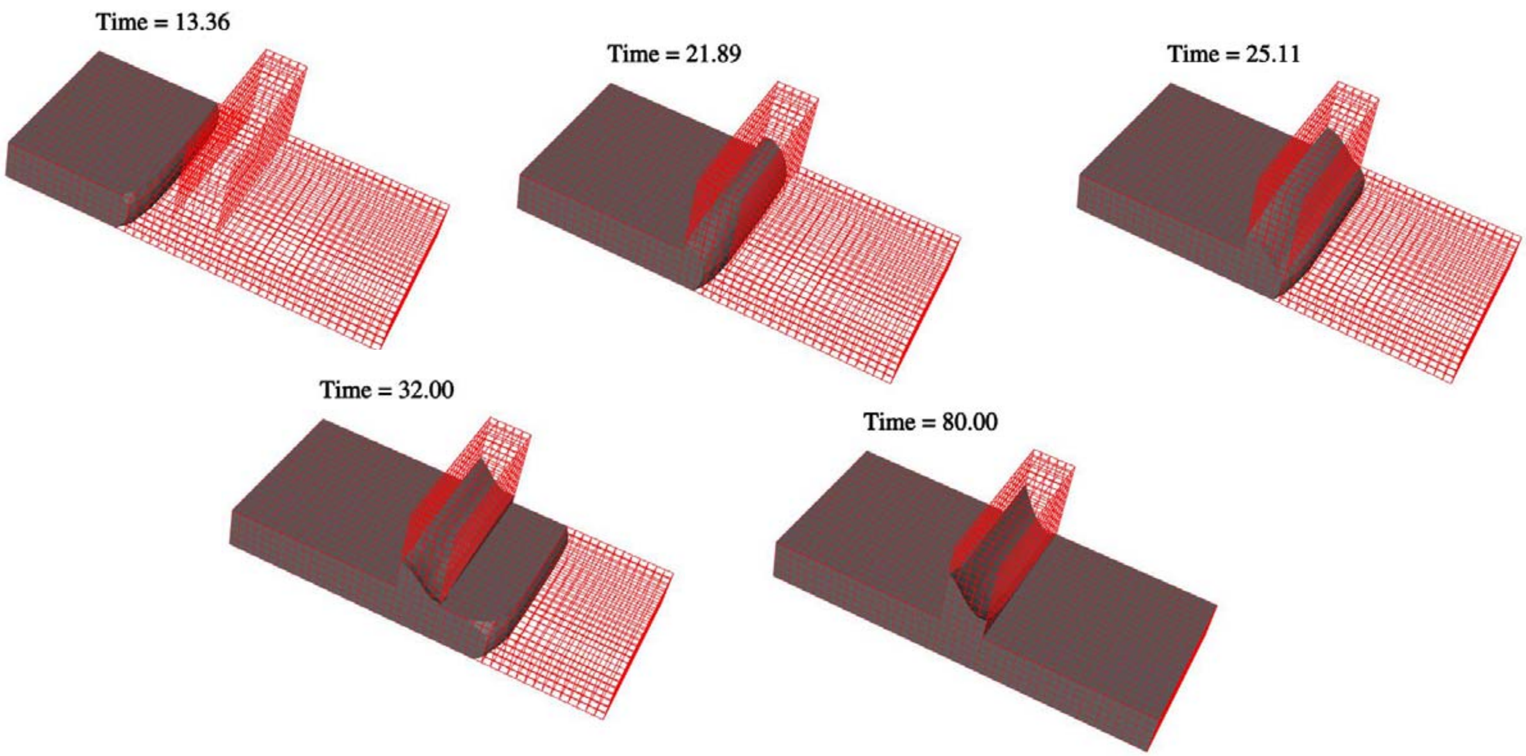


- Simulation predicts bigger bubble
- 2D calculation vs. 3D reality



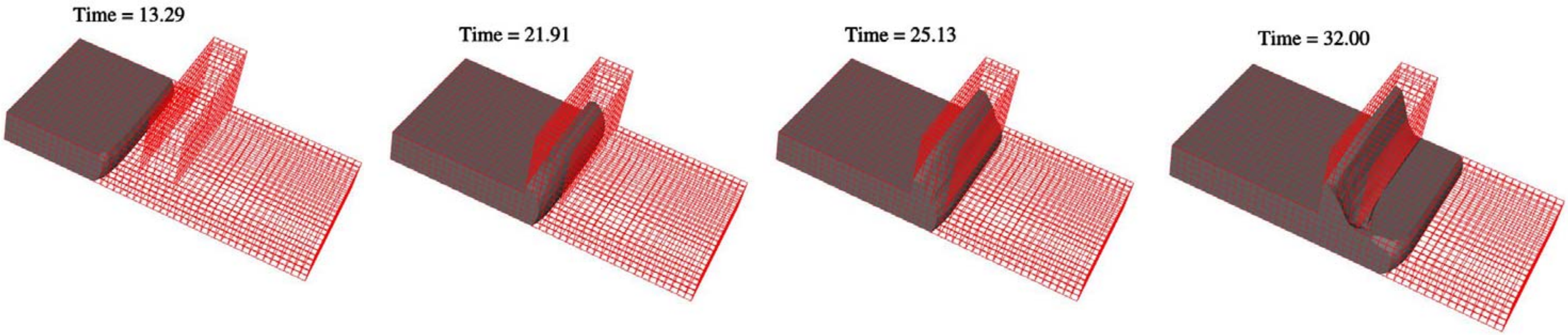
Time increasing as flows up

Correct Surface Tension & Gas Viscosity 100 Times Actual Value



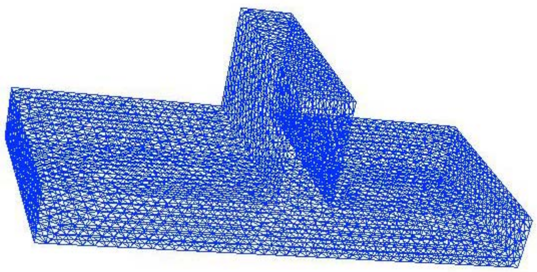
- 3D curvature makes it easier for air bubble to escape
- After 80s the bubble is smaller, but still present

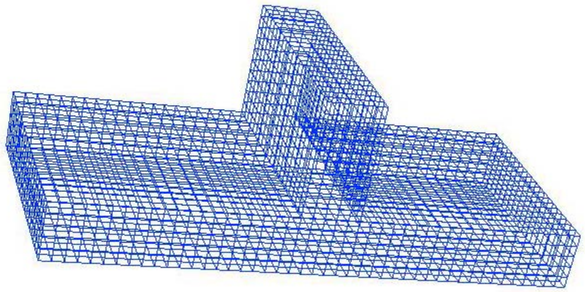
Less Surface Tension & Realistic Gas Viscosity



Lower surface tension, even with realistic gas viscosity, allows more air to escape making bubble smaller

Comparison of Stabilization Methods on 3D Notch Problem for Tets and Hexes run on 24 processors



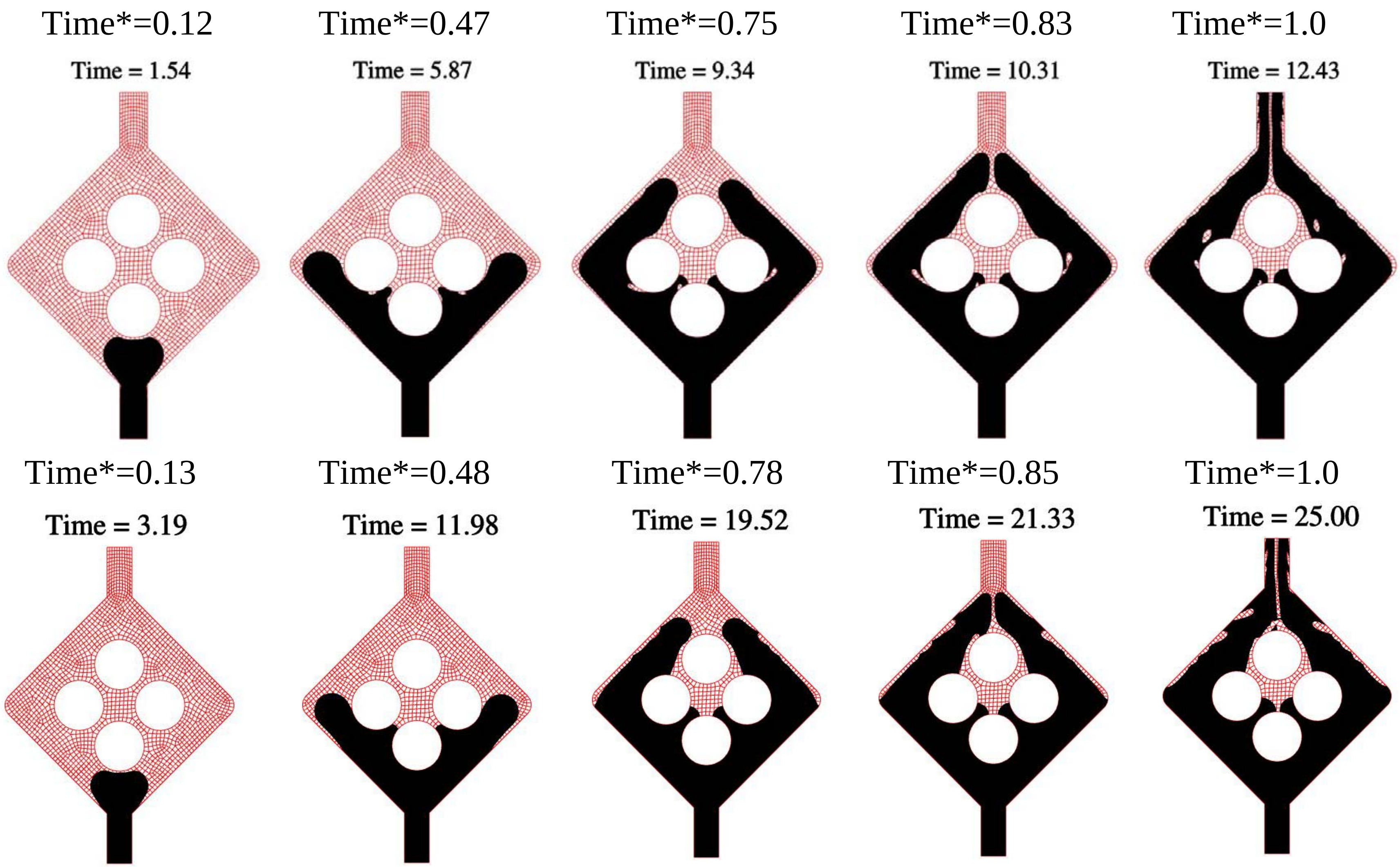


Stabilization method	Element type	#elem.	#unk.	Precond/ solver	Assembly	Solve per Newton	Linear its	Mass conservation
PSPG	hex	5500	28224	Gmres/ilut (2)	0.27 s	6.0s	250	poor
PSPP	hex	5500	28224	Ilu/bicgstab	0.25 s	0.5s	50	poor
PSPP	tet	42595	35076	Ilu/bicgstab	0.4s	0.3s	45	poor
PSPP_OFF_INTERFACE	hex	5500	28224	Ilu/bicgstab	0.25 s	0.5s	50	poor
MINI	tets	42595	162861	Gmres/ilut (2)	1.1s	2.0s	50	good

Conclusions and Future Work

- Coupled finite element/level set method can be used for modeling mold filling processes
- Results from simulations compare well to experimental validation data
- Choice of stabilization method depends on Capillary number of regime and how importantance of surface tension
  - PSPG needs to be used at a low level to ensure mass conservation for moderate capillary numbers, which in turn does not allow for solution with Krylov based methods
  - PSPP works well for viscous flows and even for moderate capillary numbers if it is implemented only away from the free surface
  - MINI element works for a range of capillary numbers and shows good mass conservation, though it is an expensive choice requiring GMRES/ILUT (2) with static condensation of the bubble
- Future work will explore matrix free method such as CBS coupled with level-set

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