SAND2008-7695C

Finite Element Analysis of Multilayer Coextrusion

Presented: Rekha Rao
Sandia National Laboratories, Albuquerque, NM USA

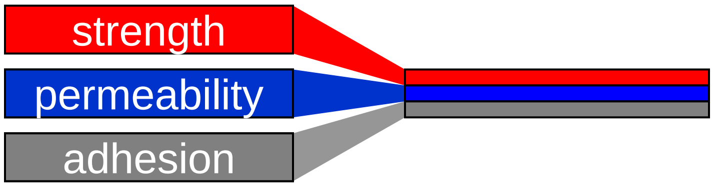
Thomas Baer
Proctor and Gamble, Cincinnati, Ohio

Robert Collins, Randy Mrozek, Joseph Lenhart, Randy Schunk, and Lisa Mondy
Sandia National Laboratories, Albuquerque, NM USA

AIChE Annual Meeting
Philadelphia, PA
November 16-21, 2008

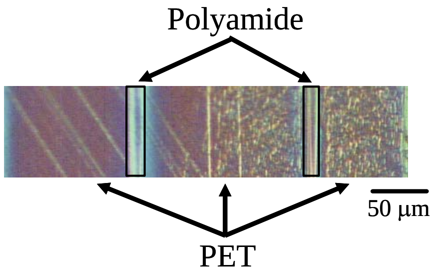
Multilayered Materials

Multilayered coextrusion combines multiple polymers in a layered structure to produce properties not found in a single polymer



Current Applications

Packaging (bottles, bags, etc.)
Protection coatings
Barrier properties



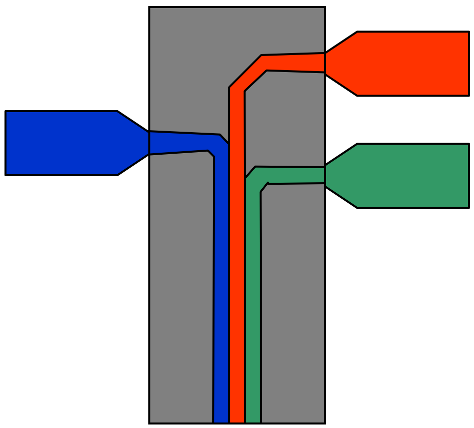
Emerging Technologies

Energy storage devices
Display devices
Sensors
Optical devices
Barrier materials
Membranes
Microcomposites
Armor applications
Responsive clothing

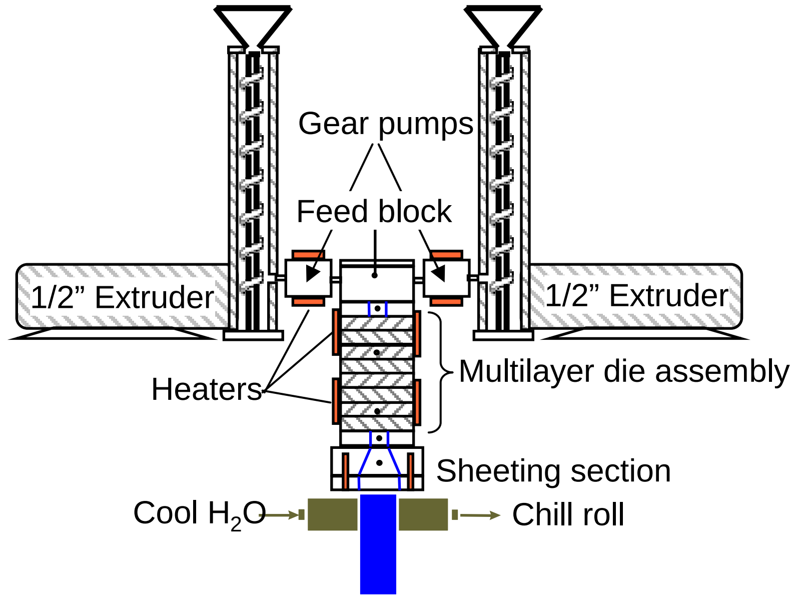
Cargotech Airliner®
maintains temperature during extended transport

Multilayer Coextrusion Processing

Multiple Extruders



Multiplication Die

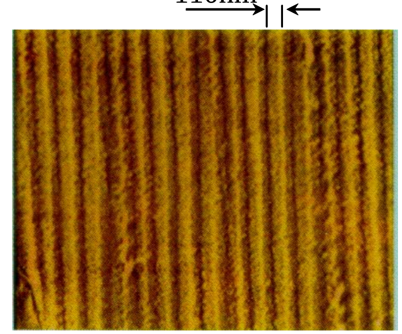


- Multilayer die assembly increases the number of layers within the same cross-section
  - Decreases layer thickness
- Gear pumps provide precise flow rate control
- Sheeting die creates ~ 1 mm tape

3M

$\delta_{PS} = 23.8 \pm 4.0$ (μm)
$\delta_{PP} = 22.9 \pm 5.1$ (μm)

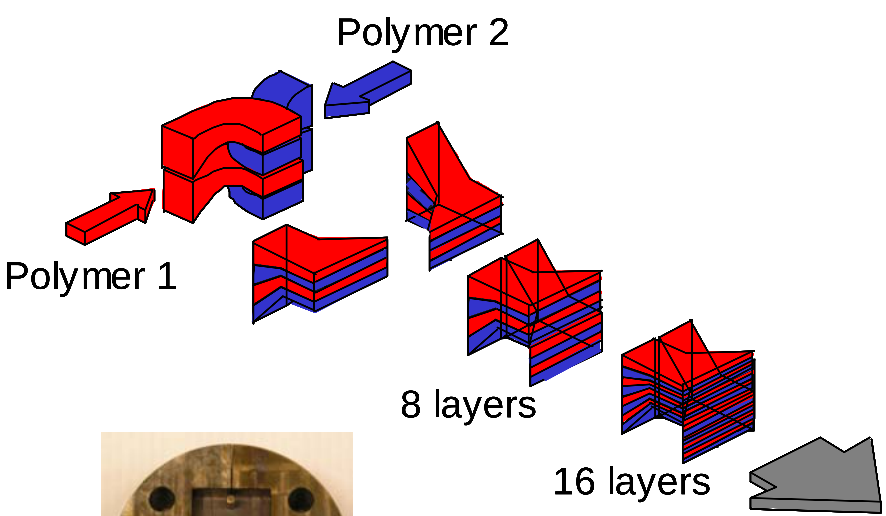
110nm

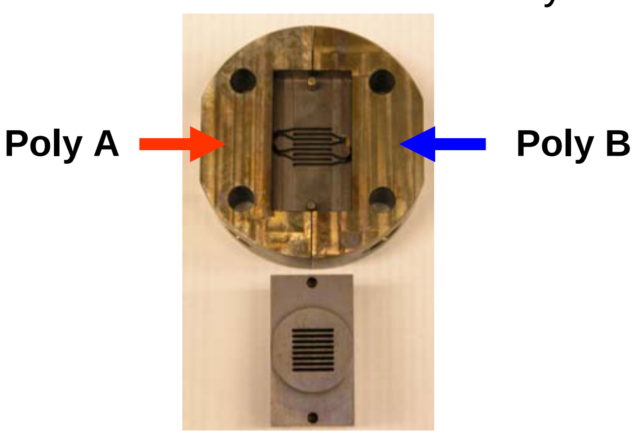


PC/PMMA multilayer, Dow Chem.

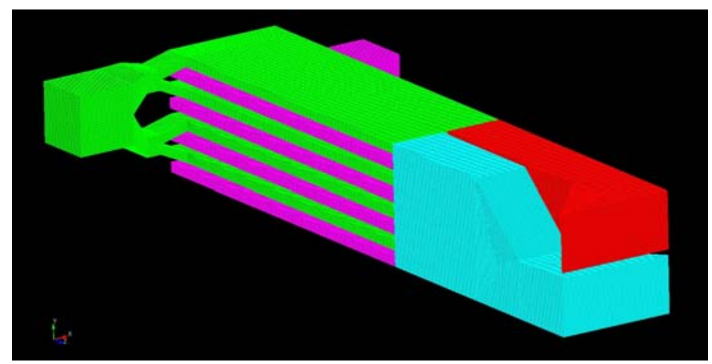
Multiplication Scheme

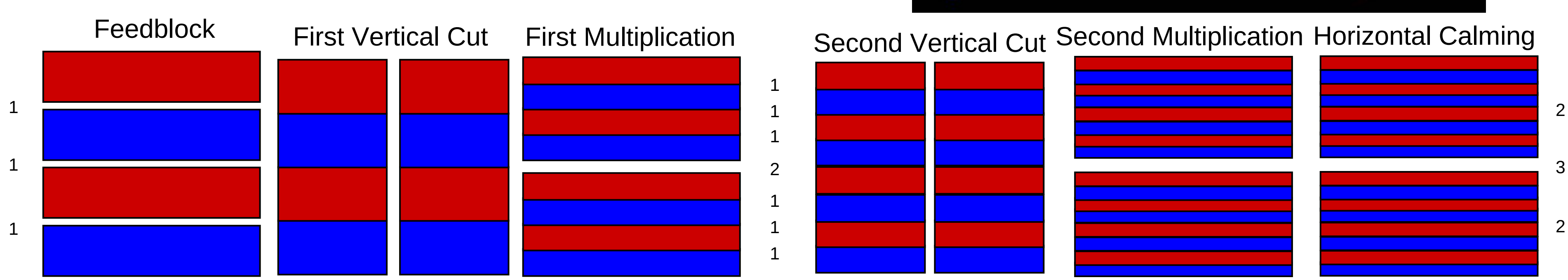
Multiplication Scheme



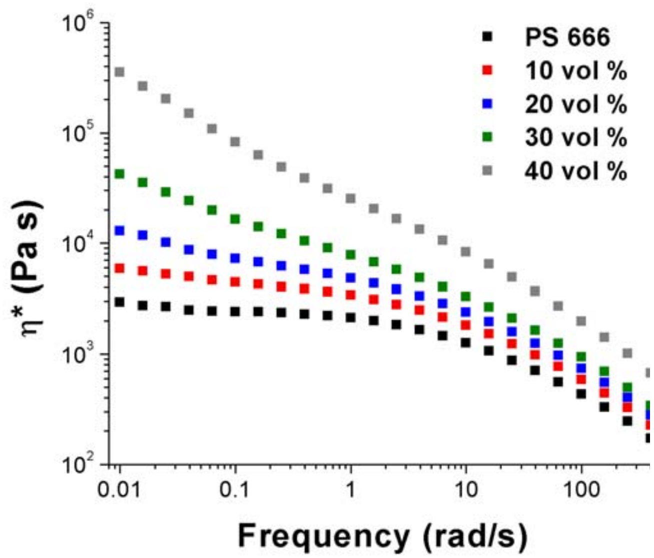


- Feedblock produces initial layered structure
- Each multiplication element doubles the number of layers
- Stacking “n” multiplication dies results in 2^{n+3} layers
- Layer stability is largely dependent on uniform laminar flow
- Thin layers (submicron) can easily break-up due to instabilities

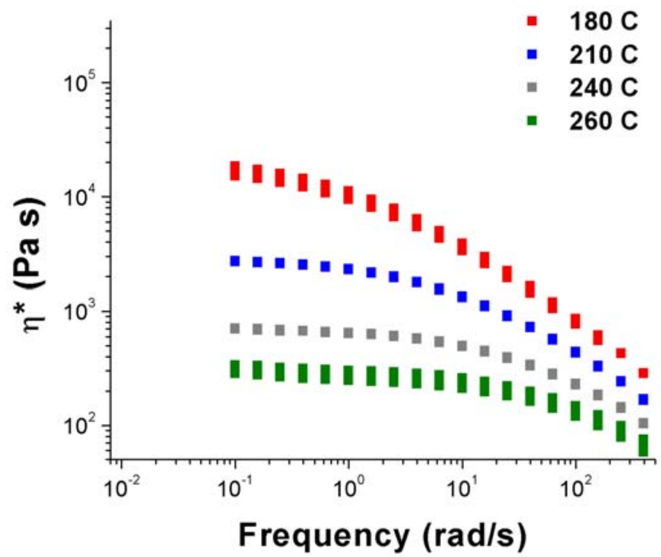




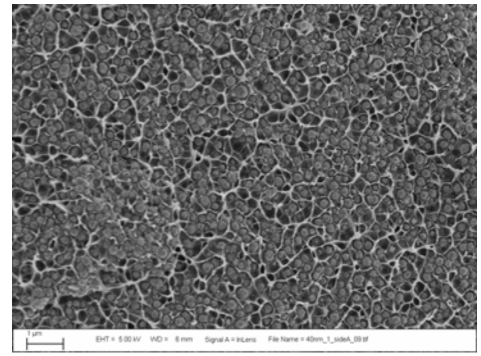
Characteristic Material Properties and Processing Parameters



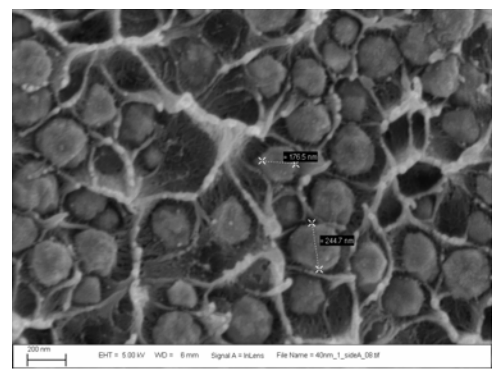
Viscosity of PS loaded with 200 nm Ni



Viscosity of PS as a function of temperature



30 vol % 200 nm Ni



- Viscosity range 10^3-10^5 Pa s
- Density range 1-5 g/cm^3
- Velocities 0.25-4 cm/s
- Interfacial tension, ?

Free Surface Flows: Coupling Fluid Flow to Pseudo-Solid Mesh Motion

- Technique for mapping mesh nodes in response to boundary deformation
- Displacement of nodes determined by solution of quasi-static problem:

$$\nabla \cdot \mathrm{T}_{mesh} = 0, \quad \mathrm{T}_{mesh} = f(\lambda_{ps}, \mu_{ps}; \nabla d_{mesh})$$

- Mesh node displacements are solved for simultaneously with other variables
- Deformation driven by boundary constraints:

Geometric

$$P(x,y,z) = 0$$

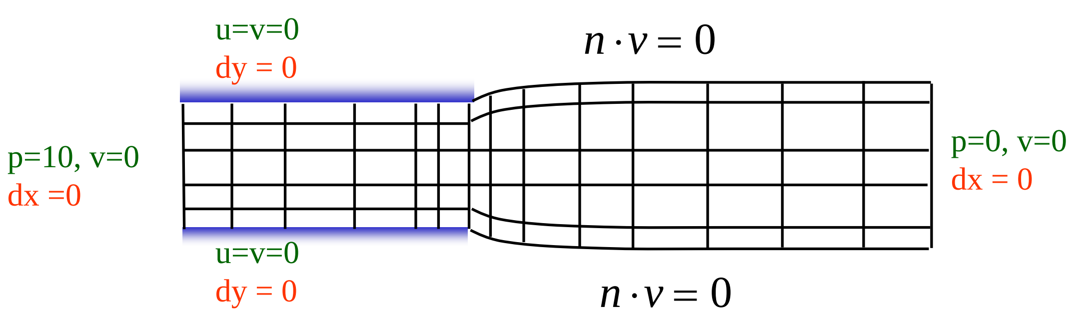
$$\vec{d} = \vec{D}_0$$

$$n_1 \cdot n_2 = \cos(\theta)$$

Coupled

$$n \cdot v = 0$$

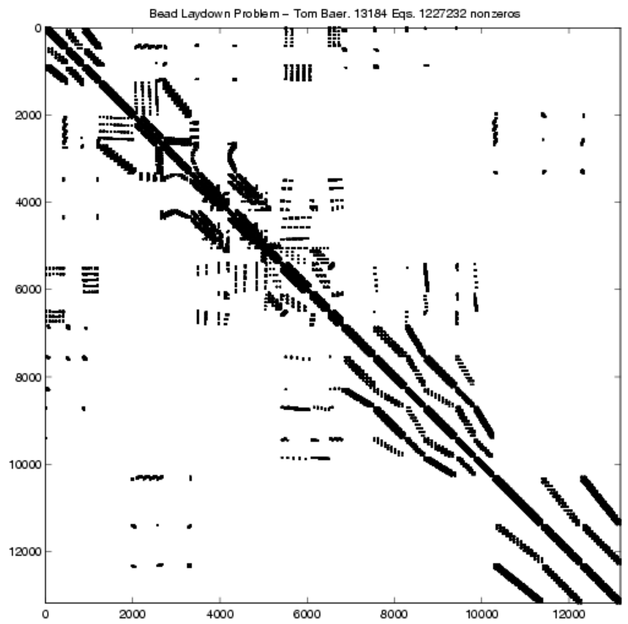
$$T = T_{melt}$$



Arbitrary Lagrangian Eulerian (ALE) mesh motion: The mesh moves with the material at boundaries and arbitrarily, as a nonlinear elastic solid, elsewhere.

Sackinger, Schunk, and Rao, 1994; Cairncross et al, 2000; Baer et al, 2000

Why Are 3D Free Surface Problems Hard?



Typical problem graph for incompressible flow

$$\rho \frac{Du}{Dt} = -\nabla P + \mu \nabla^2 v + \rho g$$

$$\nabla \cdot u = 0$$

$$\nabla \cdot \mathrm{T}_{mesh} = 0, \quad \mathrm{T}_{mesh} = f(\lambda_{ps}, \mu_{ps}; \nabla d_{mesh})$$

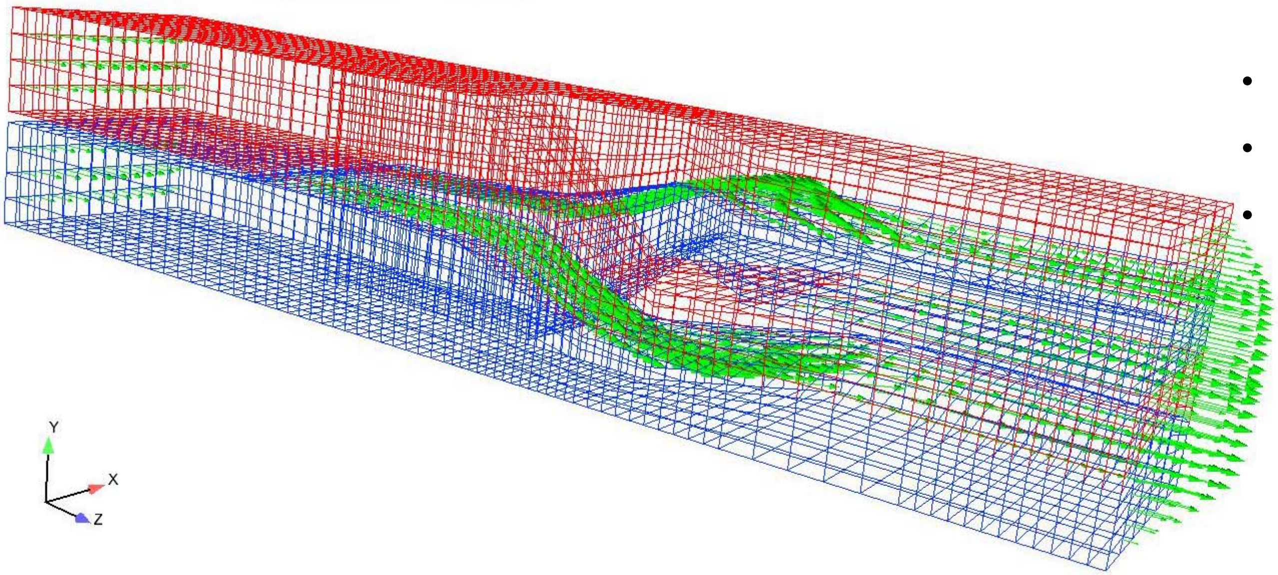
- Incompressibility constraint and distinguishing conditions (DC), e.g. kinematic, and boundary conditions (BC) lead to non-diagonally dominant matrices
- In 2D, direct solver can be used with LBB elements
- In 3D, only Krylov-based iterative solvers are feasible
- Stabilization for the continuity equation is used to allow for equal order interpolation and improve the matrix condition number, but DC/BCs are still a problem
- Solution requires heavy duty preconditioner-solver pairing such as ILUT(1-3)/GMRES, which are not very scalable
- Rotated conditions are applied by hand and require much user intervention to yield well-behaved mesh and matrix

Dohrman-Bochev Stabilization (PSPP) (Dohrmann, and Bochev, 2004)

$$R_i^c = \int_D \phi^i [\nabla \cdot u] dV + \sum_{Elem} \tau_{pspp} (\phi^i - \pi\phi^i)(p - \pi p) dV$$

$$\pi p = \int_{V_e} p dV \Big/ \int_{V_e} dV$$

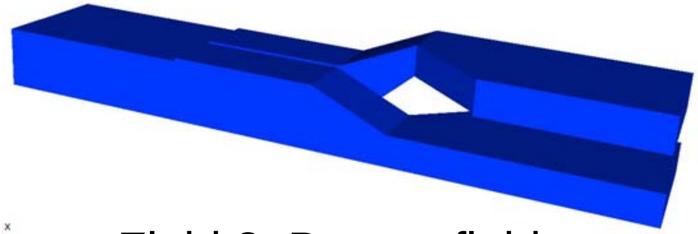
3D Mesh of Two-Layer Coextrusion Multiplication Region to Four-Layer Structure



- 9276 8-Node hexahedral elements
- 12040 Nodes
- 84280 total degrees of freedom

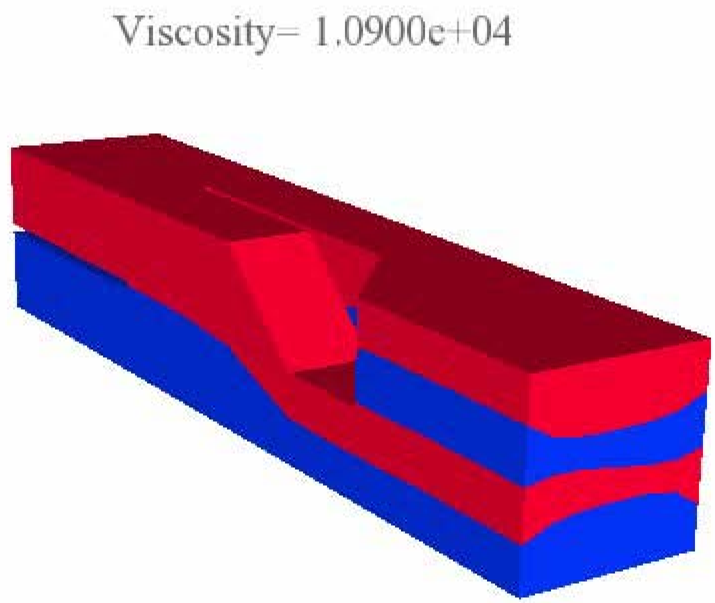
- Flow splitters and duct wall all have no slip boundary conditions
- Free surface exists between red and blue fluid in the downstream region, where surface tension and kinematic condition are applied
- Inflow boundaries have constant applied pressure
- Boundary conditions must be applied to momentum equations and mesh equations
- Sixteen different side sets in the mesh

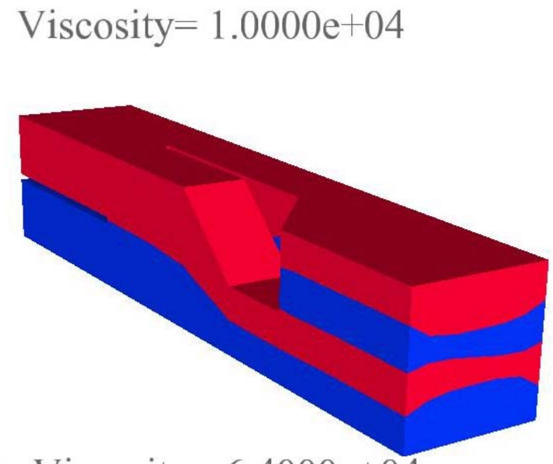
Fluid 1: Top fluid

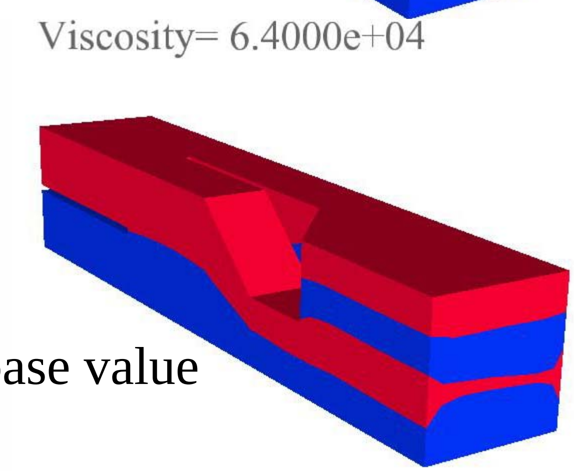


Fluid 2: Bottom fluid

Continuation in Red Fluid Viscosity at a Constant In Flow Pressure

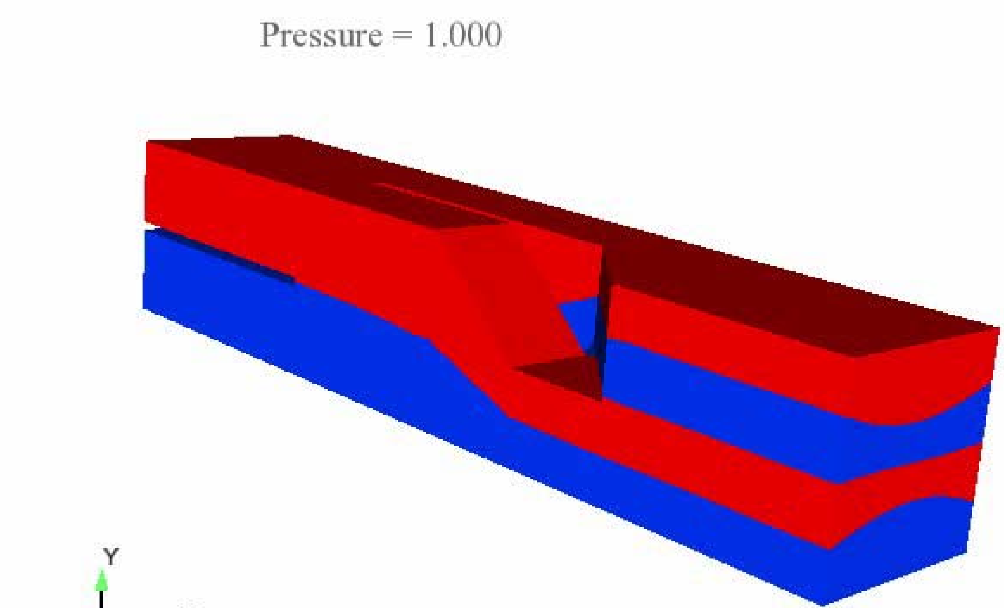


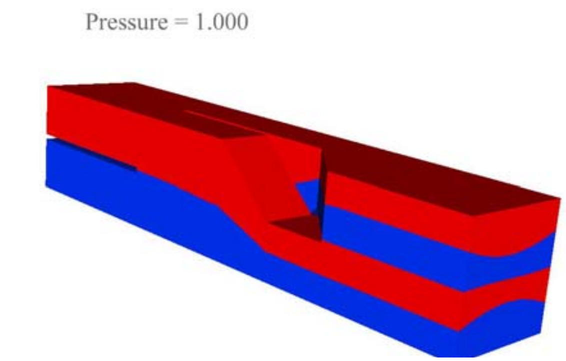


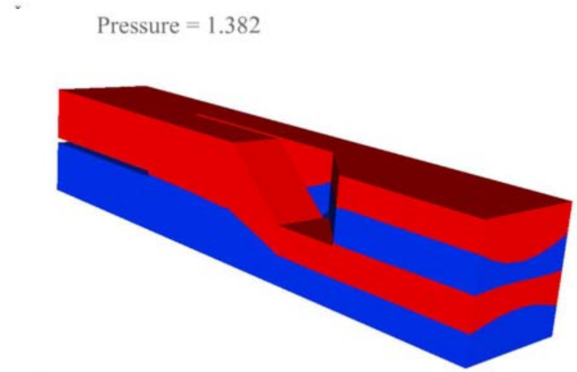


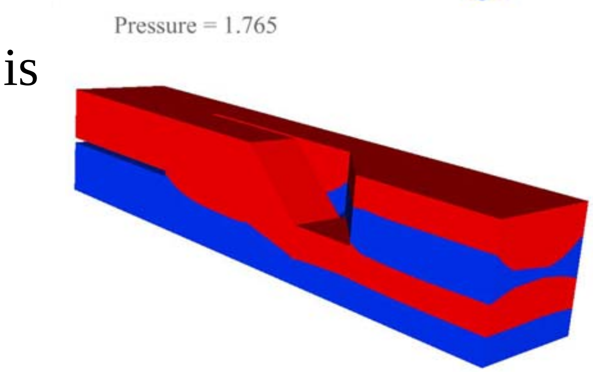
- Red fluid viscosity is increased while blue fluid stays at base value of 10,000 Poise
- Blue fluid squeezes out red fluid until the bottom red layer is nearly gone
- Simulations discontinued as mesh becomes too deformed
- 3D deformed geometry remeshing would be helpful
- Boundary conditions could be relaxed from no slip

Continuation in Red Fluid Inflow Pressure at a Constant Equal Viscosity for Both Phases



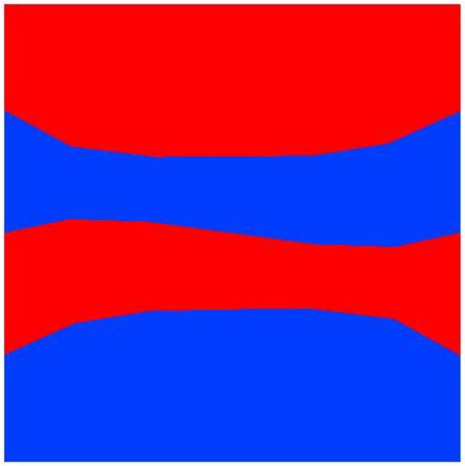


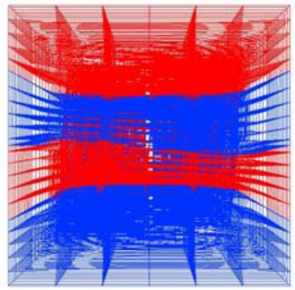


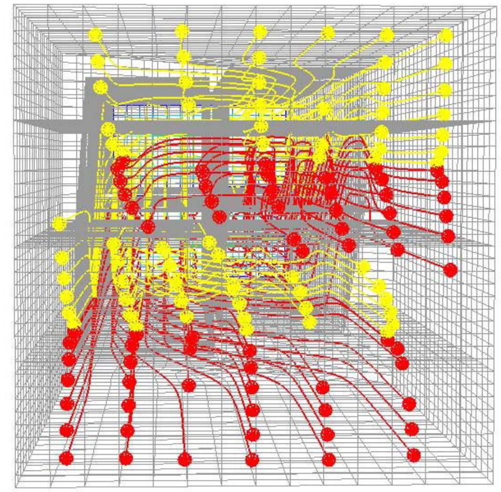


- Pressure of red fluid is increased until mesh deformation become too great
- Both and blue fluid viscosity are 10,000 Poise
- Red fluid squeezes out blue fluid until the top blue layer is nearly gone
- Nondimensionalization improved solver performance, reducing average iterations from 180 to 30

Can We Use From Fixed Mesh Solution Particle Tracking To Determine Layer Thicknesses?



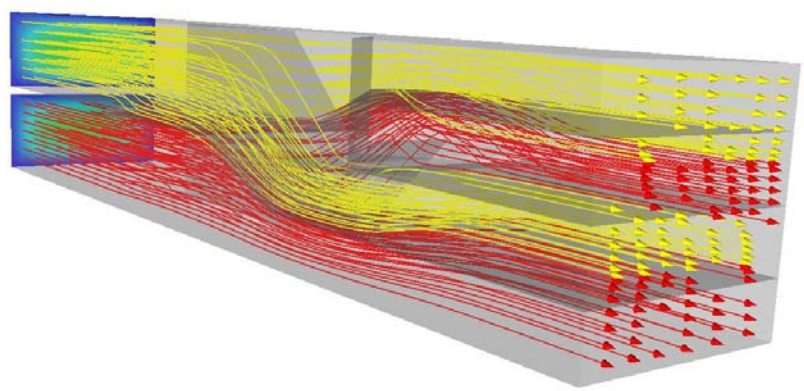




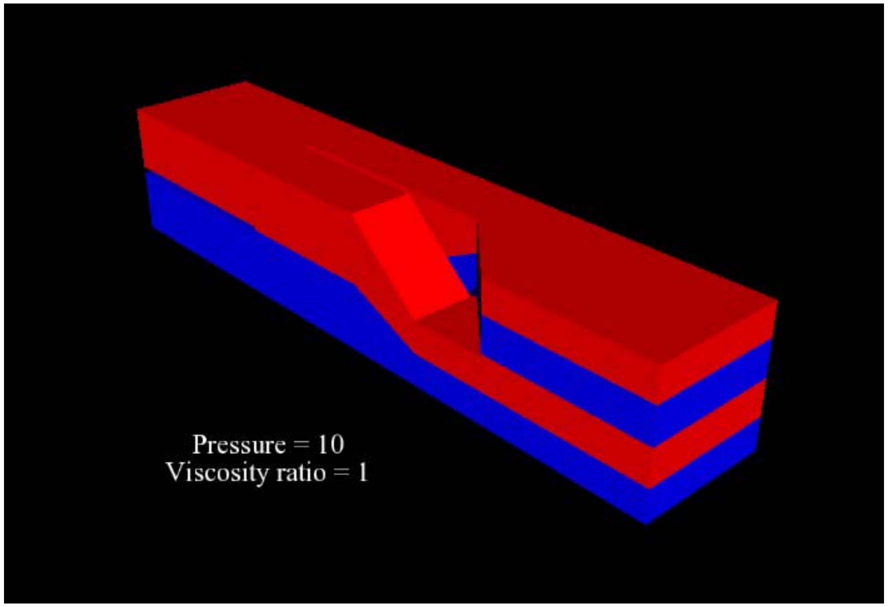
Solution for equal properties and flow rates using kinematic condition between layers

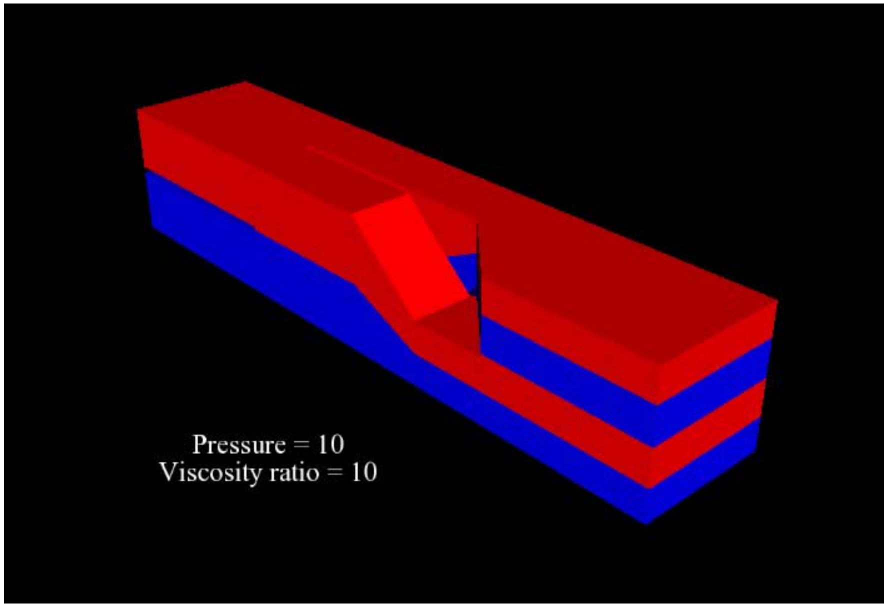
Particle traces indicate flow and layer thickness from fixed mesh solution for equal properties and flow rate

- Particle tracking from the inflow from the fix mesh solution predicts layer thickness and shape different from moving mesh solution
- Lack of kinematic condition could be the reason for the dissimilar results



Simulation of two-layer coextrusion with level-set interface tracking



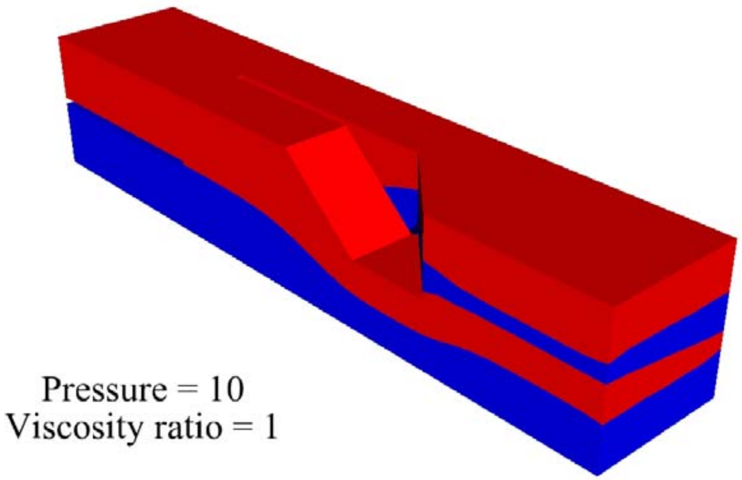


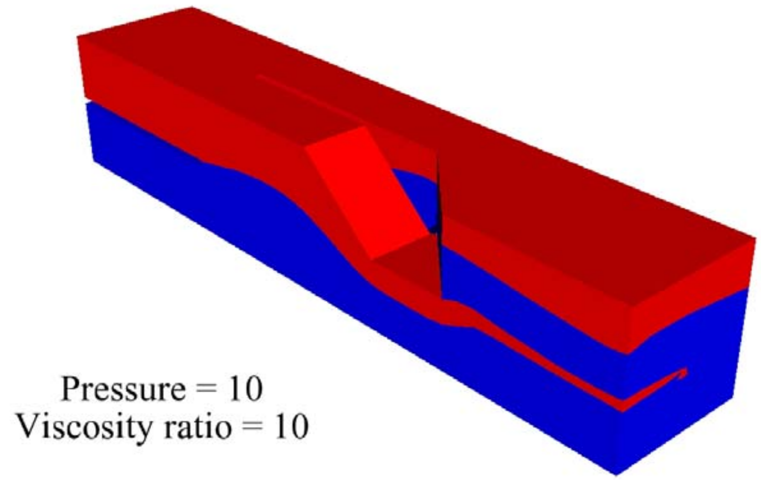
- Time-dependent simulations of two-layer coextrusion using level-set interface tracking

- Blue fluid squeezes out red fluid, thinning the bottom red layer

- At high viscosity ratios, the more viscous (blue) fluid layers merge in part of the channel, destroying the integrity of the lamilae

Simulation of two-layer coextrusion with level-set interface tracking





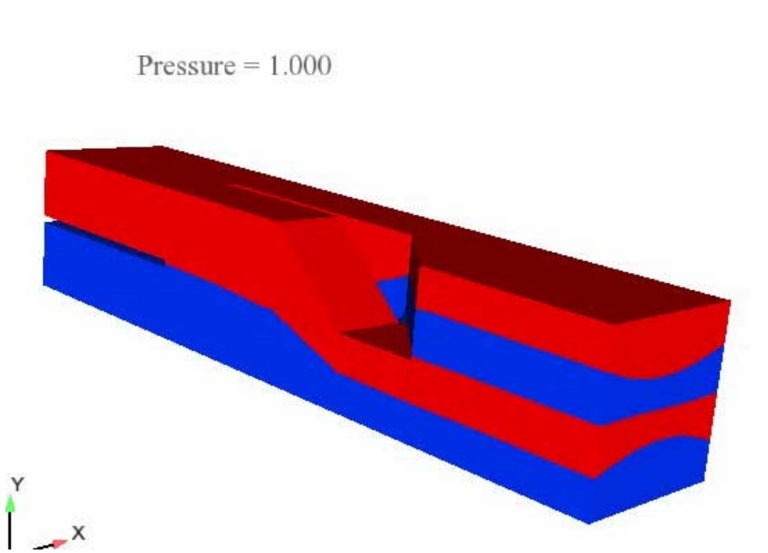
- Time-dependent simulations of two-layer coextrusion using level-set interface tracking

- Blue fluid squeezes out red fluid, thinning the bottom red layer

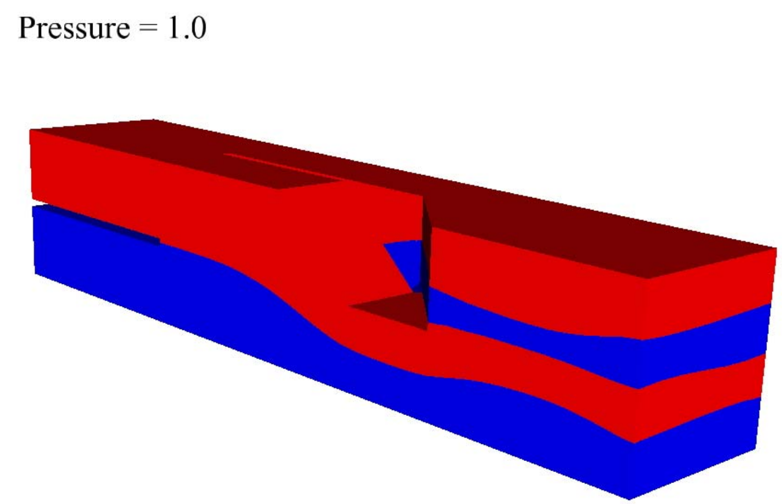
- At high viscosity ratios, the more viscous (blue) fluid layers merge in part of the channel, destroying the integrity of the lamilae

Comparison of ALE and Level-Set Coextrusion Simulations

ALE simulation



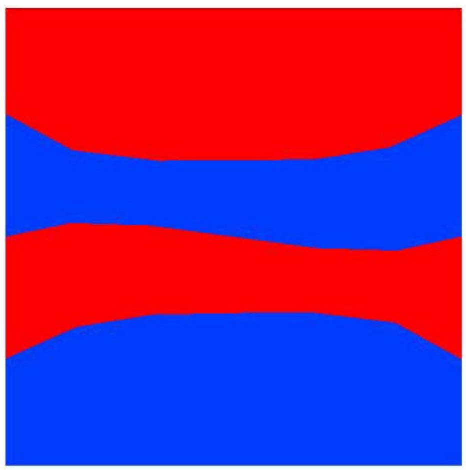
Level-set simulation

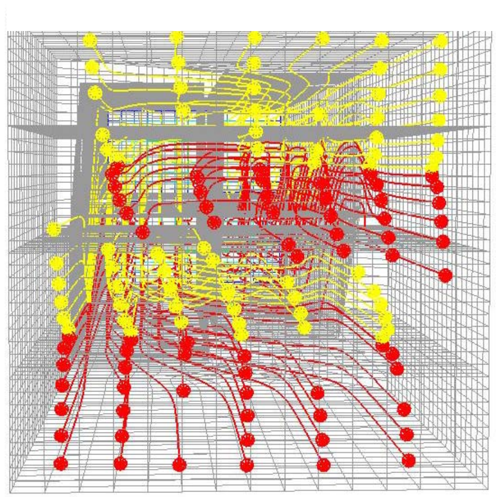


- In both simulations, the fluid viscosities are each 10000 Poise
- Blue fluid squeezes out red fluid until the bottom red layer is nearly gone
- Differences are due to boundary conditions along the walls contacting the free surface – ALE simulations use a no-slip condition, while level-set simulations use a Navier-slip condition on these walls

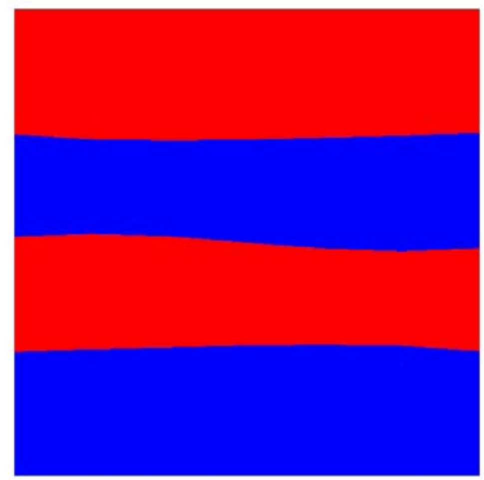
Comparison of ALE and Level-Set Coextrusion Simulations

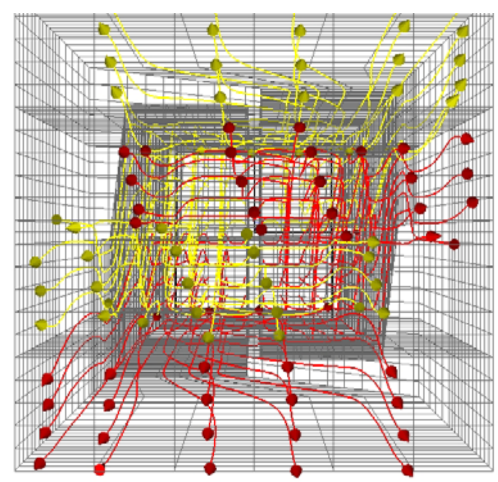
ALE simulation



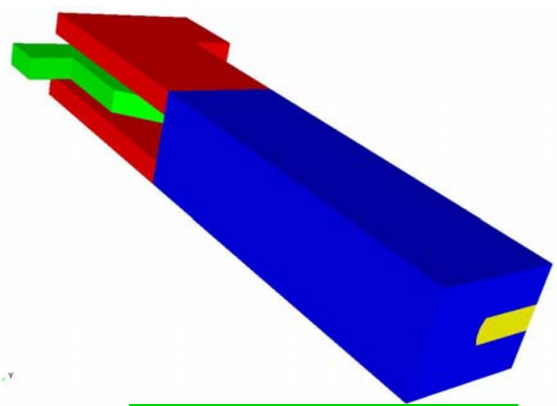


Level-set simulation

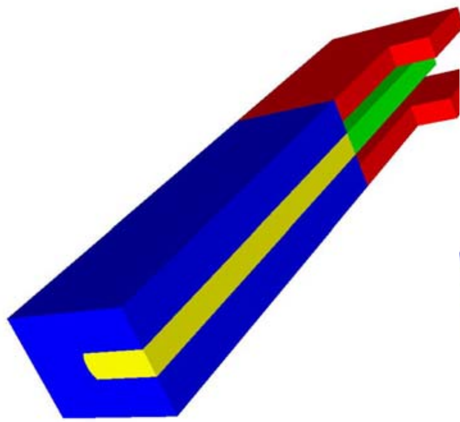




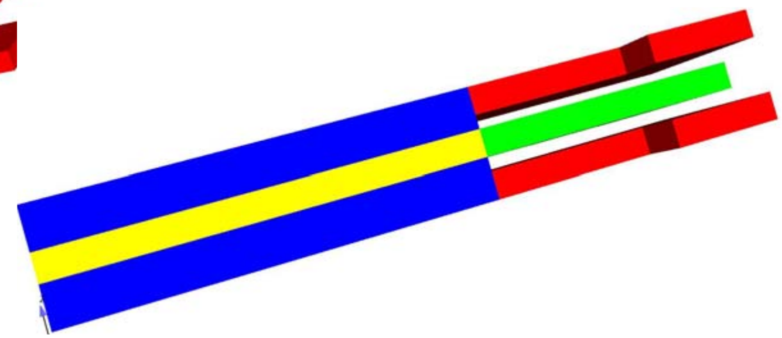
Simplified 3D Mesh of Three-Layer Coextrusion



Left side of three-layer mesh



Right side of three-layer mesh

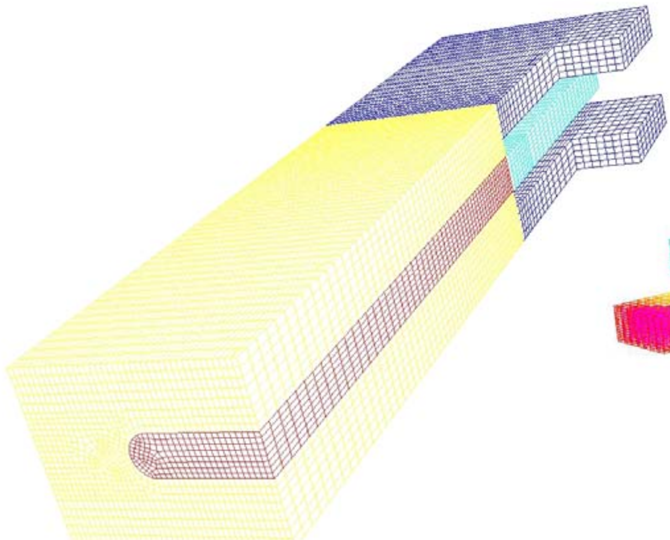


Side view shows thickness of die based on current design

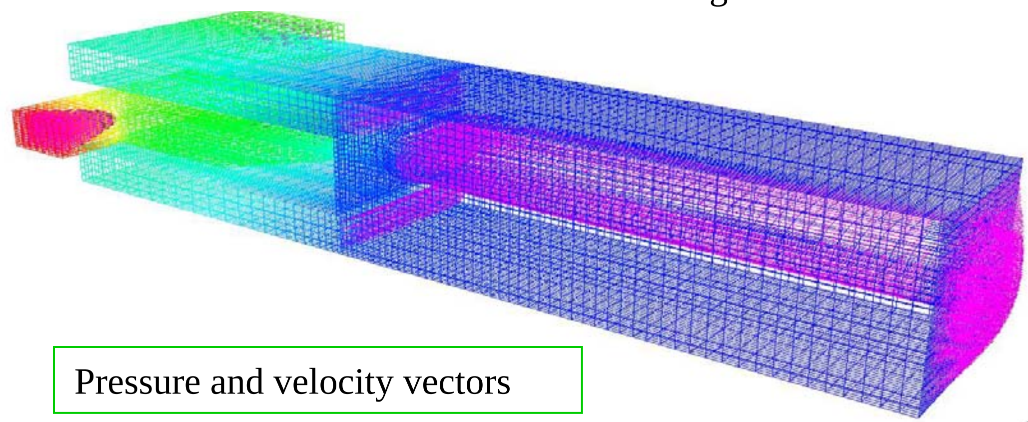
- Gradual drawdown of encapsulating fluid layer (shown in green) to potentially create offset for capacitor.
- The offset fluid transitions from green to yellow in the free surface region
- The red encapsulating fluid maintains it cross-section in the die and then the fluid transitions to blue in the free surface region
- Free surface ALE with a moving mesh simulations will show if encapsulation of yellow fluid by the blue fluid will occur and what the final cross-section will be

Boundary Conditions for Three-Layer Offset Die

- 76593 8-Node hexahedral elements
- 85108 Nodes
- 368080 total degrees of freedom



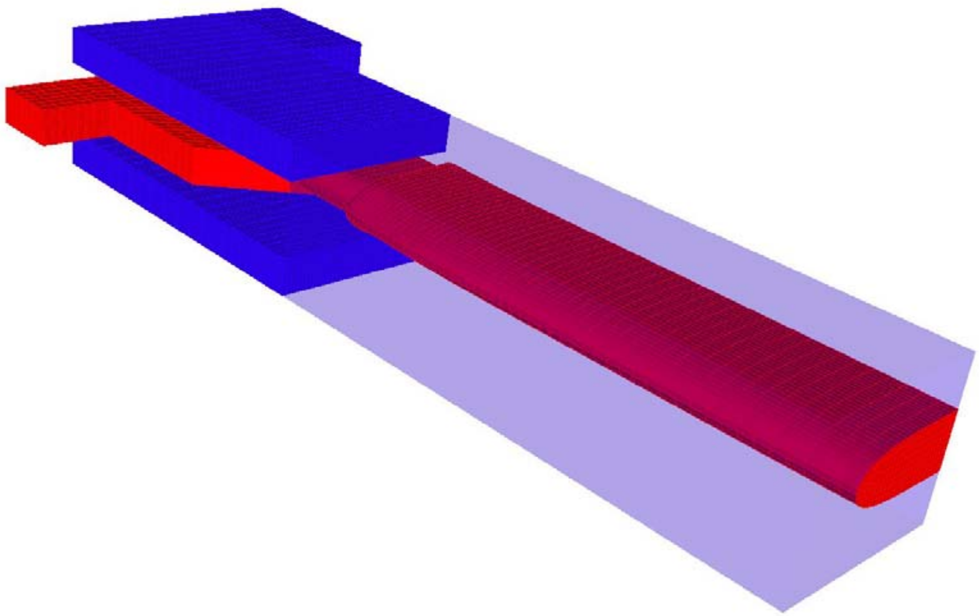
Initial undeformed mesh



Pressure and velocity vectors

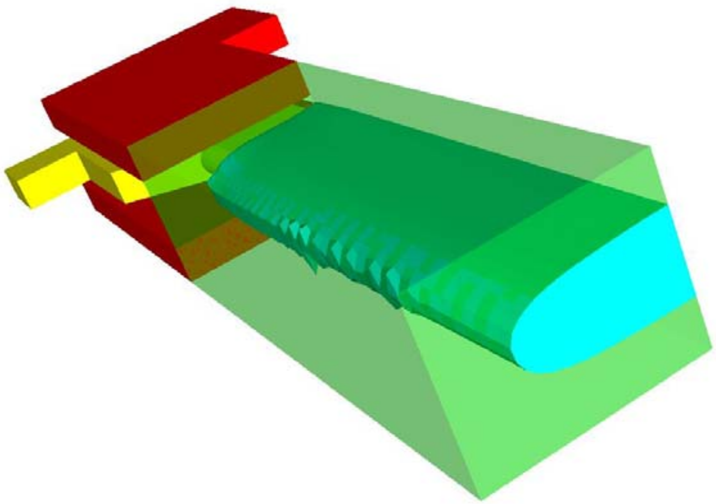
- Duct walls begin with small amount of slip on the surface to approximate a rolling motion condition and then converge to no slip boundary conditions
- Free surface exists between red and yellow fluid in the downstream region, where surface tension and kinematic condition are applied
- Inflow boundaries have constant applied pressure
- No mesh equations in die region
- Boundary conditions must be applied to momentum equations and mesh equations
- Twenty-two different side sets in the mesh

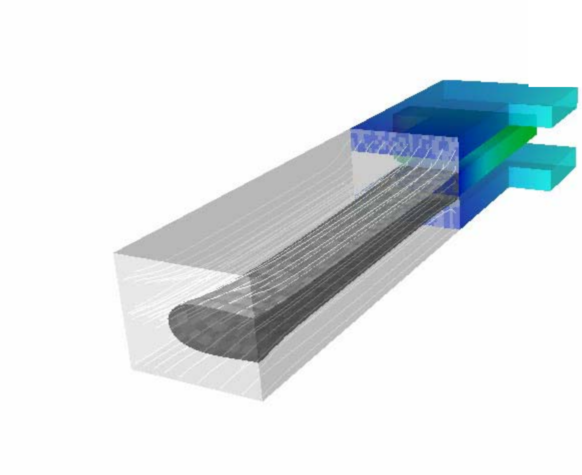
Simplified 3D Mesh of Three-Layer Coextrusion

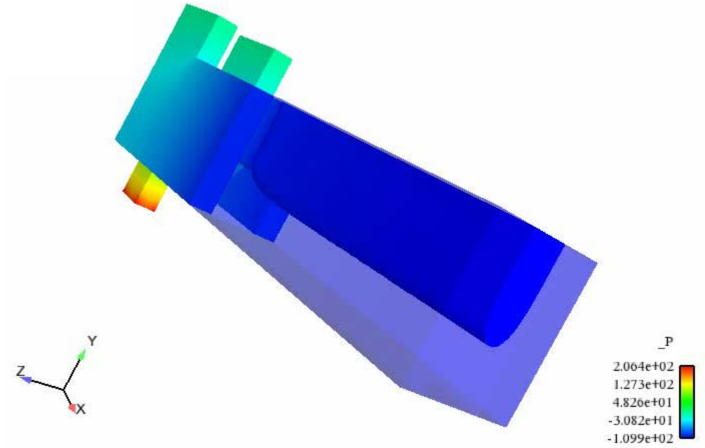


- The encapsulating fluid has been made transparent to better visualize the shape of the free surface.
- The "die swell" of the fluid core as it leaves the upstream die is clearly visible even for a Newtonian fluid.
- The fluid core tends to remain in a flatter configuration because of the upper and lower fluid streams compress it.

Effects of Shear-Thinning on Three-Layer Offset Die

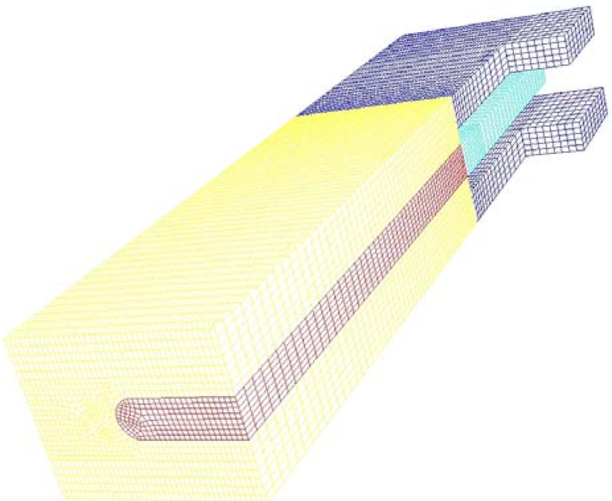


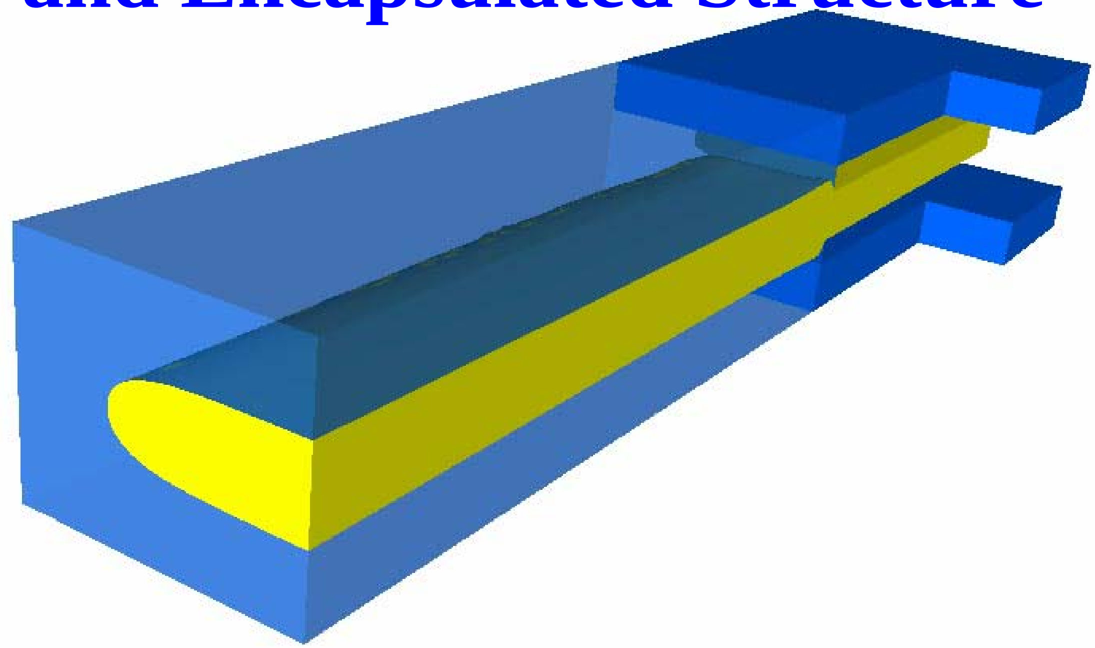




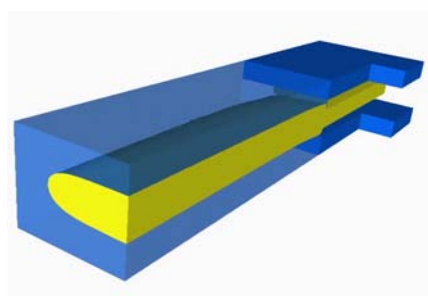
- As the fluid becomes more shear-thinning, the inner layer flattens and thins.
- Velocity packets show flow rearrangement leaving the die lip.

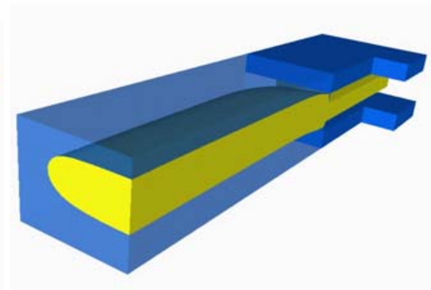
Three-Layer Coextruder Design with an Offset to Produce and Encapsulated Structure

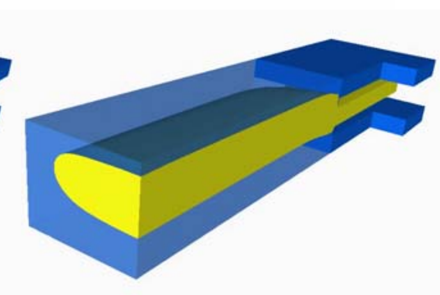




Initial undeformed mesh shows no die swell







- Movie shows continuation steps as flow rate of top blue inflow is decreased
- Flow rate imbalance leaves layer mismatch
- Die swell is seen as the fluid exits the die even for a Newtonian fluid

Conclusions and Future Work

- Finite element modeling has been used to better understand a multilayer coextrusion process for manufacturing composite materials with filled polymers
  - Effects of viscosity/density/pressure mismatch
  - Effects of geometry
- Several numerical techniques have been used including
  - 3D ALE moving mesh solutions
  - 3D level set methods

For future work, we would like to look at

- Redesigning splitter dies, adding quieting regions, etc
- Finer mesh/more layers
- Slip boundary conditions on solid surfaces/ Blake wetting condition
- Linear stability analysis to create and operating window
- Shear rheology in capillary viscometer with nanoparticle filled PS
- More complex fluids, shear-thinning, particle filled, viscoelastic effects?