

Modeling of Extrusion-Based 3D Printing of Cementitious Materials

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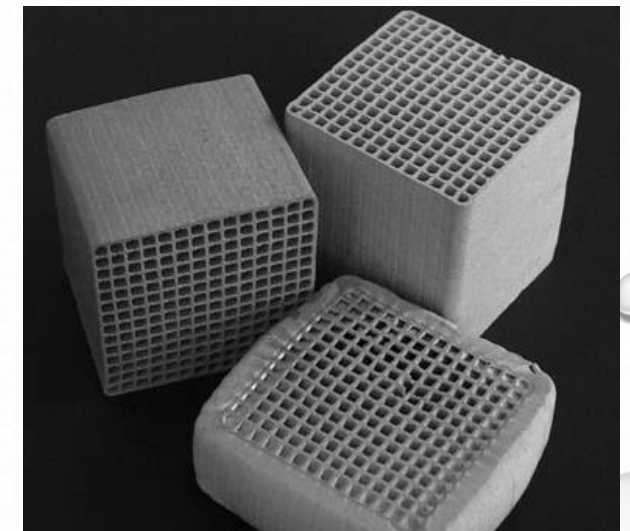
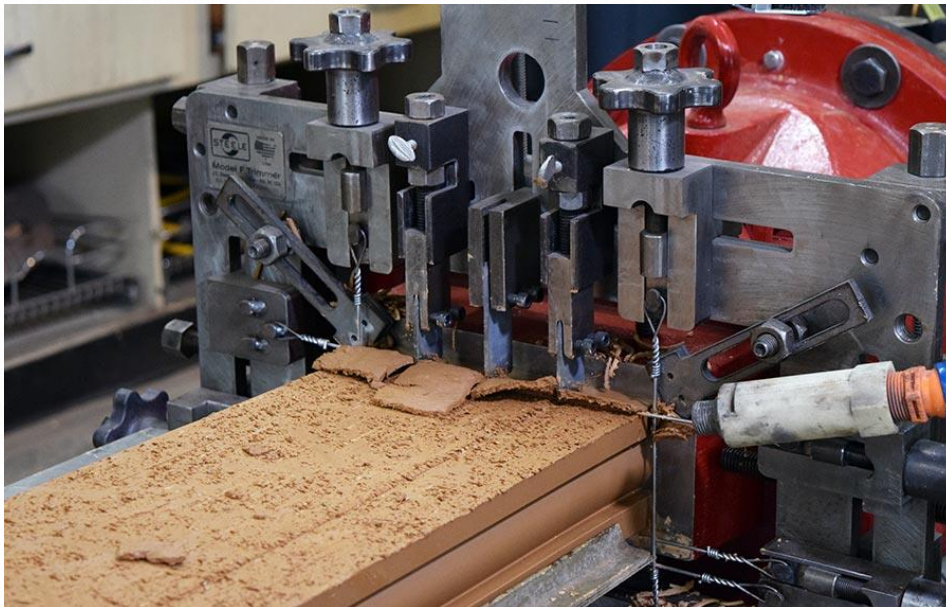
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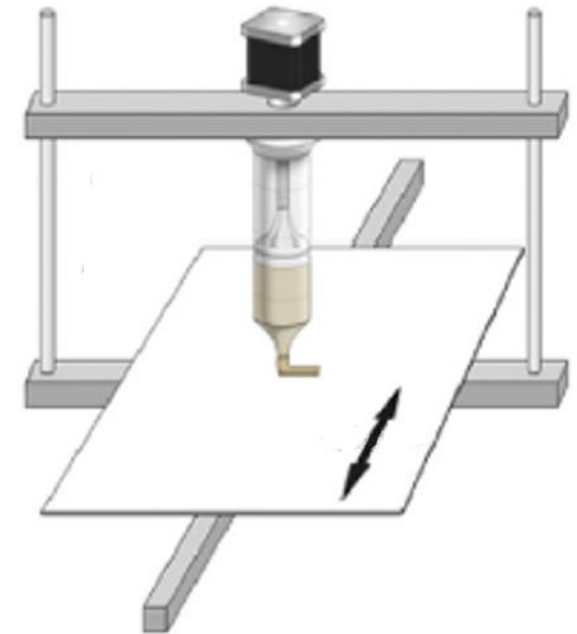
Extrusion Based Additive Manufacturing



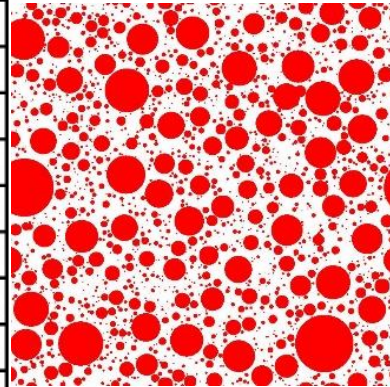
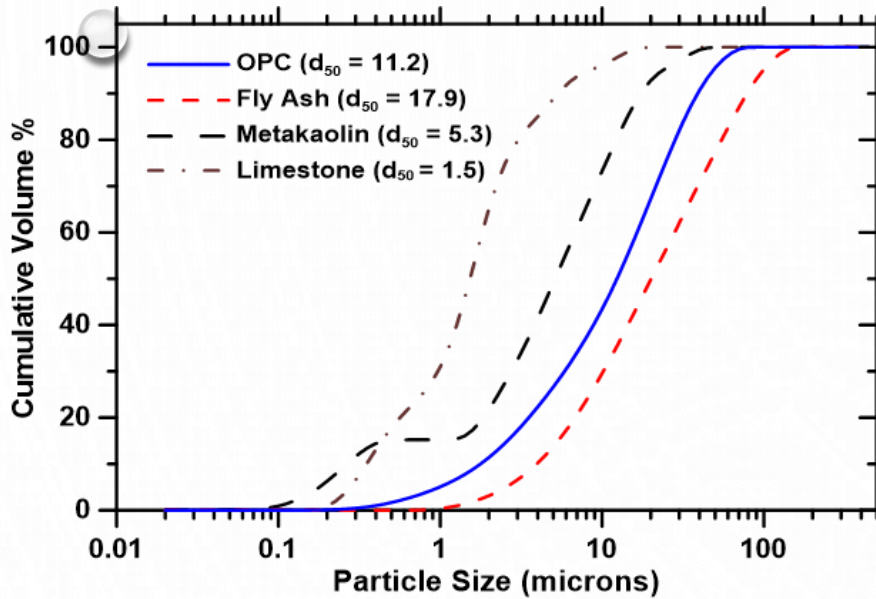


Concrete 3D Printing: Fresh state concerns

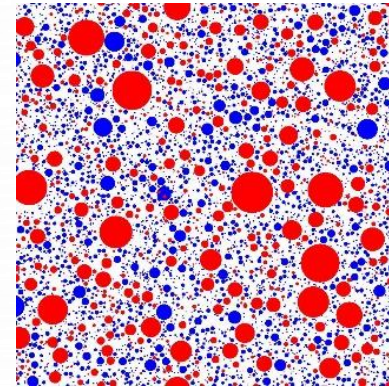
- Extrudability and Buildability (Printability)
- Open time - its influence on pumping and extrusion;
- Setting and layer cycle-time - influence on vertical build rate;
- Deformation, instabilities as successive layers are added;
- Liquid phase migration (LPM)



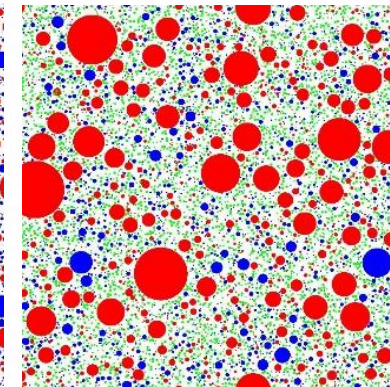
Particle packing effects



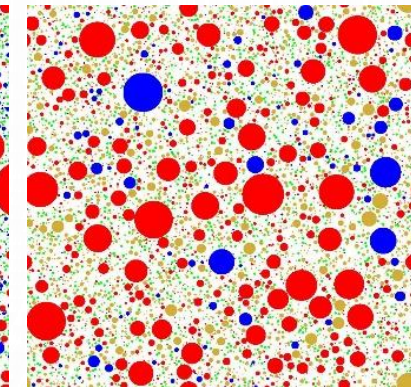
(a)
OPC



(b)
OPC-Ls (70-30)



(c)
OPC-SF-Ls (70-15-15)



(d)
OPC-SF-MK-Ls
(70-5-5-20)

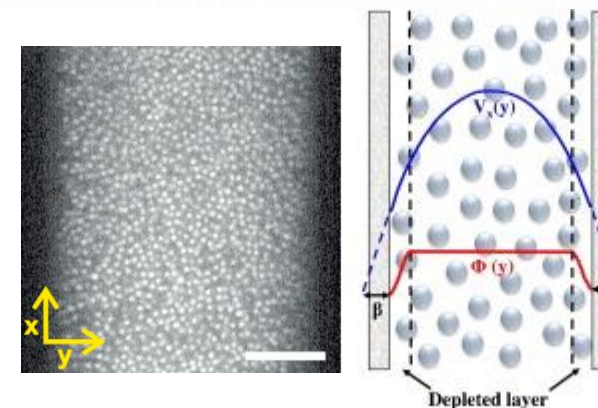
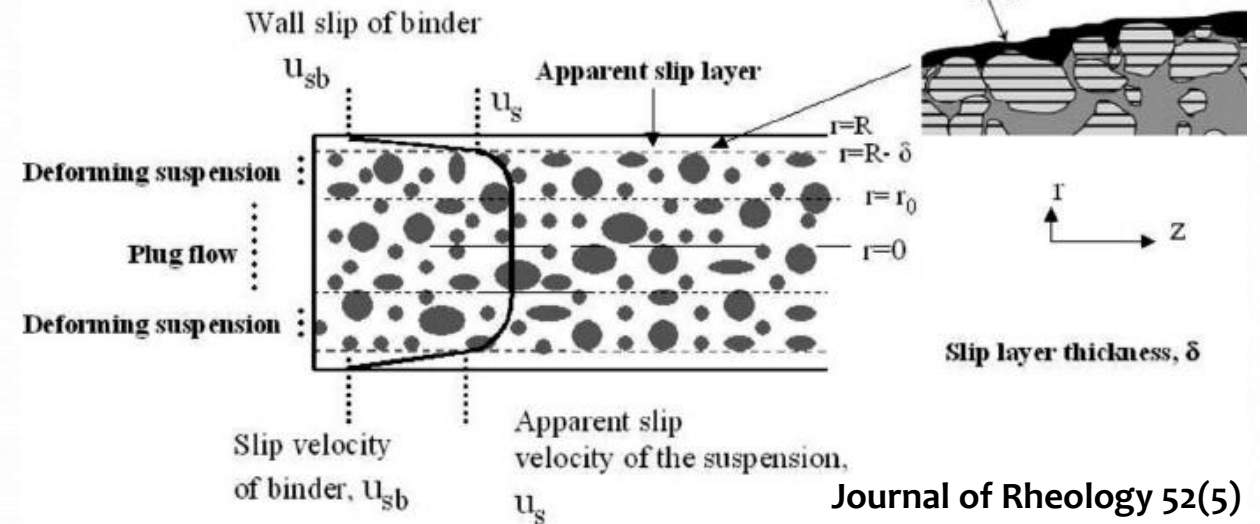
- Particle packing in the microstructure influences printability
- Selection of materials guided by extrudability and the ability to sustain overburden pressure

$$\kappa = \frac{N_d \cdot CN_{avg}}{MCD * 100} \quad (\mu m^{-4})$$

Slip in paste extrusion

- Slip – result of depletion of solid particles from the wall
 - Slip layer (lubrication layer); $V_{\text{liquid}} = 0$
- Particles crowd and lock in place, reducing Brownian motions that disturb the slip layer
 - A function of volume fraction of particles
 - Brownian motion enabled at low volume fractions
 - Importance of microstructural packing
 - Packing factor as a printability design parameter

Journal of American Ceramic Society,
<https://doi.org/10.1111/jace.16305>, 2019



Colloids and Surfaces A: Physicochemical and Engineering Aspects, 491, 2016

Printing of cement-based materials

- Issues with inadequate print quality – fresh state
 - Liquid phase migration under layer built up
 - Inhomogeneous print
 - Insufficient layer stability under overburden pressure



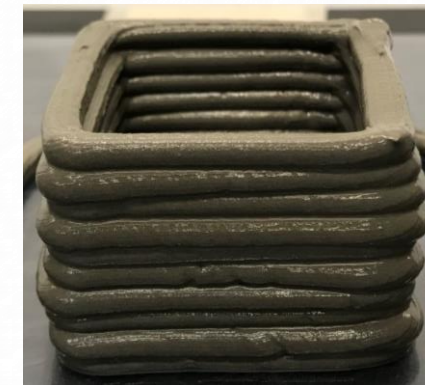
Slumping of printed mixture



Instability issue (warping)



Squeezing of bottom layers



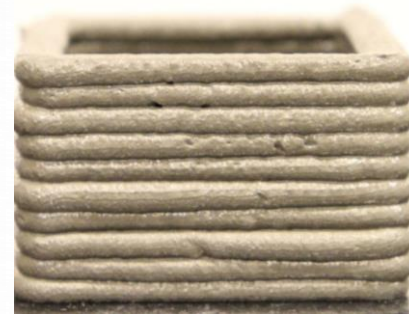
No edge retention

Some of the printable mixtures for model validation

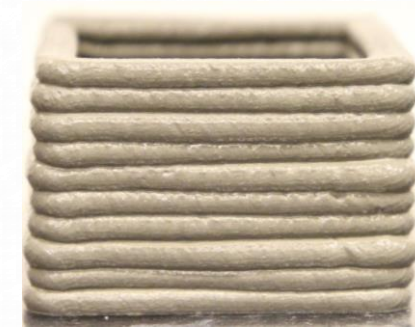
Mixture ID	Mass fraction of ingredients					Water-to-powder ratio (w/p), by mass	Super-plasticizer (% by mass of powder)	Solid volume fraction (ϕ)	Micro-structural index (ϕ/d_{50}^2), $\times 10^3 \mu\text{m}^{-2}$
	OPC	Fly ash (F)	Limestone (L); $d_{50} = 1.5 \mu\text{m}$	Micro-silica (M)	Meta-kaolin (K)				
OPC*	1.0	0	0	0	0	0.32	0	0.403	2.64
F ₃₀ *	0.70	0.30	0	0	0	0.30	0	0.439	2.12
L ₃₀	0.70	0	0.30	0	0	0.41	0	0.324	9.92
L ₁₅ M ₁₅	0.70	0	0.15	0.15	0	0.445	0	0.301	13.83
L ₃₀ -s	0.70	0	0.30	0	0	0.35	0.25	0.382	11.71



70% OPC + 15% SF + 15% LS (1.5 μm)



70% OPC + 10% SF + 10% LS (1.5 μm)

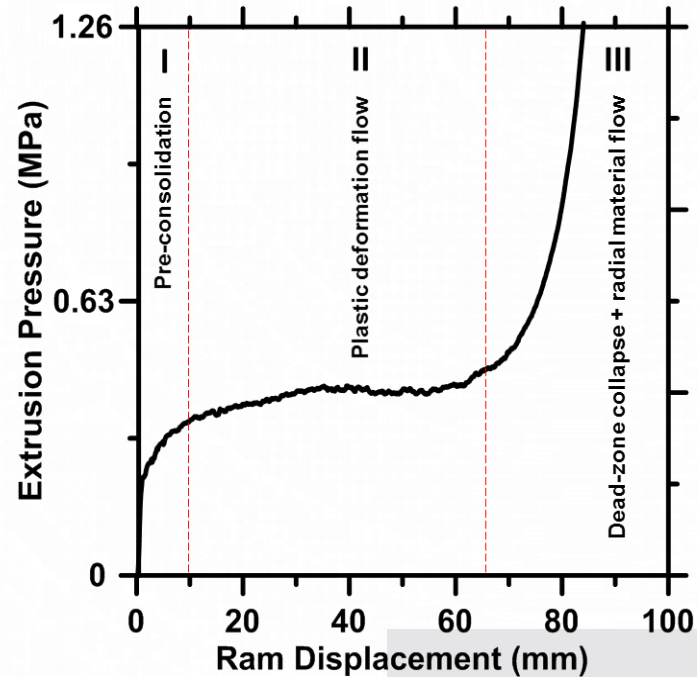
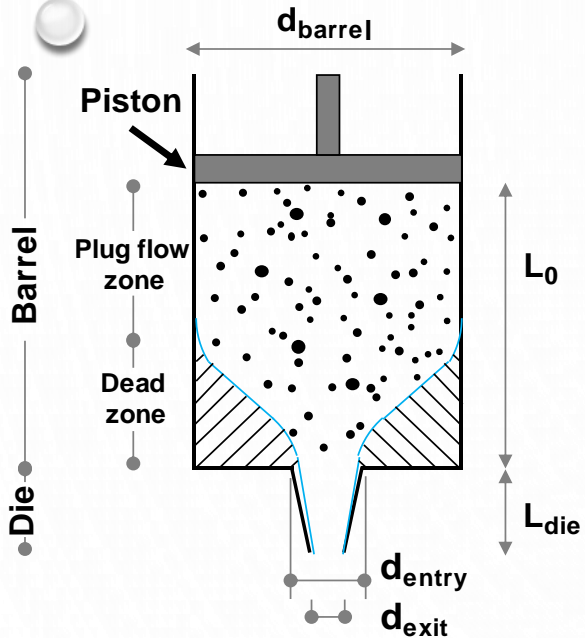


70% OPC + 5% MK + 5% SF + 20% LS (1.5 μm)

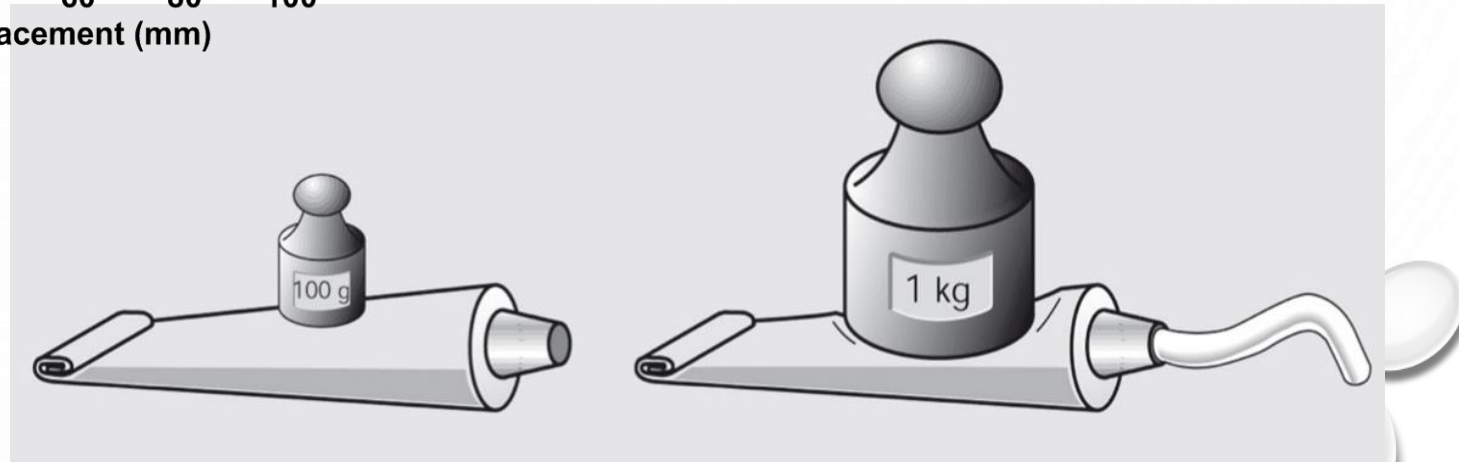
Modeling extrusion printing: Linkages between particle scale effects and processing

- Phenomenological modeling
 - Extrusion pressure linked to pressures in the barrel and the die, and the velocity of extrusion
- Analytical models
 - For frictional plastic materials
- Computational models
 - Discrete element method (DEM) simulations

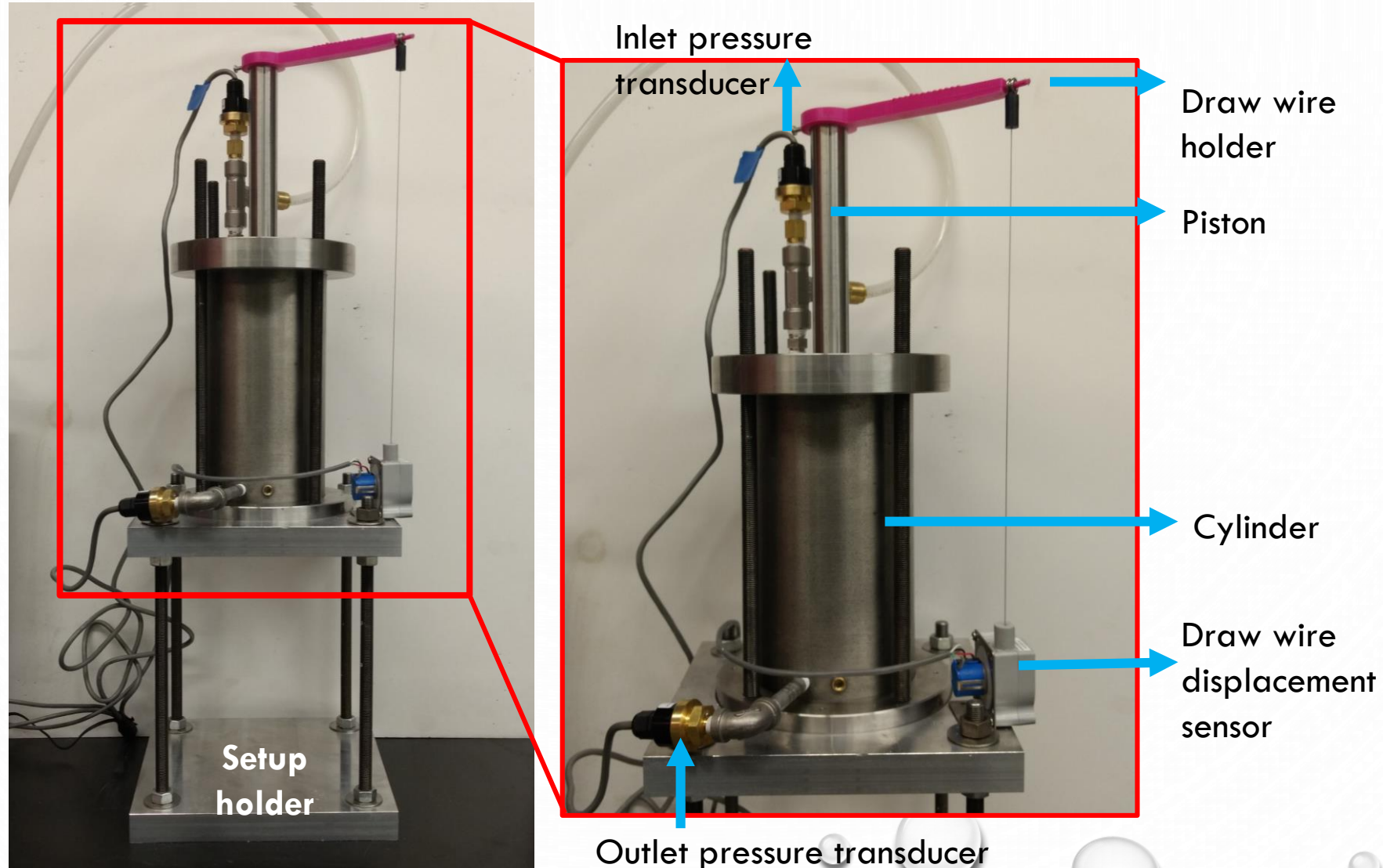
Ram extrusion of cementitious materials



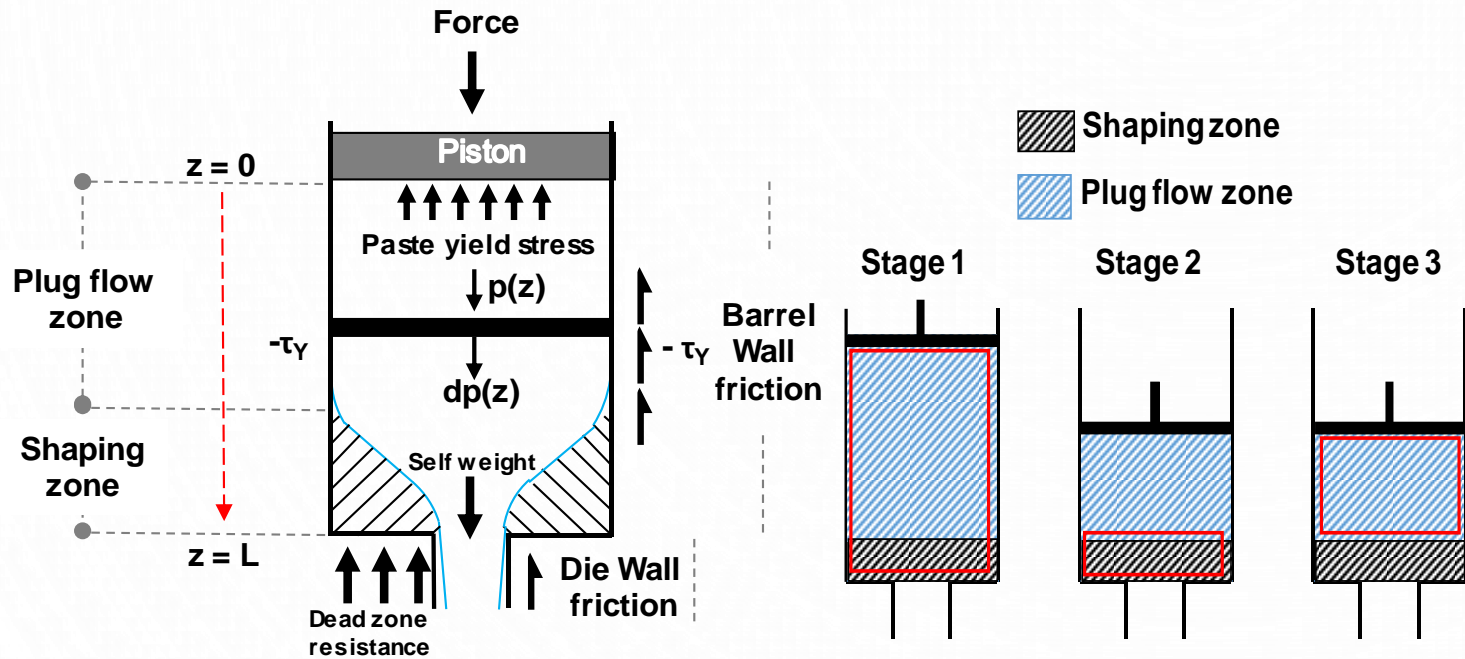
- Pre-consolidation
- Plastic deformation – extrusion flow
- Static “dead zone” region that forms the outer shell for extrusion near the die-entry



Extrusion cell





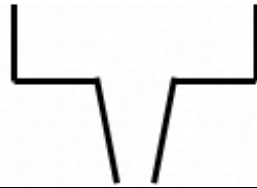
Force Balance



- Stage 1: Both plug flow and shaping zones; plastic and frictional yield stresses constant (do not evolve with axial stress)
- Stages 2 and 3: yield stresses change with particle rearrangement and LPM

Extrusion – Geometric Ratio

$$\psi = \frac{1 + \frac{L_{die}}{d_{exit}}}{\frac{d_{entry}}{D}}$$

Designation and details of die geometries						
Configuration	-	Orifice		Uniform die		Tapered die
Designation	-	O10	O4	N10-10	N4-4	N10-4
Entry diameter, d_{entry}	(mm)	10	4	10	4	10
Exit diameter, d_{exit}	(mm)	-	-	10	4	4
Length of die, L	(mm)	0	0	36	36	36
Geometric ratio, ψ	unitless	3.5	8.75	16.1	87.5	35

Analytical model: Frictional Cohesive Material Model

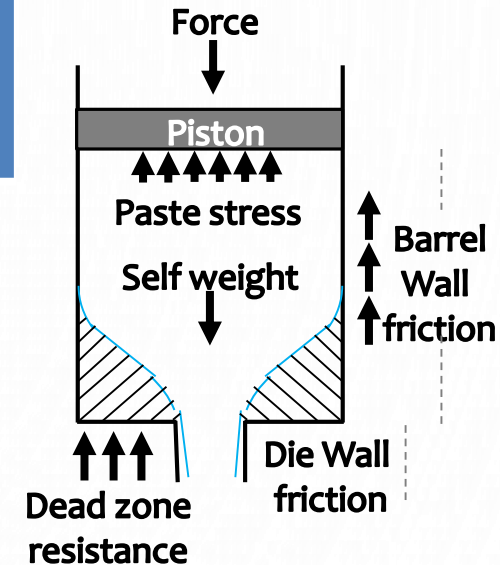
$$p(z) = \gamma \cdot \left(\frac{\alpha \cdot \tau_0}{\beta} e^{4 \frac{\beta z}{d_{barrel}}} \left(e^{4 \frac{\beta z}{d_{barrel}}} - 1 \right) + \sigma_0 \right) + 4 L_{die} \frac{d_{die}}{d_{barrel}^2} \tau_{die}$$

γ - Hill's coefficient
 α, β - Friction parameters

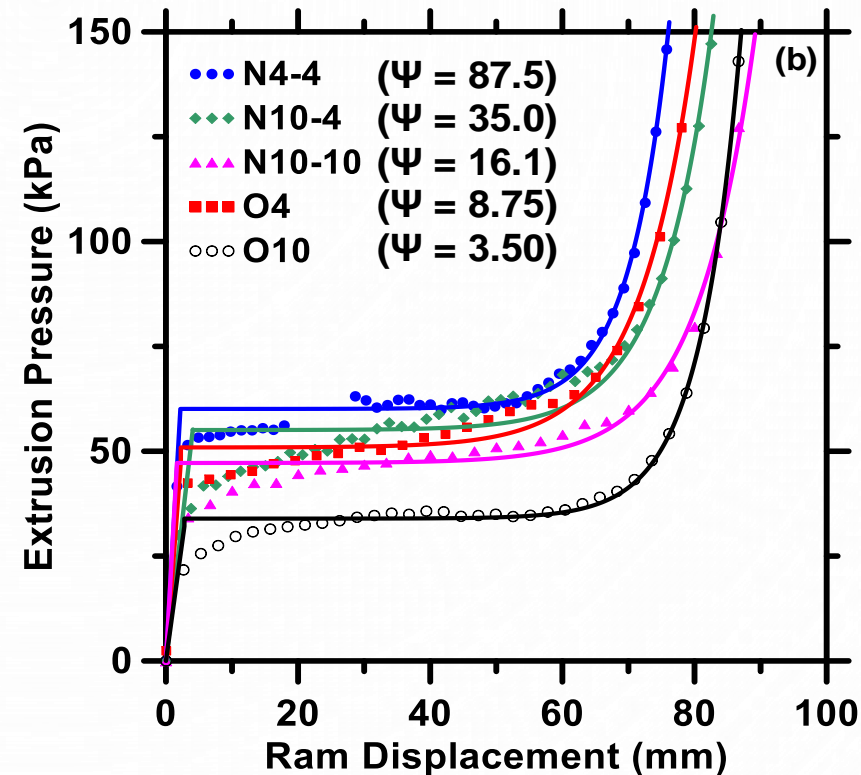
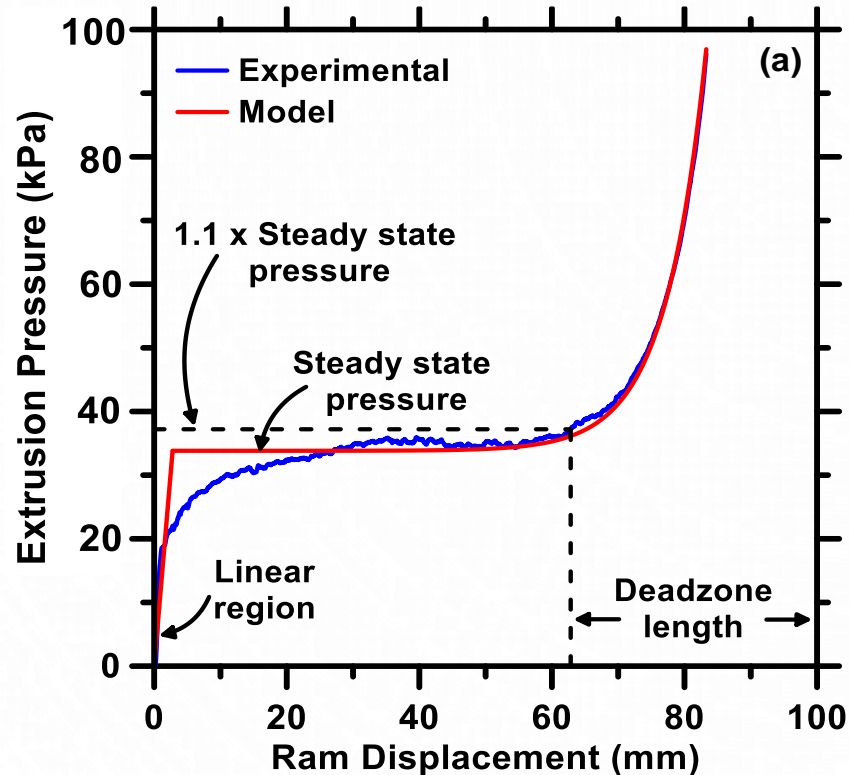
Shaping stress into the die

Shear stress in the die

- Total force expressed as a sum of axial plastic shaping force and a frictional force
- Considering force balance in a strip of paste moving along the barrel under a compressive force



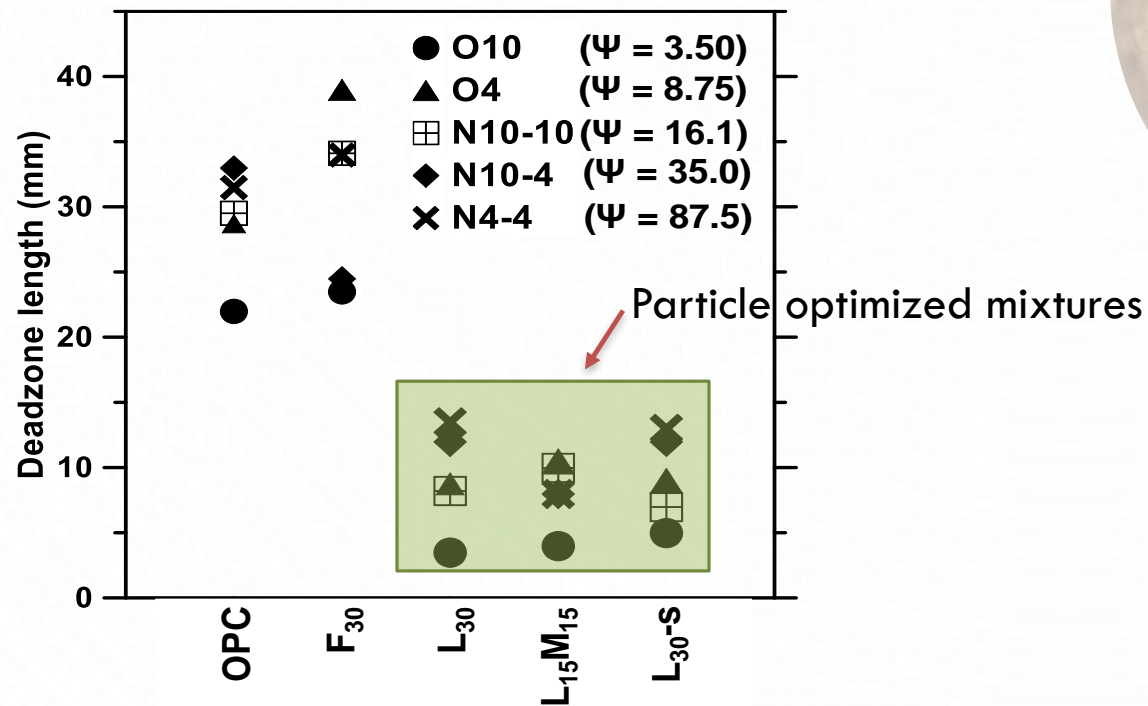
Analytical model – Geometry effects on pressure



- Attempt to link material properties (rheology etc.) to processing parameters (extruder geometry)

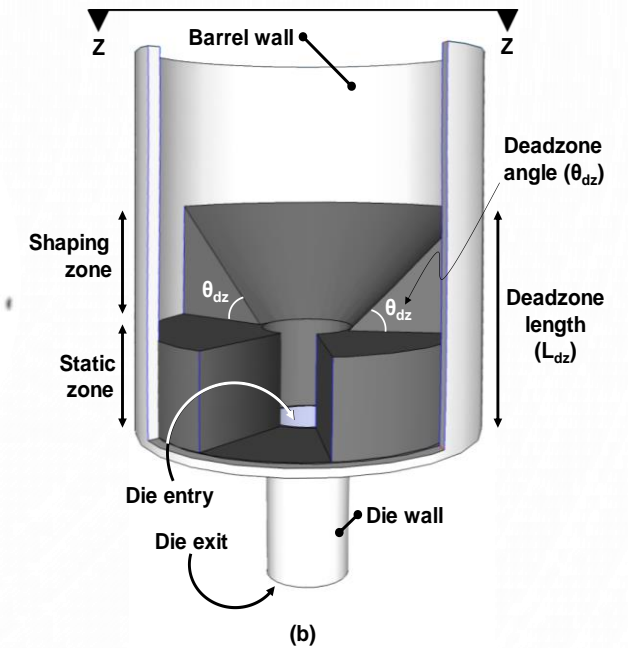
Dead zone formation

- Static zone formed at the bottom of the barrel when material forced under pressure



Section Z-Z

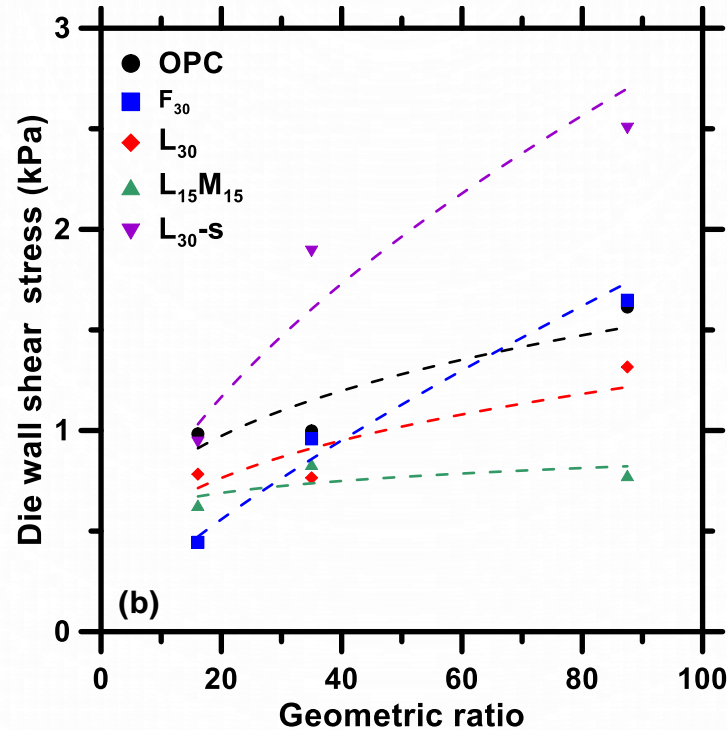
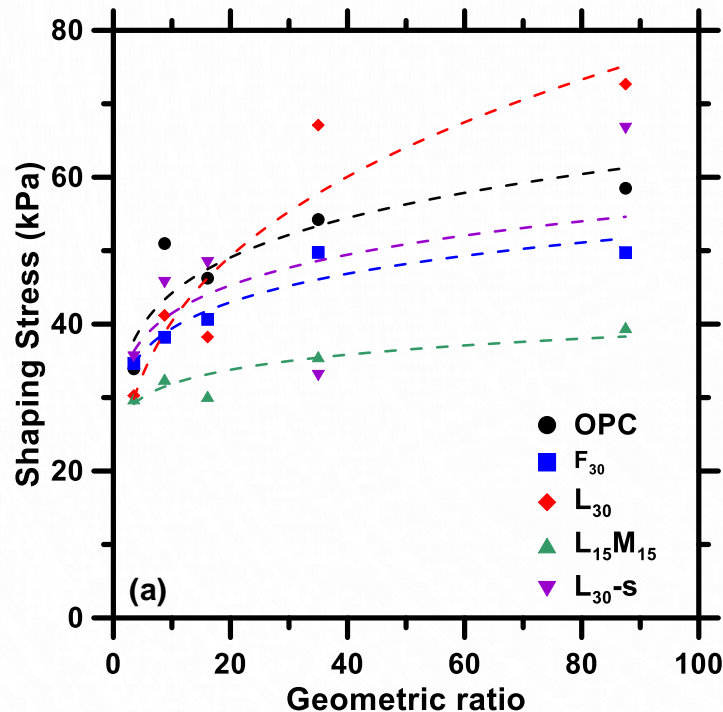
(a)



(b)

- Material does not move in this zone - forms the outer shell for extrusion near the die entry

Shaping stress and wall shear stress

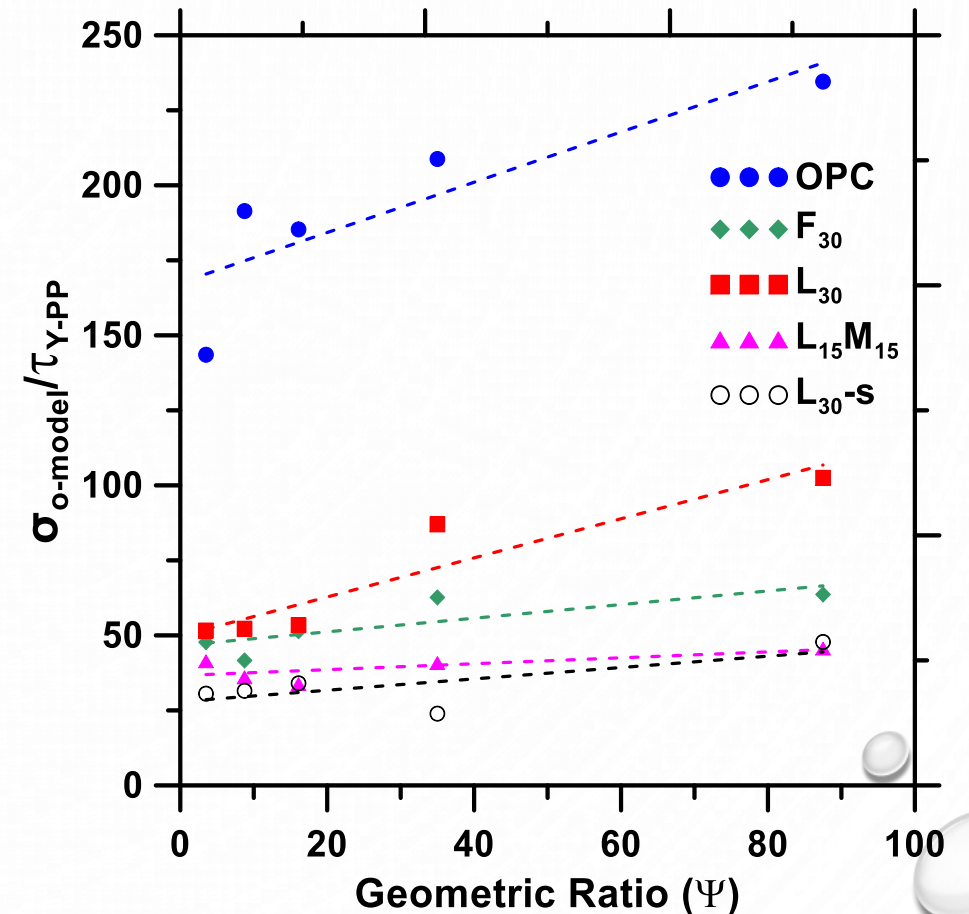


- Stresses tend to plateau out at higher geometric ratios
- Related to the length of dead zone at higher geometric ratios
- Wall shear much lower than shaping stress

- Shaping stress, the controlling geometry-linked design feature, can be predicted

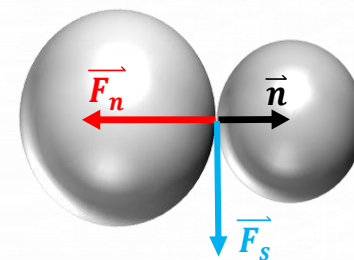
Robustness under extrusion

- Ratio of predicted extrusion yield stress to the measured shear yield stress
- Processed vs. virgin property
- Relationship with geometric ratio shows robustness of mixtures with the best packing

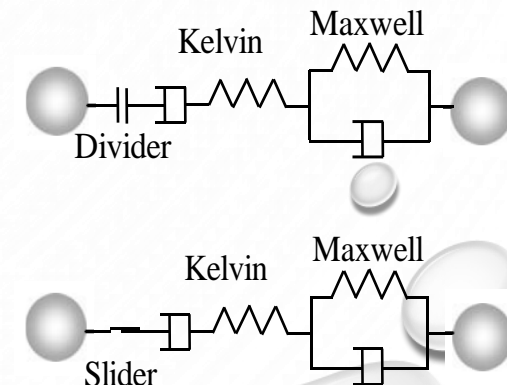


DEM Simulations of Extrusion

- Burger's model is employed to describe the particle-scale contact behavior
- Contains a Kelvin model and a Maxwell model in both normal and shear directions
- Acts over a vanishingly small area and can only transmit force
- Sustains both compressive and tensile forces
- Mohr-Coulomb law limits the shear behavior



Normal
Tangential



Model Description

- Force-displacement equation

$$-f + \left[\frac{C_k}{K_k} + C_m \left(\frac{1}{K_k} + \frac{1}{K_m} \right) \right] \dot{f} + \frac{C_k C_m}{K_k K_m} \ddot{f} = \pm C_m \dot{u} \pm \frac{C_k C_m}{K_k} \ddot{u}$$

- The total displacement u is the sum of the displacement of the Kelvin section (u_k) and Maxwell section (u_{mK} and u_{mC})

$$-u = u_k + u_{mK} + u_{mC}$$

- The force at a given step is determined by a finite difference scheme

$$-f^{t+1} = \pm \frac{1}{C} \left[u^{t+1} - u^t + \left(1 - \frac{B}{A} \right) u_k^t \mp D f^t \right]$$

- The force-displacement law for the Burger's model consists two steps:

- Updating the normal force
- Updating the shear force with the following sequence: (a) update shear force, (b) update shear strength, (c) update the linear shear force and (d) update the slip state

C_k - viscosity of Kelvin section

C_m - viscosity of Maxwell section

K_k - stiffness of Kelvin section

K_m - stiffness of Maxwell section

f - force

u - total displacement

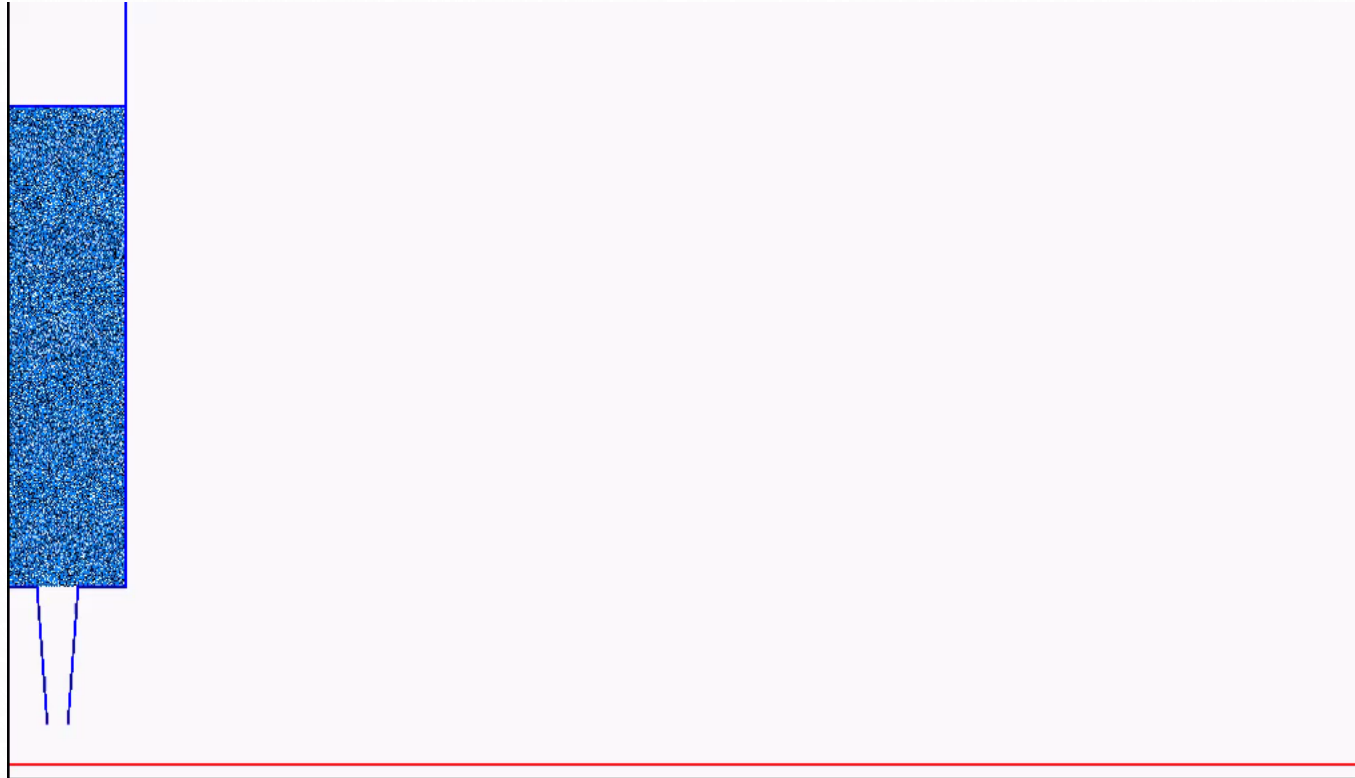
$$A = 1 + \frac{K_k \Delta t}{2C_k}$$

$$B = 1 - \frac{K_k \Delta t}{2C_k}$$

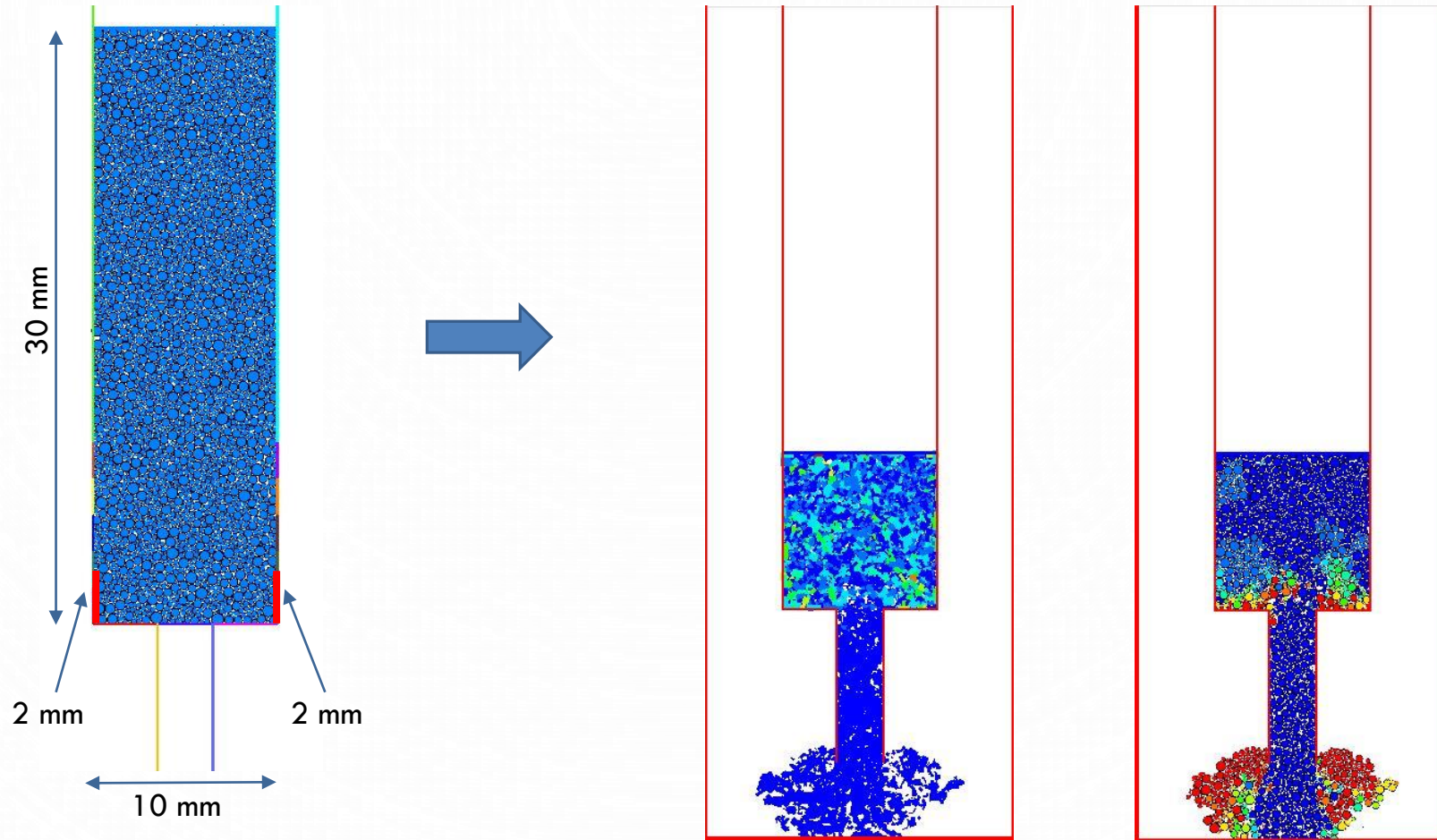
$$C = \frac{\Delta t}{2C_k A} + \frac{1}{K_m} + \frac{\Delta t}{2C_m}$$

$$D = \frac{\Delta t}{2C_k A} - \frac{1}{K_m} + \frac{\Delta t}{2C_m}$$

Simulation of 3D printing



Die entry pressure

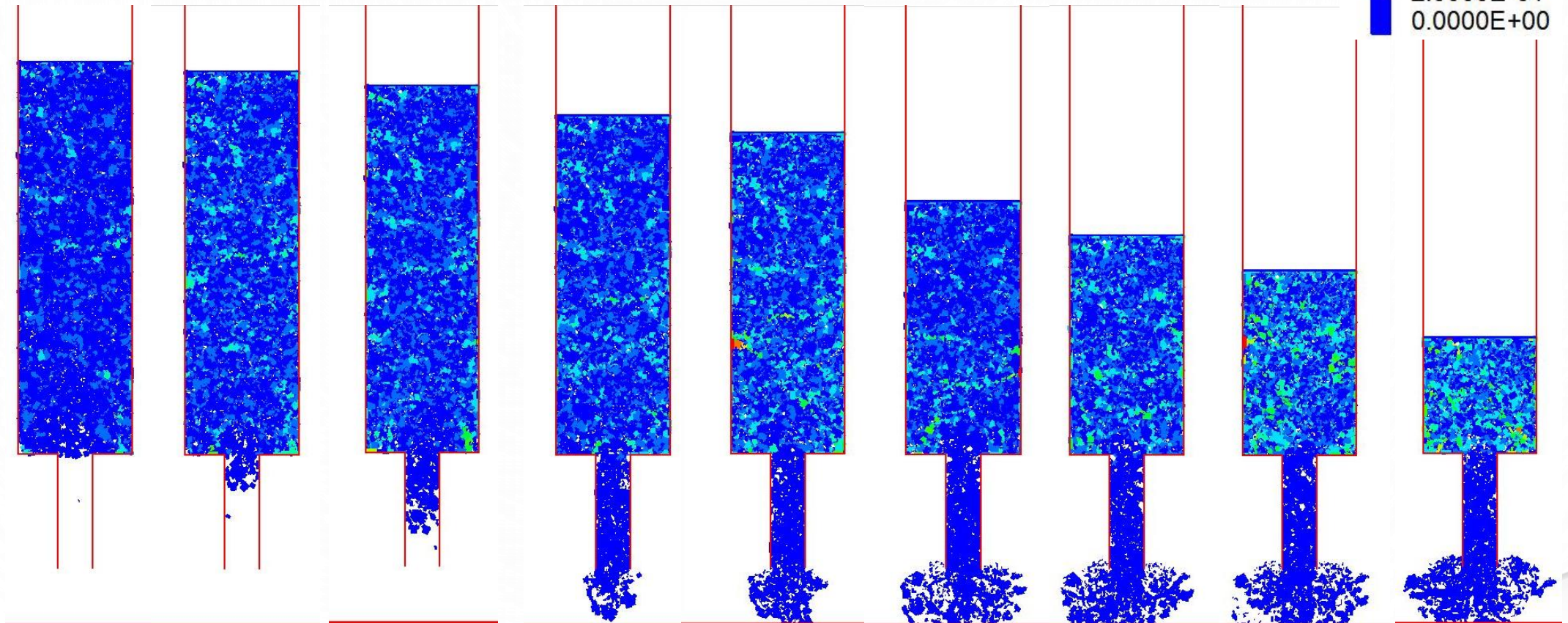
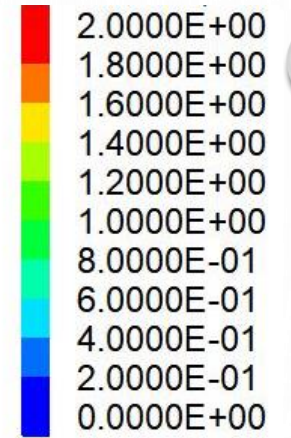


Side walls used to monitor the force

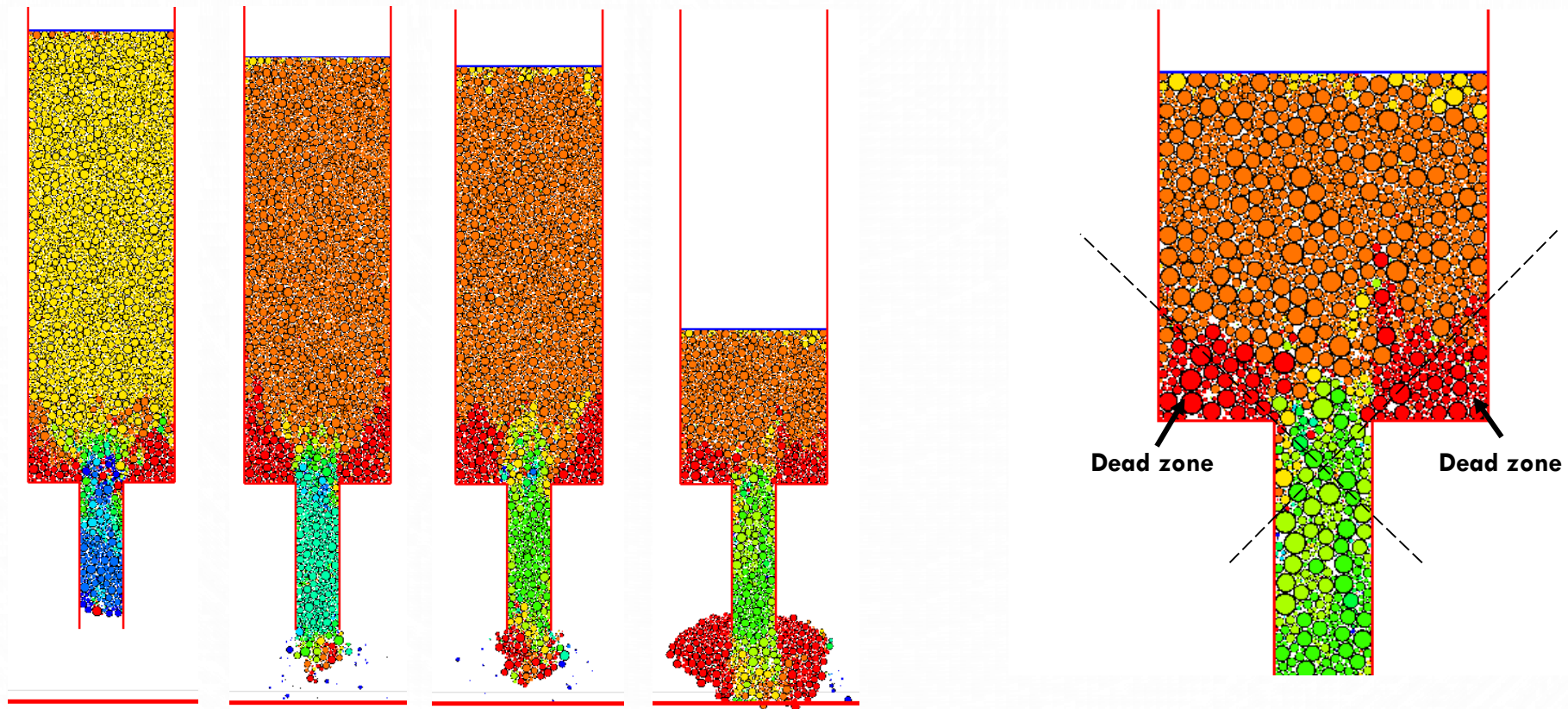
Velocity Evolution



Force Evolution



Dead zone formation



Summary/Conclusions

- Modeling helps to understand the materials-processing linkages better – mixture and process optimization
- Analytical and numerical models accurately capture : (i) the steady state pressure at which extrusion occurs, and (ii) the sudden increase in pressure corresponds to the dead zone
- Steady state pressures can be used to infer the energy required for extrusion-based printing - contributes to the design of appropriate extrusion-based printing systems
- Dead zone lengths decrease with improved microstructural packing and printability
- Dead zone lengths can be used as a convenient metric to evaluate the printability of the mixtures and the quality of the print
- Particle-scale aspects can be captured using the DEM model, to accurately design the material and the printing system

Acknowledgements

