Modeling of Extrusion-Based 3D Printing of Cementitious Materials

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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

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

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

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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

<table>
<thead>
<tr>
<th>Mixture ID</th>
<th>Mass fraction of ingredients</th>
<th>Water-to-powder ratio (w/p), by mass</th>
<th>Superplasticizer (% by mass of powder)</th>
<th>Solid volume fraction (φ)</th>
<th>Microstructural index (φ/d₅₀²) x 10³ μm⁻²</th>
</tr>
</thead>
<tbody>
<tr>
<td>OPC</td>
<td>OPC; Fly ash (F); Limestone (L); d₅₀ = 1.5 µm; Microsilica (M); Metakaolin (K)</td>
<td>0.32</td>
<td>0</td>
<td>0.403</td>
<td>2.64</td>
</tr>
<tr>
<td>F₃₀</td>
<td>0.70</td>
<td>0.30</td>
<td>0</td>
<td>0</td>
<td>0.30</td>
</tr>
<tr>
<td>L₃₀</td>
<td>0.70</td>
<td>0</td>
<td>0</td>
<td>0.41</td>
<td>0</td>
</tr>
<tr>
<td>L₃₀M₁₅</td>
<td>0.70</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.445</td>
</tr>
<tr>
<td>L₃₀₅</td>
<td>0.70</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.35</td>
</tr>
</tbody>
</table>

- **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

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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

\[
\psi = 1 + \frac{L_{\text{die}}}{d_{\text{exit}}} - \frac{d_{\text{entry}}}{D}
\]

<table>
<thead>
<tr>
<th>Designation and details of die geometries</th>
<th>Orifice</th>
<th>Uniform die</th>
<th>Tapered die</th>
</tr>
</thead>
<tbody>
<tr>
<td>Configuration</td>
<td>-</td>
<td>O10</td>
<td>N10-10</td>
</tr>
<tr>
<td>Designation</td>
<td>-</td>
<td>O4</td>
<td>N4-4</td>
</tr>
<tr>
<td>Entry diameter, (d_{\text{entry}}) (mm)</td>
<td>10</td>
<td>4</td>
<td>10</td>
</tr>
<tr>
<td>Exit diameter, (d_{\text{exit}}) (mm)</td>
<td></td>
<td></td>
<td>10</td>
</tr>
<tr>
<td>Length of die, (L) (mm)</td>
<td>0</td>
<td>0</td>
<td>36</td>
</tr>
<tr>
<td>Geometric ratio, (\psi) unitless</td>
<td>3.5</td>
<td>8.75</td>
<td>16.1</td>
</tr>
</tbody>
</table>

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Analytical model: Frictional Cohesive Material Model

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

\( \gamma \) - Hill’s coefficient
\( \alpha, \beta \) - Friction parameters

- 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

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

- Particle optimized mixtures

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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 extrusional 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
Model Description

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

- 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

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\( C_k \) - 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
\( A = 1 + \frac{K_k \Delta t}{2C_k} \)
\( B = 1 - \frac{K_k \Delta t}{2C_k} \)
\( C = \Delta t \left( \frac{1}{2C_k A} + \frac{1}{K_m} + \frac{\Delta t}{2C_m} \right) \)
\( D = \Delta t \left( \frac{1}{2C_k A} - \frac{1}{K_m} + \frac{\Delta t}{2C_m} \right) \)
Simulation of 3D printing
Die entry pressure

Side walls used to monitor the force

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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