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NOMAD XIII Final Presentation

Printability of Particle-Laden Inks

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Org 1556

Presented at the NOMAD XIII Final Presentations on August 4, 2026

U.S. DEPARTMENT of ENERGY NNSA National Nuclear Security Administration

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SAND2026-24726PE

INTRODUCTIONS

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BYU

- PROJECT DESCRIPTION
- EXPERIMENTAL RESULTS
- PARTICLE PACKING SIMULATIONS
- SUSPENSION MODELING
- PRINTING TESTS
- CONCLUSIONS

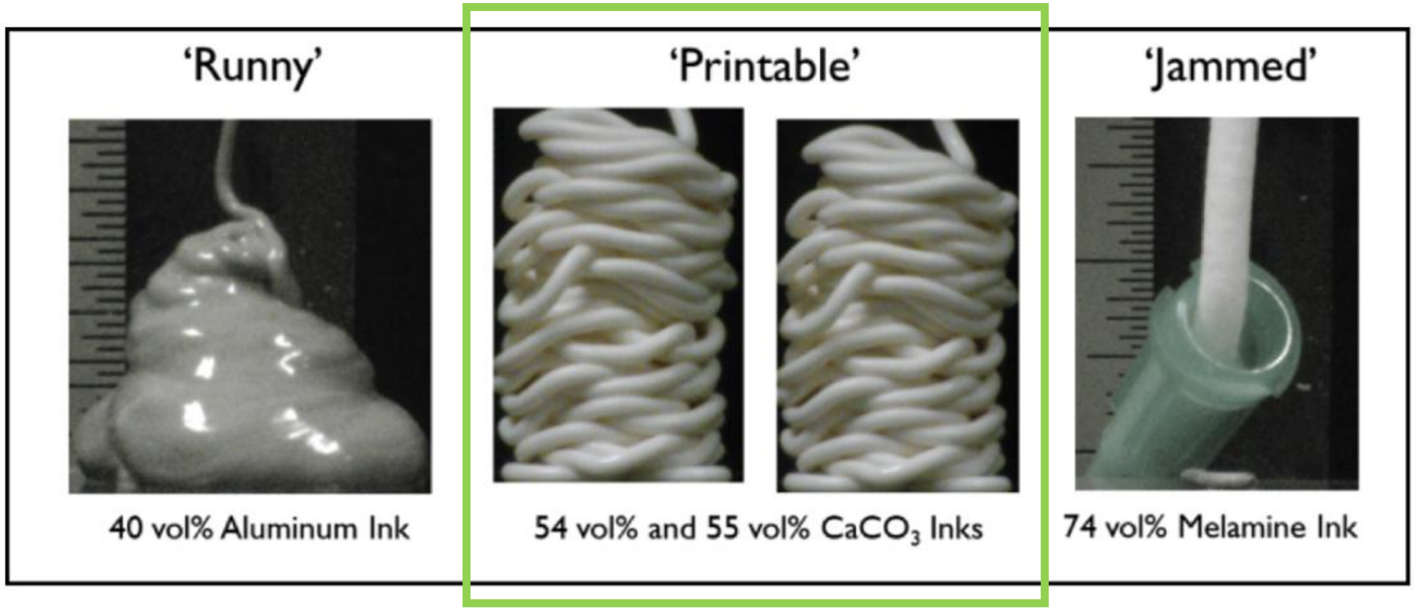
Agenda

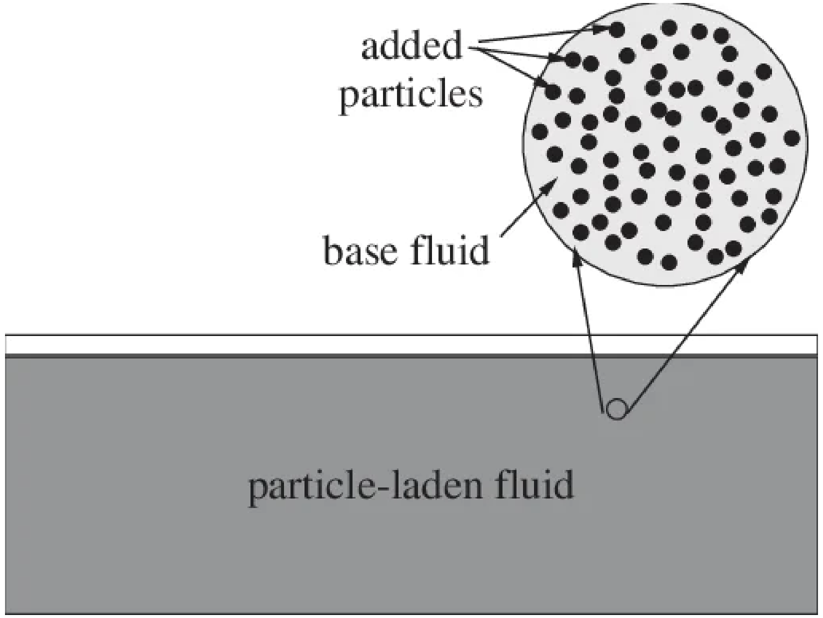
BACKGROUND

Our project addresses the additive manufacturing technique called direct ink write printing.

- 3D printing technique that extrudes ink through a syringe nozzle onto a substrate
- Ink is a complex, shear thinning fluid composed of base (liquid) and filler (solid particles). Inks must hold their original shape after printing
- Shear Thinning: material viscosity decreases as shear stress increases

Inks are characterized as runny, printable, or jammed.



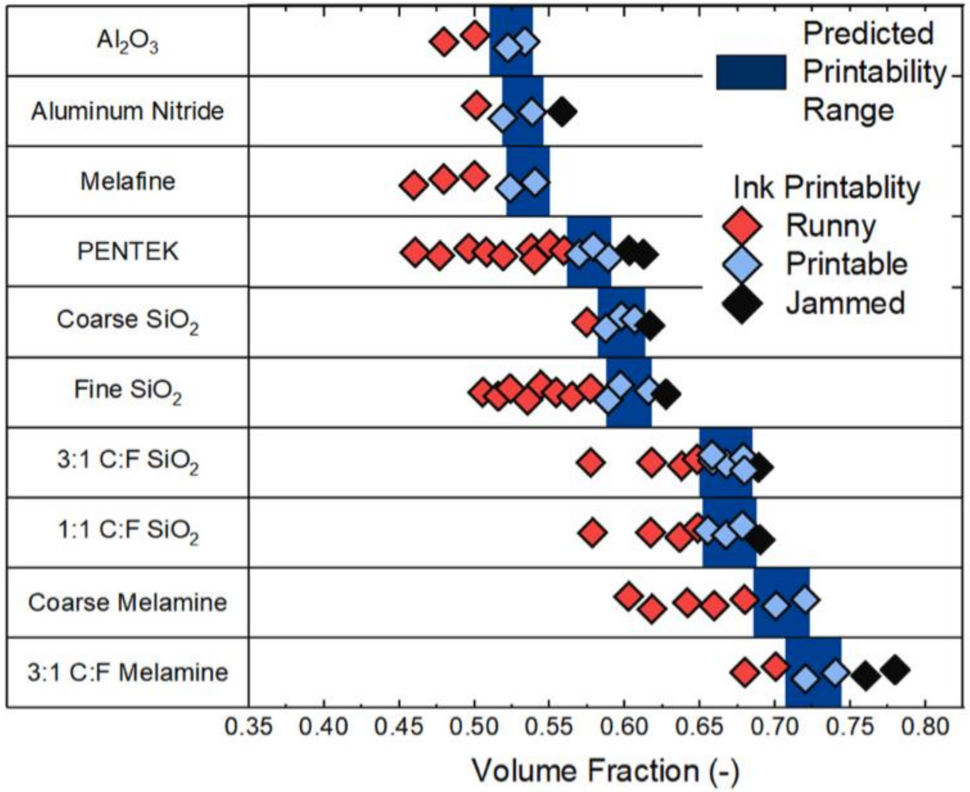


Griebler et al., Additive Manufacturing 99, 104651 (2025); Zohdi, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science. (2018).

BACKGROUND

We can characterize whether inks will be printable or runny using the packing fraction.

- Packing fraction is volume % of mixture that is the filler
- The maximum packing fraction can be determined using particle characteristics
- Inks that are 90%-94% of the max packing fraction are printable



The purpose of this project is to use experimental models to predict the maximum packing fraction and printability region and leverage complementary modeling to provide guidance towards reformulating inks to improve filler particle loading.

Griebler et al., Additive Manufacturing 99, 104651 (2025)

PROJECT OVERVIEW

Experimental

- Characterize particle morphology for materials of interest
- Shear characteristics of different volume fractions using rheology
- Determine maximum packing fraction
- Printability tests

Particle Modeling (LAMMPS)

- Calibrate friction models using experimental maximum packing fraction
- Create capability to analyze any coarse-to-fine particle ratio without mixture morphology

Suspension Modeling (Goma)

- Modeling extrusion of printable ink
- Track particle migration during extrusion using suspension balance models
- Quantify swell of extruded substance using mesh moving algorithm

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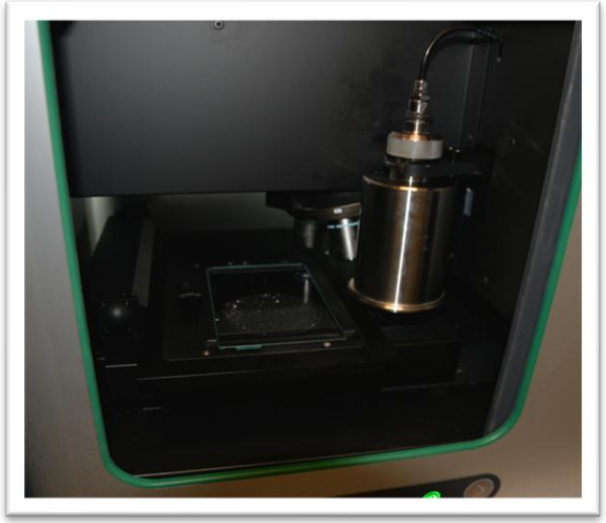
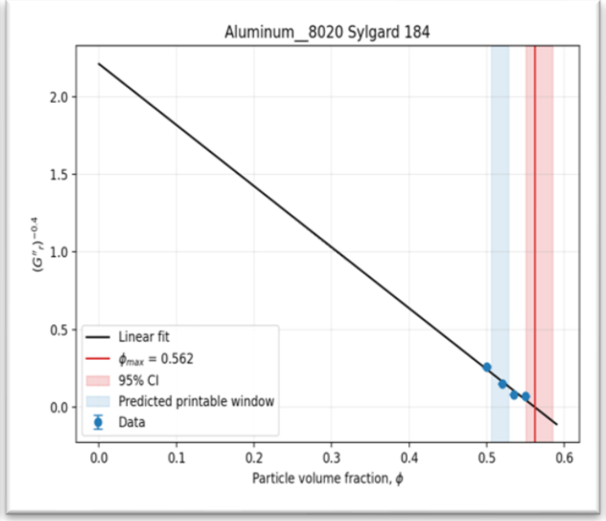
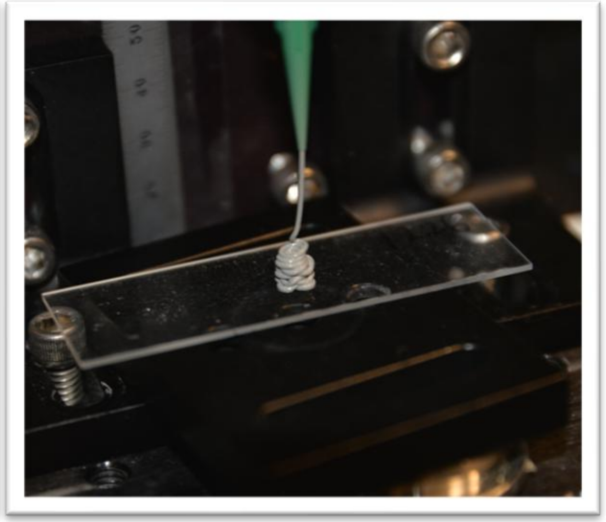
EXPERIMENTAL WORKFLOW

Morphology → Rheology → Data Analysis → Printing







CHARACTERIZING FILLER PARTICLES: MORPHOLOGY

What is Morphology?

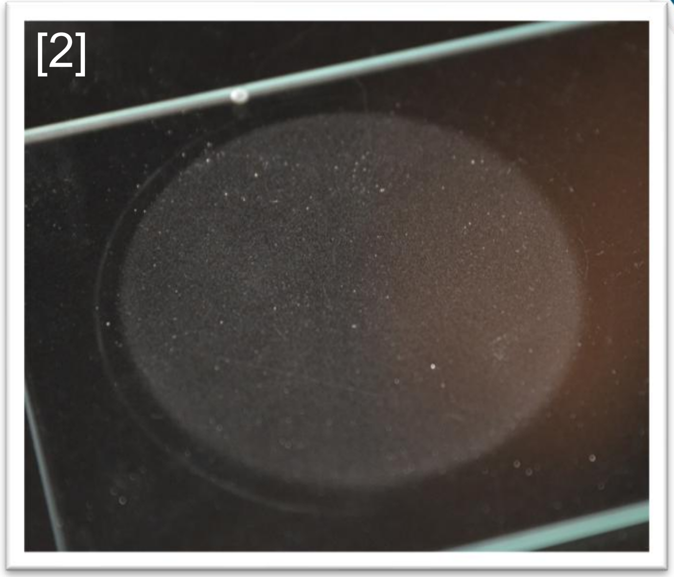
- The study of form and structure
- For this project: the study of particle size, shape, and structure

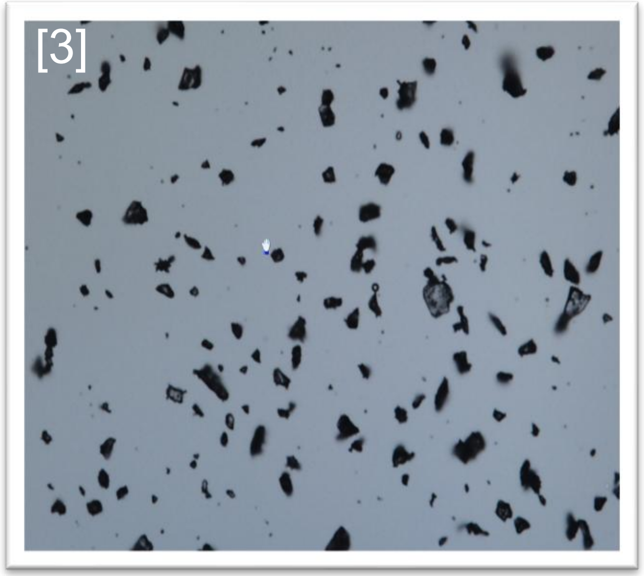
How does this work?

- Use Morphologi 4-ID to characterize each individual particle
- Gain dispersity (σ) and aspect ratio (AR) data
- Plug data into filler characteristics model from literature to calculate maximum packing fraction

$$\phi_{m,\mathrm{FCM}} = 5.95 + 1.897\sigma^2 - 9.04AR + 0.407(\sigma^2)^2$$

$$+3.756AR^2 - 1.409AR\sigma^2$$



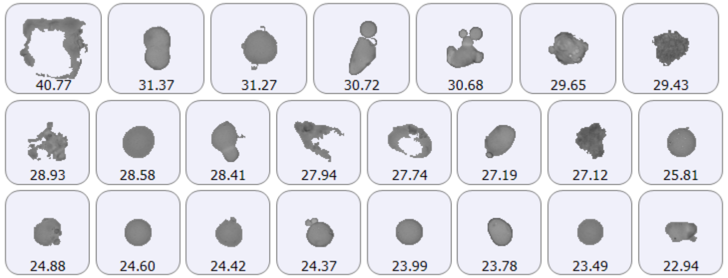


Griebler et al., Additive Manufacturing 99, 104651 (2025)

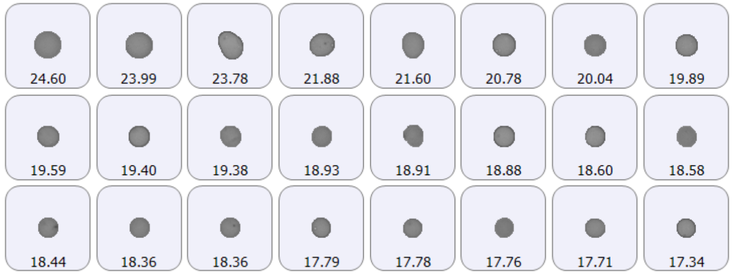
LIMITATIONS IN MORPHOLOGY ANALYSIS

Solidity

- Particles with low solidity usually are overlapping or clumped
- Determined that to be recorded, particles must be >0.9 solidity



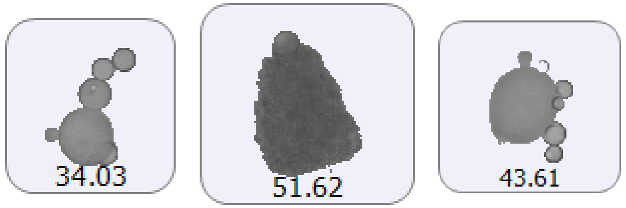
1:1 SiO2 Unfiltered



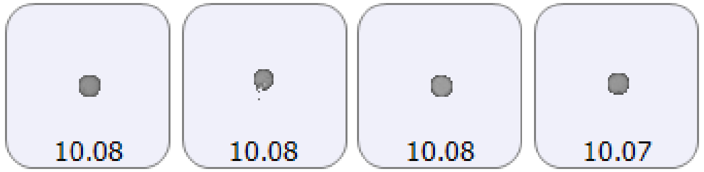
1:1 SiO2 >0.9 Solidity

Circle Equivalent Diameter

- Particles tend to aggregate, leads to diameter readings that are too high
- The particles used are between 1-10um
- Determined that particle diameter must be <15um



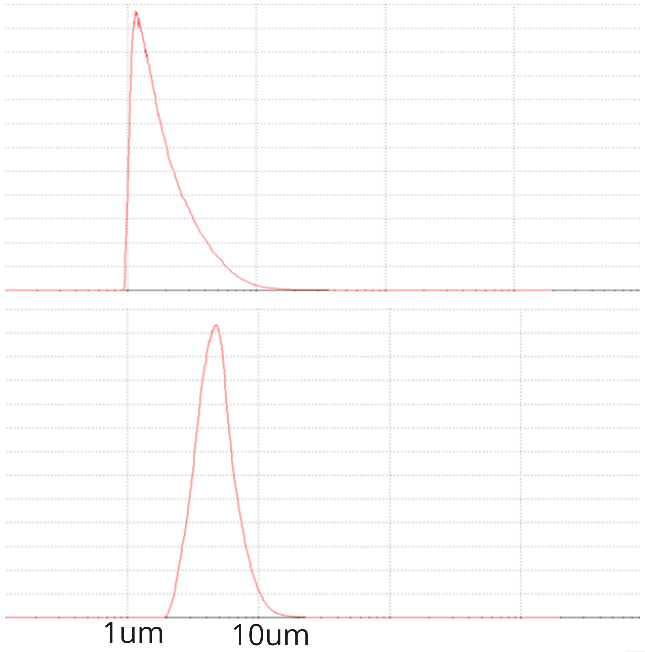
3:1 SiO2 Unfiltered



3:1 SiO2 Filtered

Detection Limit

- Morphologi 4-ID machine cuts off any particles below 1um, causes inaccuracies for smaller particles
- This is an unavoidable systematic error



1um Alumina vs. Molecular Sieves
CE Diameter

Griebler et al., Additive Manufacturing 99, 104651 (2025)

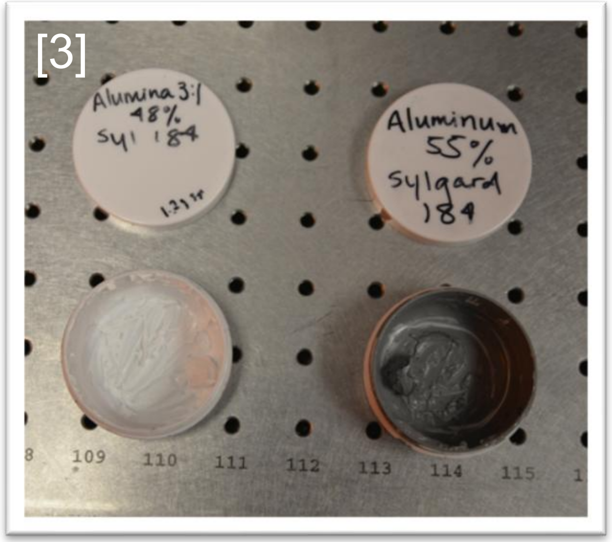
CHARACTERIZING VISCOELASTIC FLUIDS: RHEOLOGY

What is Rheology?

- The study of flow and deformation
- For this project: the study of how each ink mixture deforms during printing

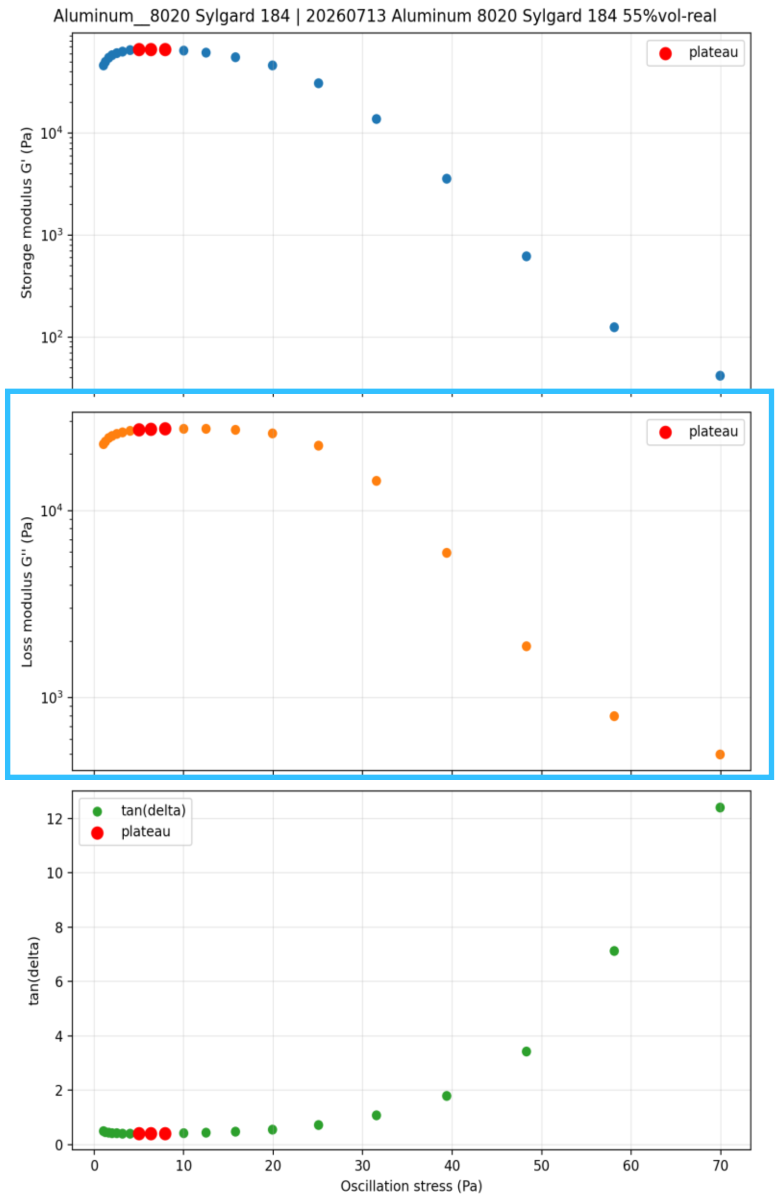
How does this work?

- Particles mixed with Sylgard 184 fluid base
- Small-amplitude oscillatory shear (SAOS) produced by rheometer

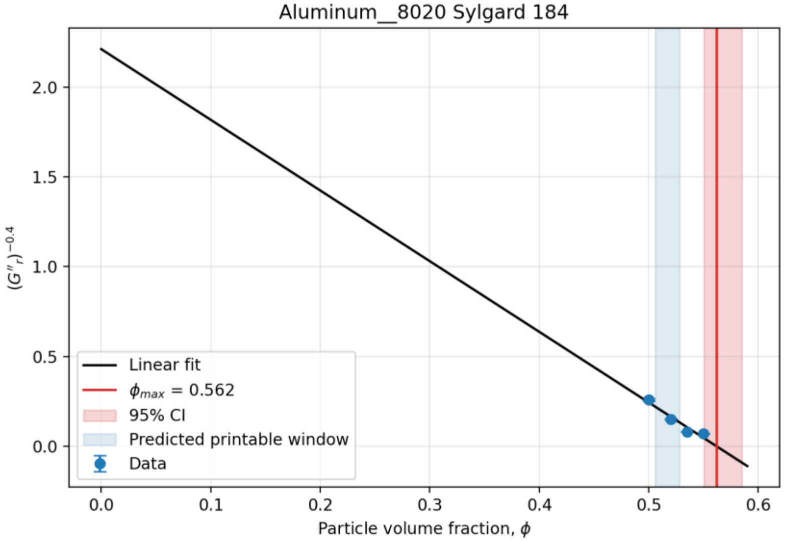


EXTRACTING MAXIMUM PACKING FRACTION FROM RHEOLOGY

- Measure the low-stress oscillatory rheology to obtain:
  - G': Storage Modulus; elastic, solid-like response
  - G": Loss Modulus; viscous, fluid-like response
  - Tan(δ): relative fluidity vs. solidity
  - Axial stress: normal force response
- Identify the linear viscoelastic plateau to obtain G''_{SAOS}
- Normalize loss modulus $G''_r = \dfrac{G''_{\mathrm{SAOS}}}{G''_0}$
- Estimate maximum packing fraction $(G''_r)^{-0.4}$ vs. $\phi \rightarrow \phi_{max}$



Viscoelastic Plateau Python Solver



Maximum Packing Fraction Python Solver

$$G''_{\mathrm{SAOS}} = G''_0 \left(1 - \frac{\phi}{\phi_{max}}\right)^{-2.5\phi_{max}}$$

Krieger-Dougherty Rheology Model

Griebler et al., Additive Manufacturing 99, 104651 (2025)

FROM EXPERIMENTAL RESULTS TO PRINTABILITY PREDICTIONS

Material	Blend	Predicted Morphology ϕ_{max}	Printable Window (90-94%)	Rheology Tested ϕ	Predicted Rheology ϕ_{max}	Printable Window & Error Range
Alumina	Fine (1um)	55.25%	50-52%			
Alumina	Coarse (10um)	67.82%	61-64%			
Alumina	1:1	53.2%	48-50%			
Alumina	3:1	61.34%	55-58%	48%, 50%, 52%, 55%, 57%	59.64%	**53-56%** **50-73%**
Alumina	5:1	57.6%	52-54%			
Alumina	1:3	59.4%	53-56%			
Aluminum	4:1	53.01%	48-50%	50%, 52%, 53.5%, 55%	56.18%	**50-53%** **49-55%**

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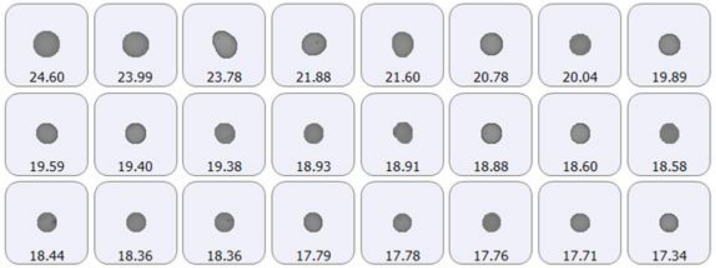
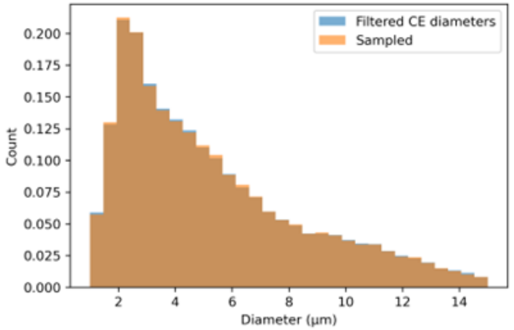
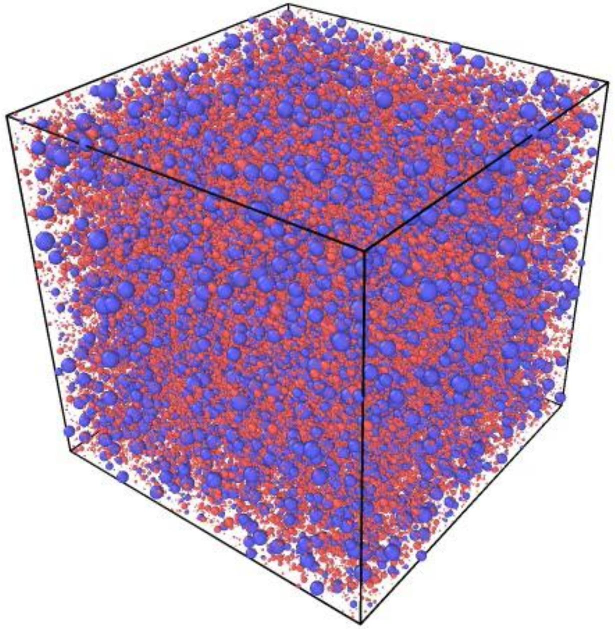
OVERVIEW OF LAMMPS

Morphology

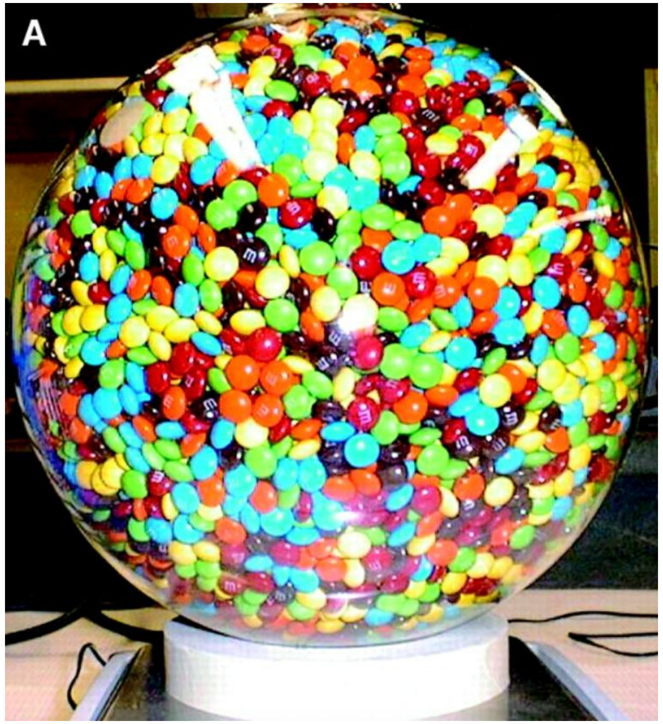




Sampling



LAMMPS



Donev et al., Science 303, 5560 (2004)

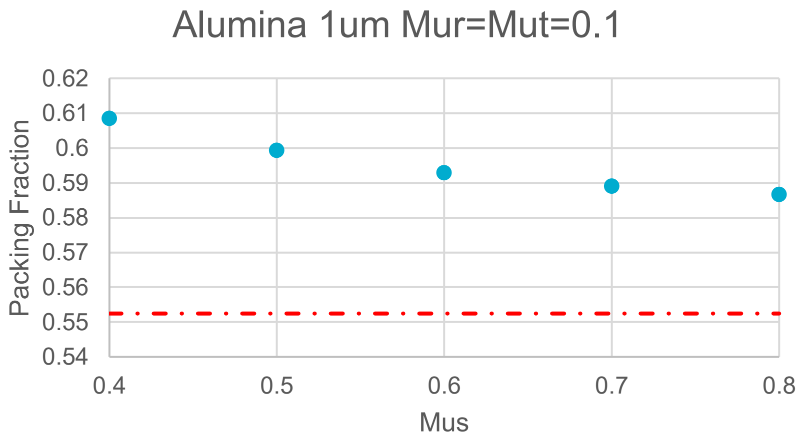
CALIBRATING FRICTION FOR DIFFERENT MATERIALS

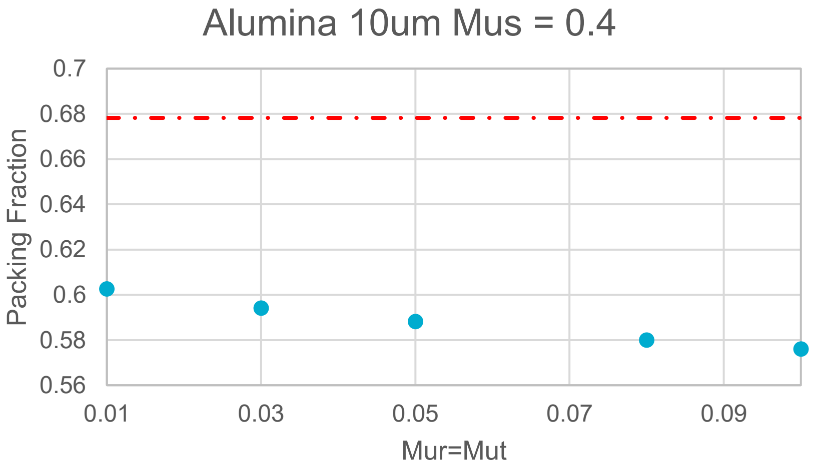
Friction

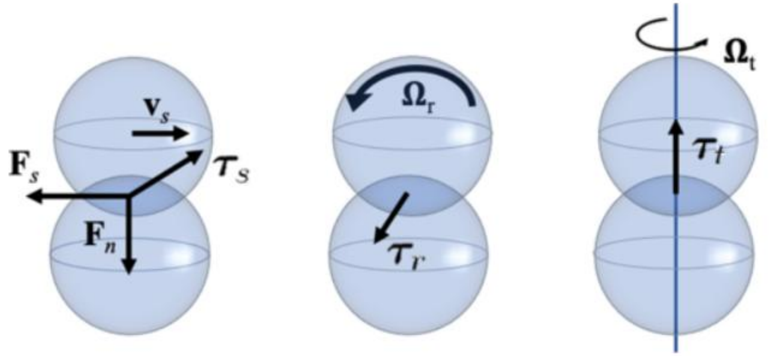
- Sliding, Rolling, Twisting
- Good values for 10um Alumina Found to be 0.01,0.01,0.01
- Good values for 1um Alumina Found to be 0.8, 0.15, 0.15
- Smaller particles are susceptible to aggregation and are irregular shapes

1um Alumina Mus = 0.8, Mur=Mut=0.15	
Data	0.552
Simulated	0.577
Error	4.5%

10 um Alumina Mus = 0.01, Mur=Mut=0.01	
Data	0.678
Simulated	0.663
Error	2.2%



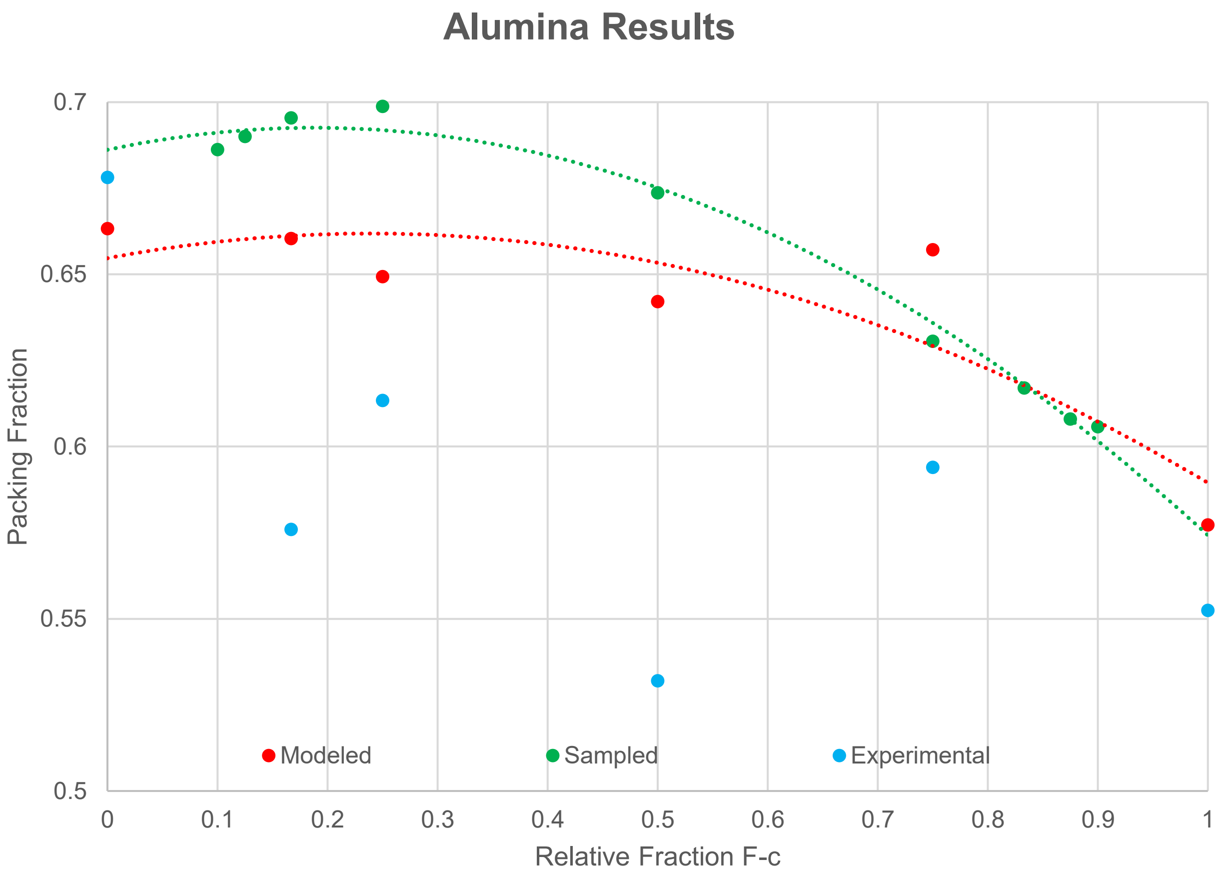




Santos et al., Phys. Rev. E 102, 032903(2020)

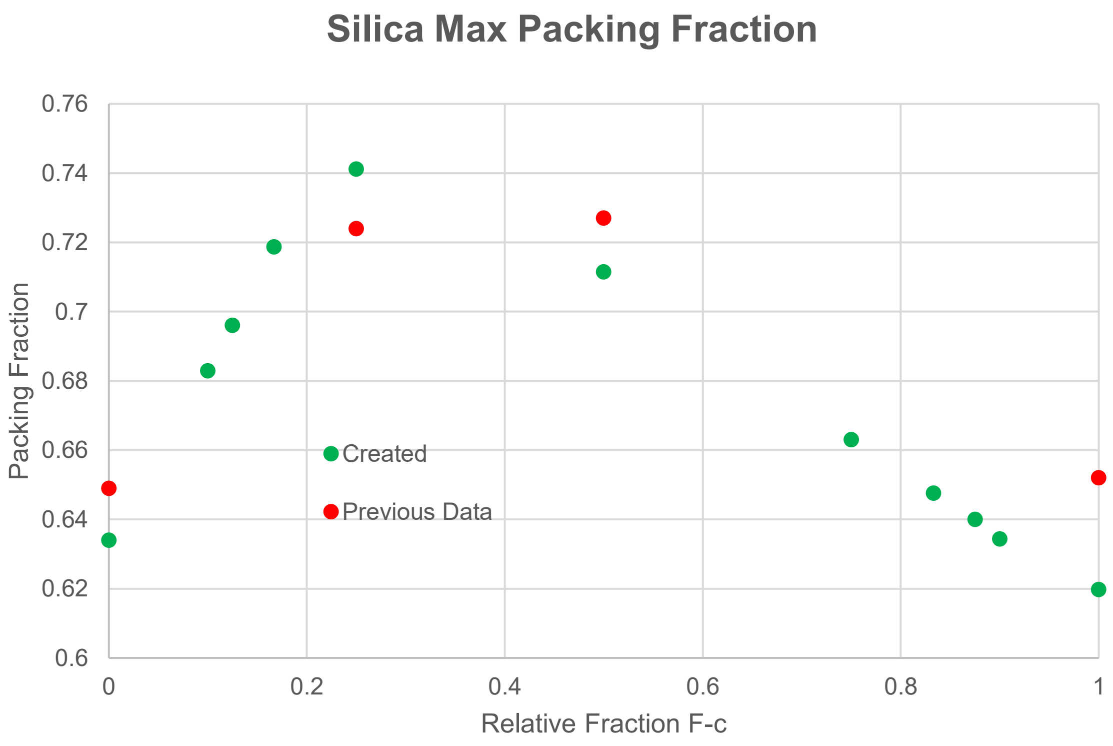
LAMMPS RESULTS

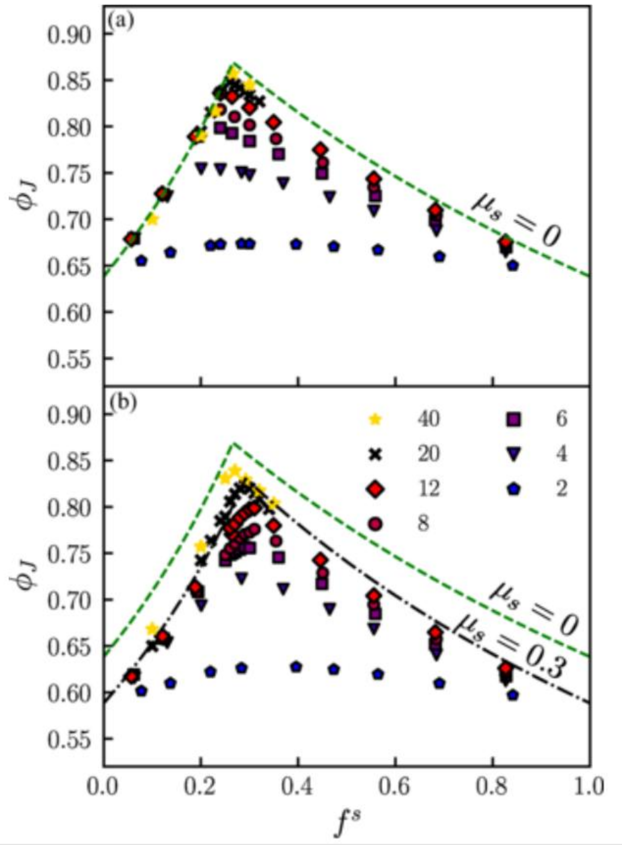
- Predictive part of Project
- Make any ratio we want
  - Cuts down on testing time
  - Friction calibration still needed for each different material
- Large differences between gathered data and when it is simulated. Upwards of 20%
- Created samples still follow expected trend
  - Peaks around 0.25 or a ratio of 3:1 Coarse to fine Alumina



APPLICATION OF LAMMPS TOWARDS OTHER MATERIALS

- Silica results From Created Ratios





The effects of friction on max packing fraction

Griebler et al., Additive Manufacturing 99, 104651 (2025)

Srivastava et al., Phys. Rev. Research 3, L032042, (2021)

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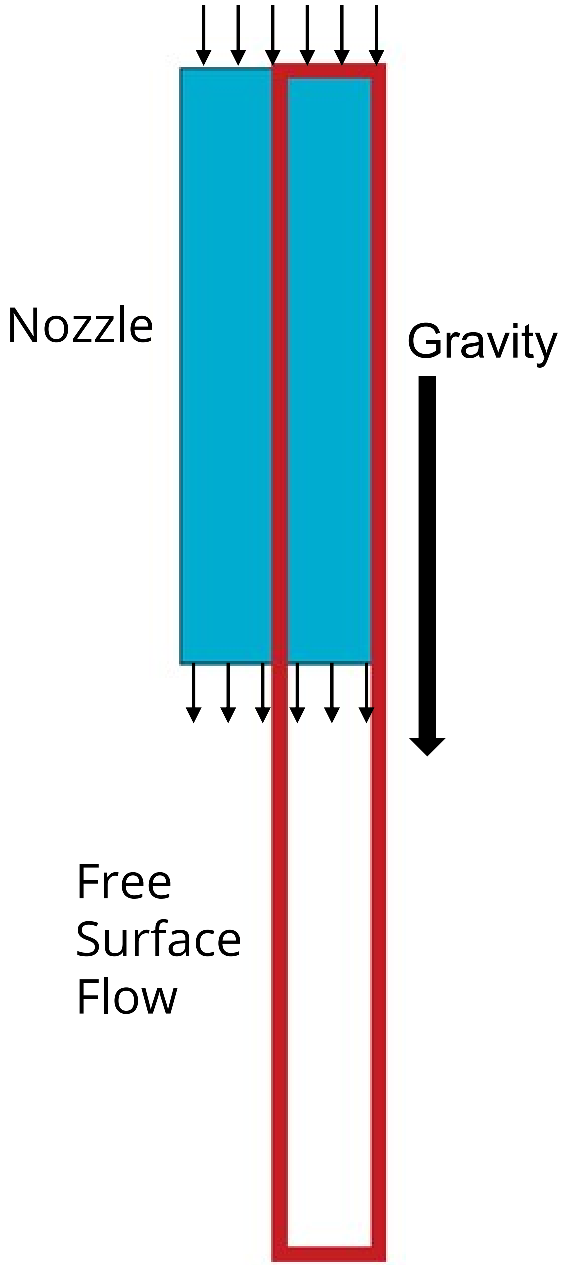
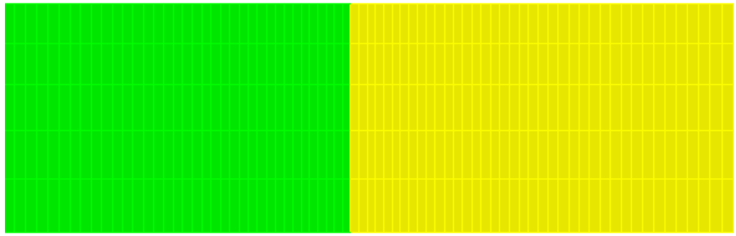
MODEL DESCRIPTION



Mesh Parameters and Boundary Conditions

- Axisymmetric mesh of pipe (3.1 cm length, 0.084 cm diameter)
- Enforce no slip condition on outer wall
- Enforce zero transverse velocity at center line
- Flow pressure (6 MPa) and concentration flux defined at inlet
- Die swell mesh identical to pipe flow portion w/ arbitrary mesh motion

Numerical Setup



- Transient solution
- Backward Euler method
- Steady state solution for Newtonian fluid is initial guess

Material Definition

- Particle diameter and packing fraction from experimental results
- Hydrodynamic diffusivity or suspension balance model
- Suspension liquid constitutive equation

52% ALUMINA 3:1

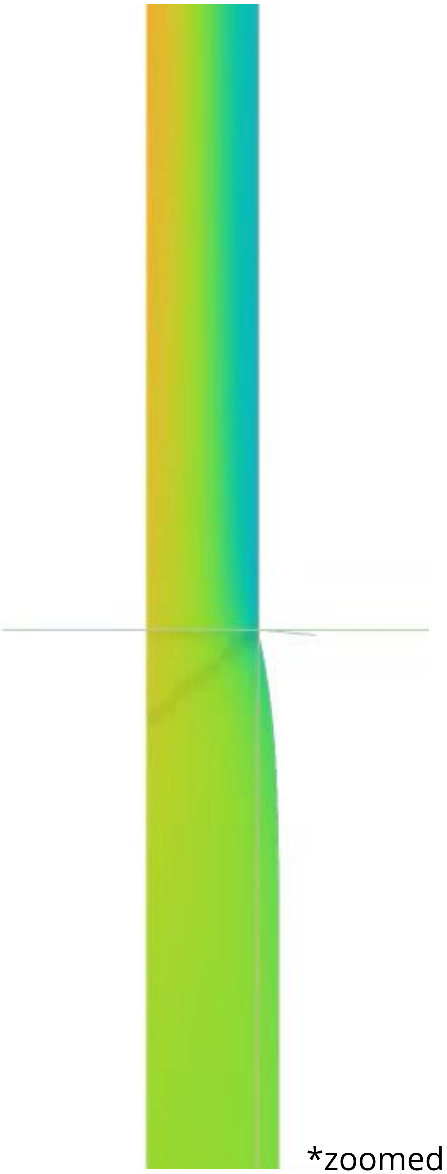
Maximum packing = 59%

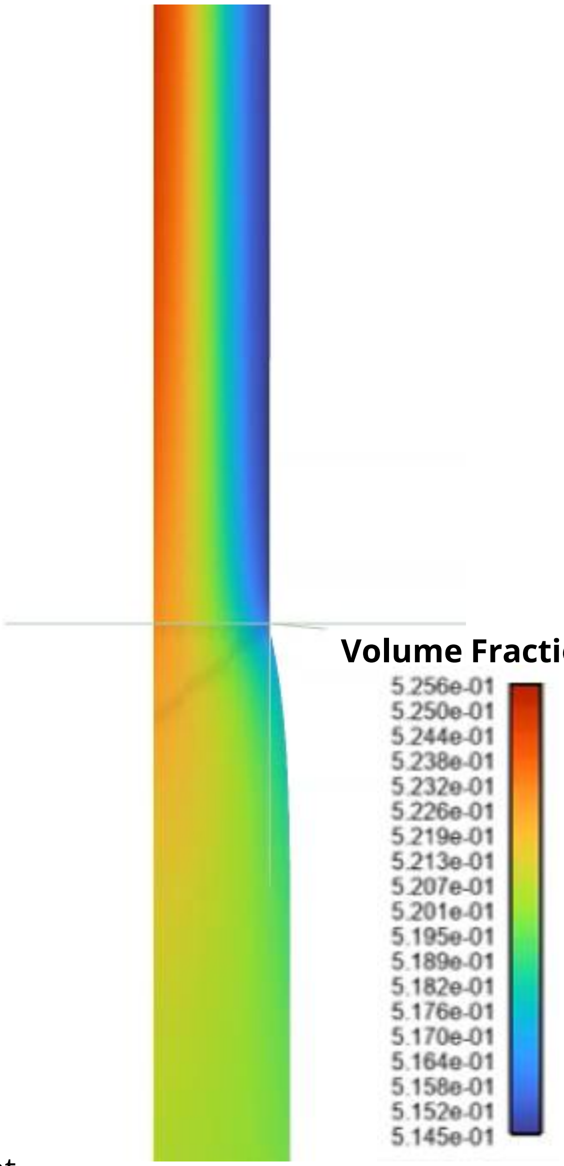
Continuous viscosity = 45750 dyne-sec/cm2

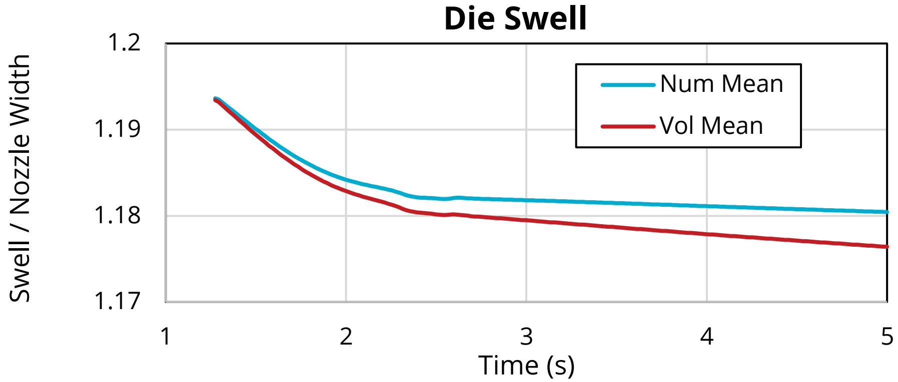
Hydrodynamic diffusivity model

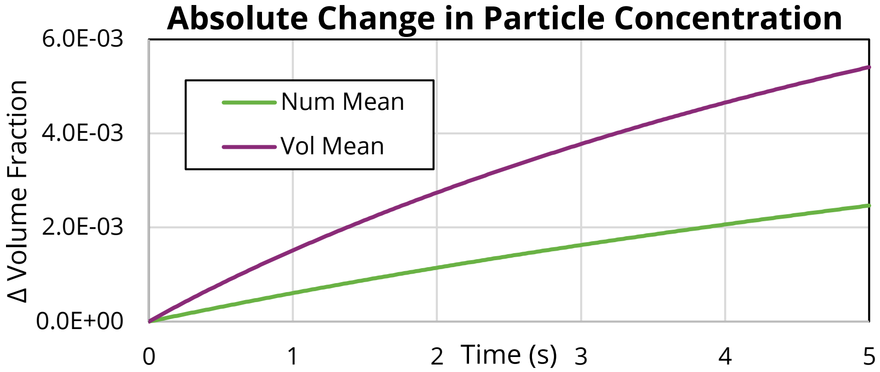
Number Mean Diameter (4.45 µm)

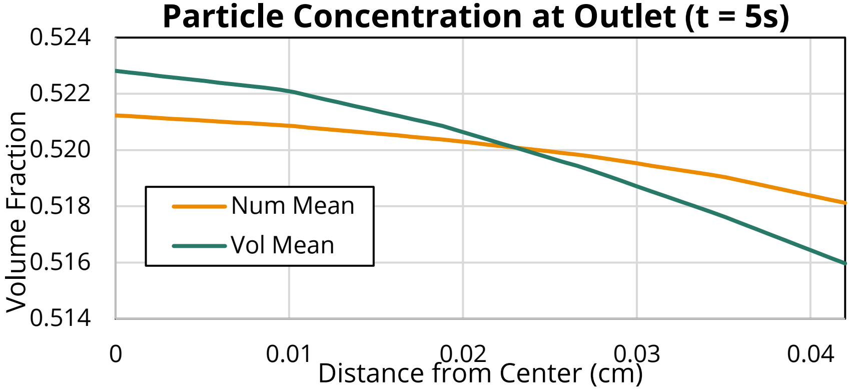
Volume Mean Diameter (7.39 µm)











*zoomed in at nozzle outlet

52% ALUMINA 3:1

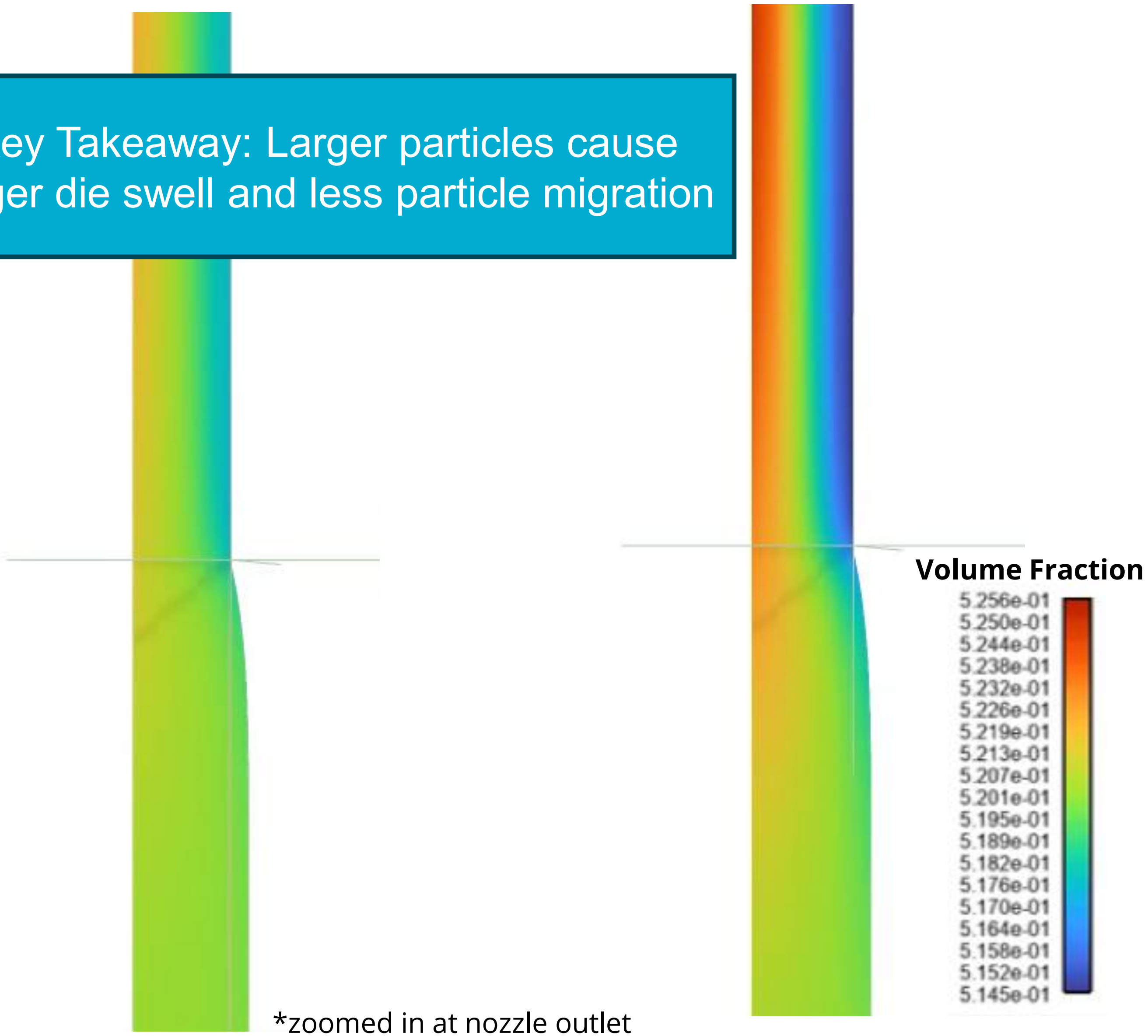
Number Mean Diameter (4.45 μm) Volume Mean Diameter (7.39 μm)

Maximum packing = 59%

Continuous viscosity = 45750 dyne-sec/cm2

Hydrodynamic diffusivity model

Key Takeaway: Larger particles cause larger die swell and less particle migration



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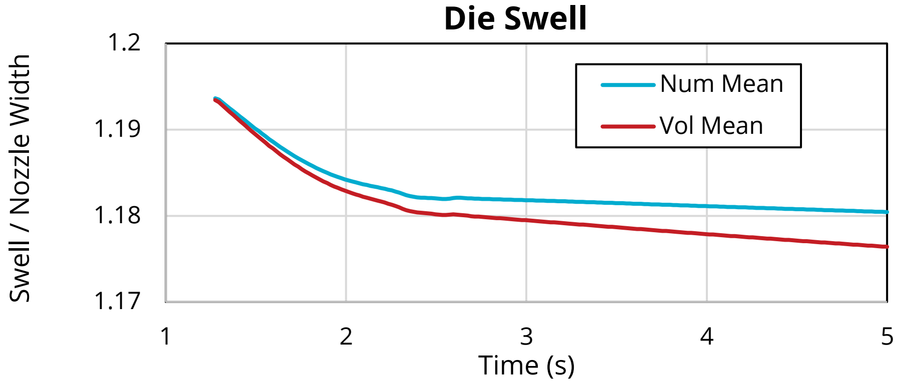
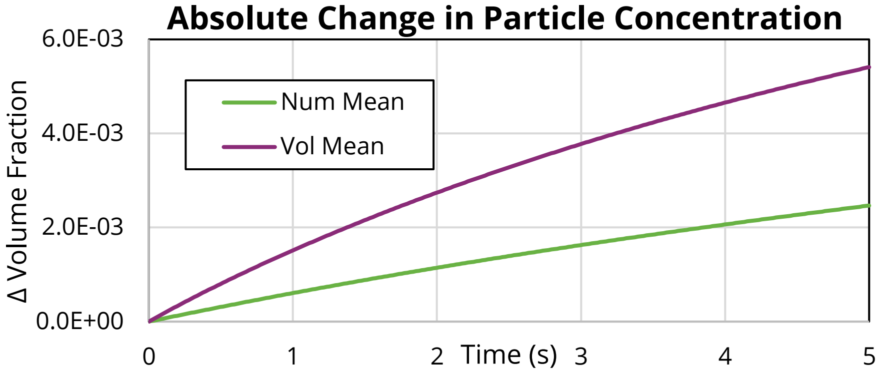
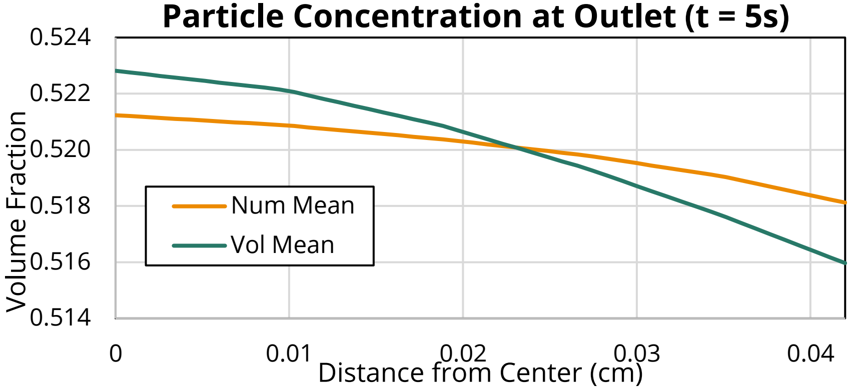






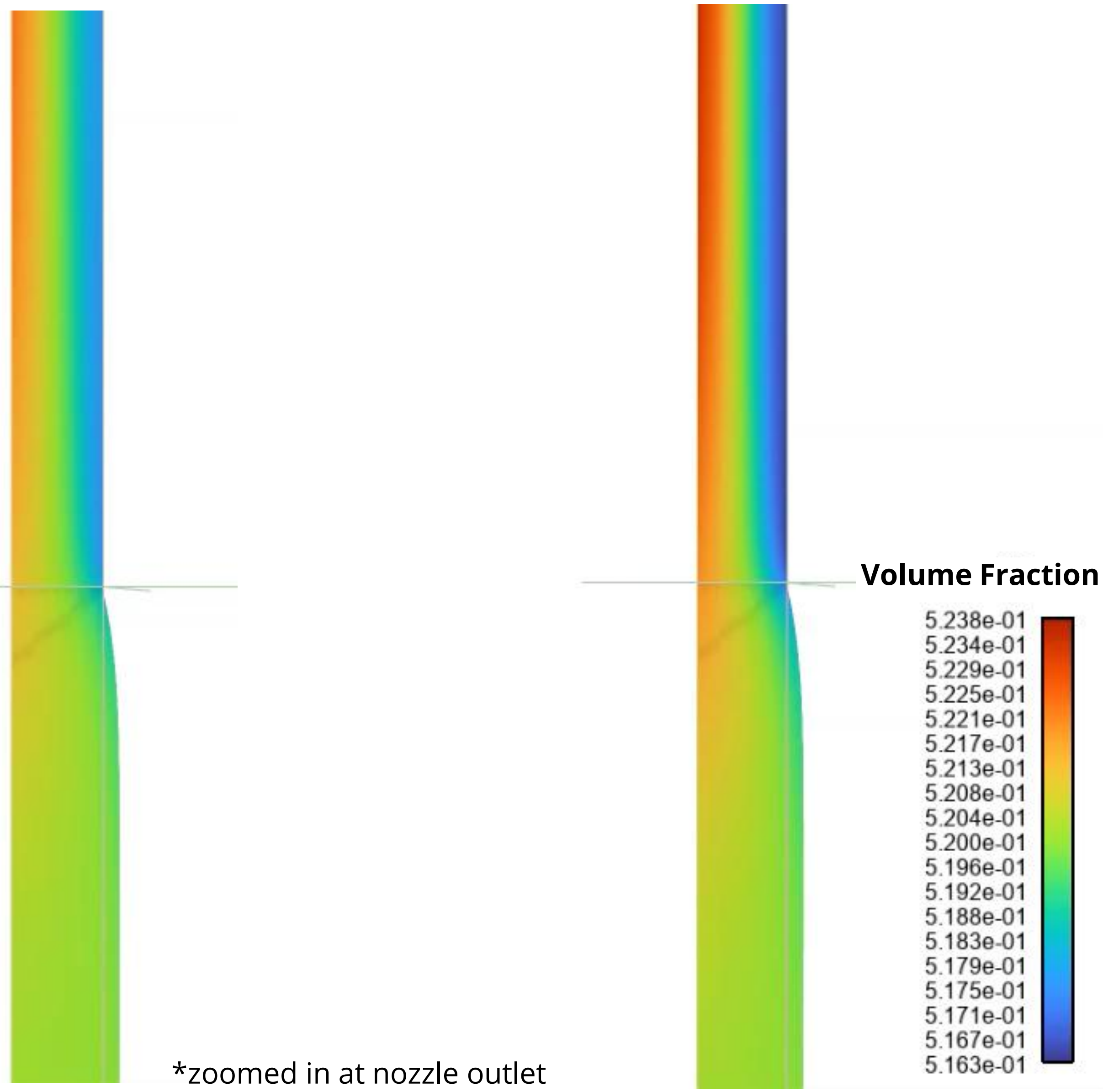
52% ALUMINA 3:1

Maximum packing = 59%

Continuous viscosity = 45750 dyne-sec/cm2

Number mean particle diameter (4.45 μm)

Hydrodynamic Model | Suspension Balance Model



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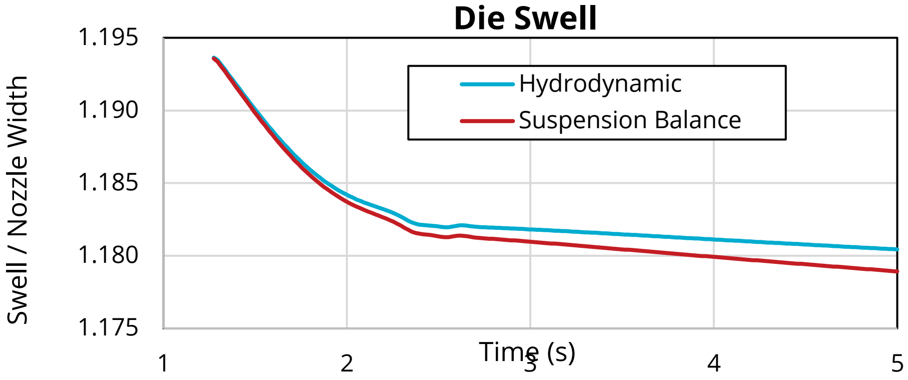
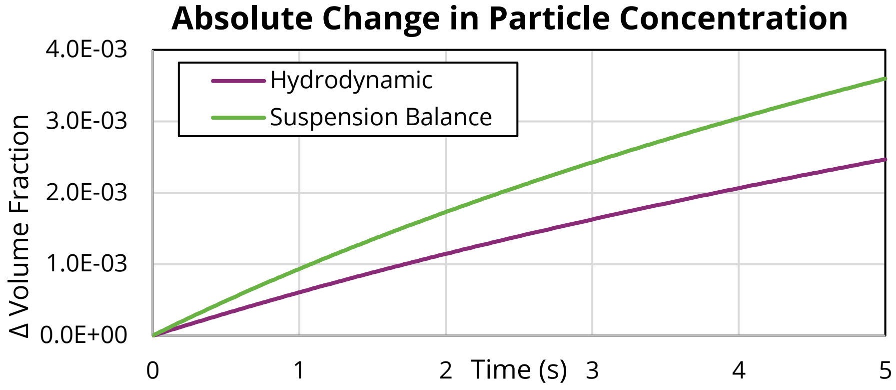
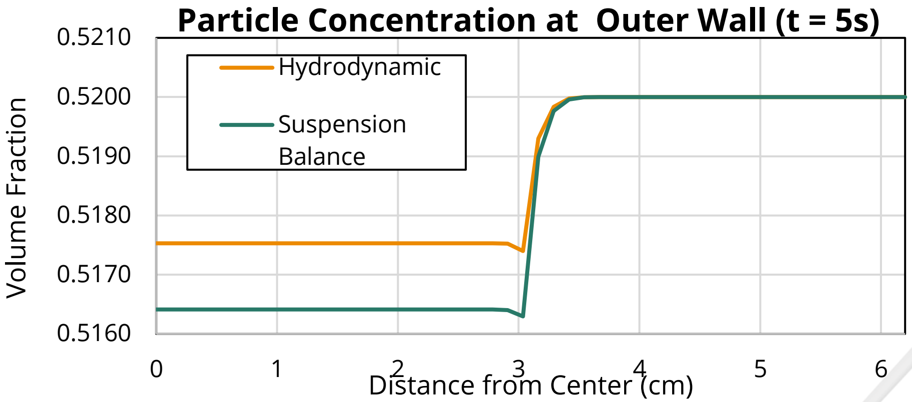






52% ALUMINA 3:1

Maximum packing = 59%

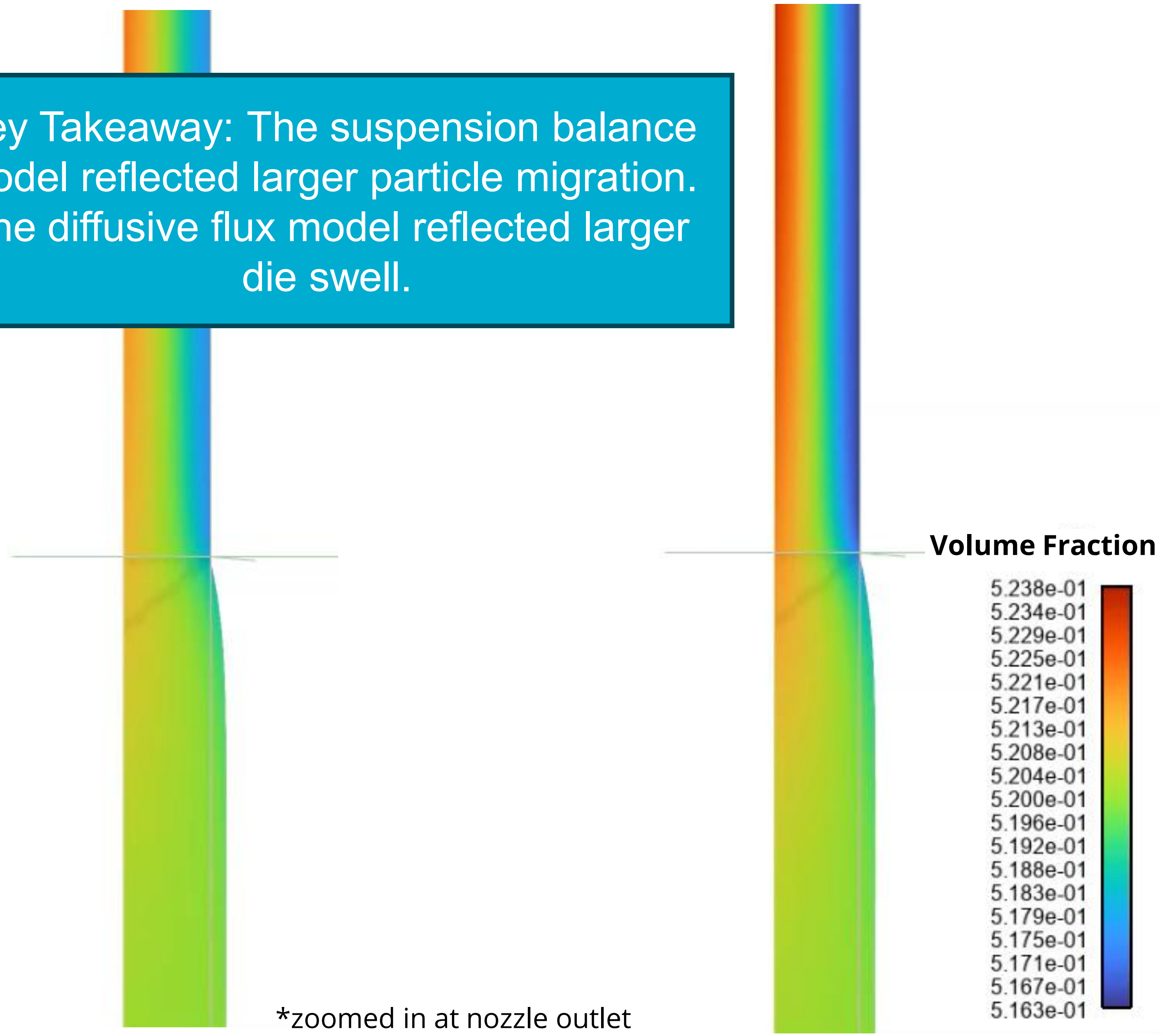
Continuous viscosity = 45750 dyne-sec/cm2

Number mean particle diameter (4.45 μm)

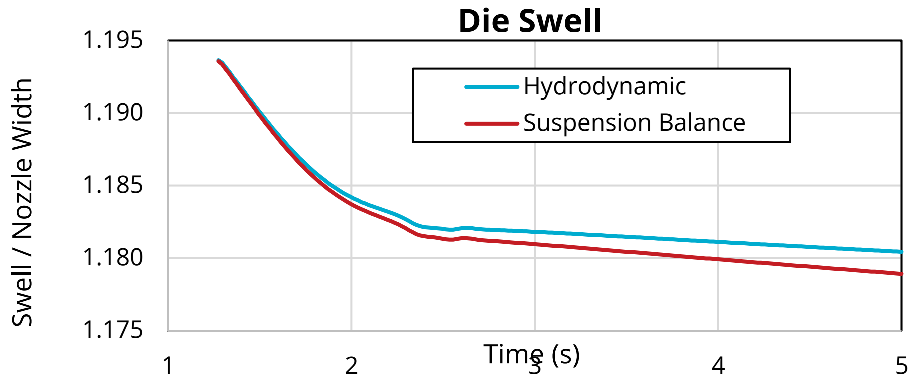
Hydrodynamic Model

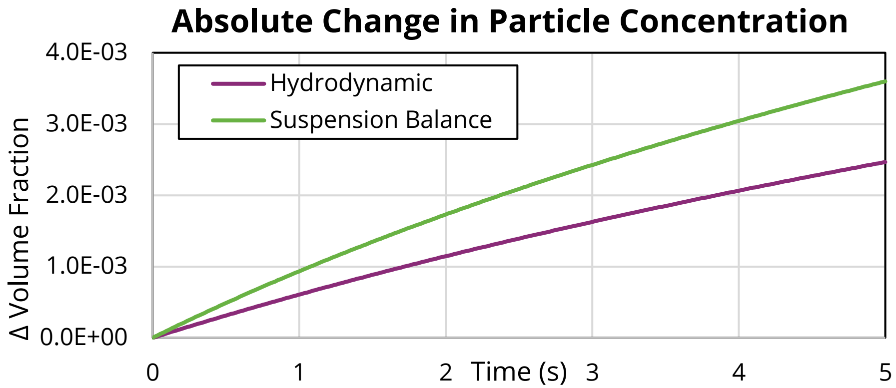
Suspension Balance Model

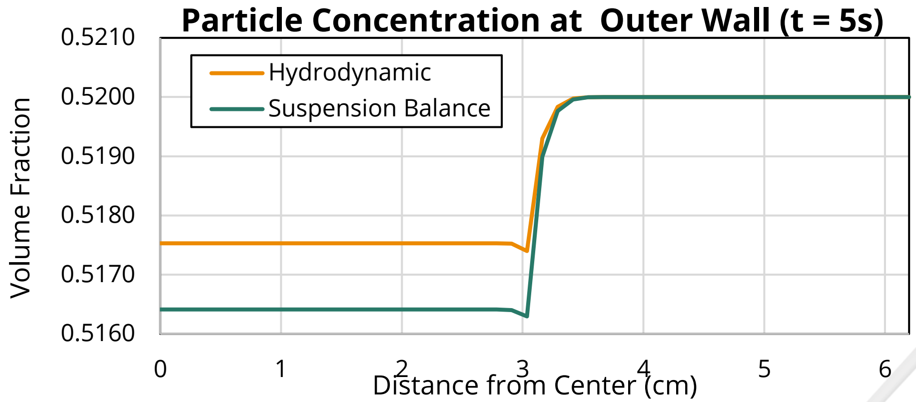
Key Takeaway: The suspension balance model reflected larger particle migration. The diffusive flux model reflected larger die swell.



*zoomed in at nozzle outlet

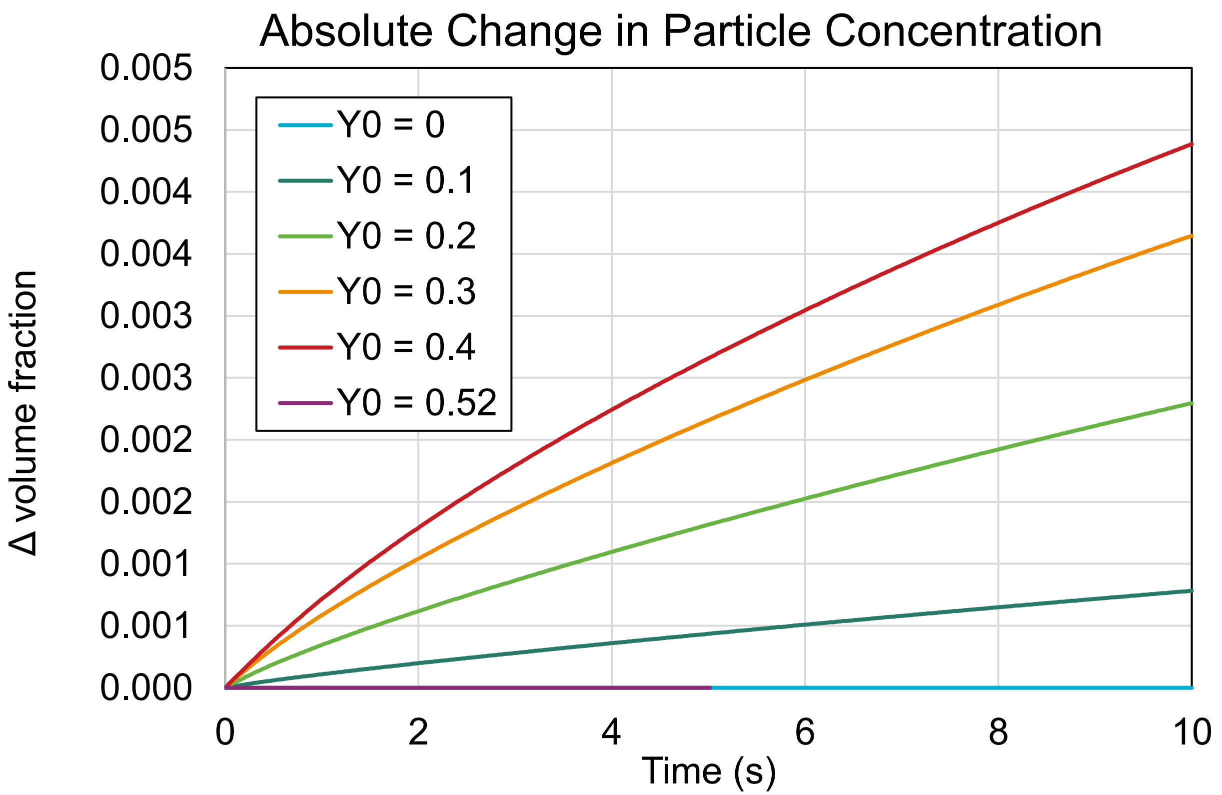


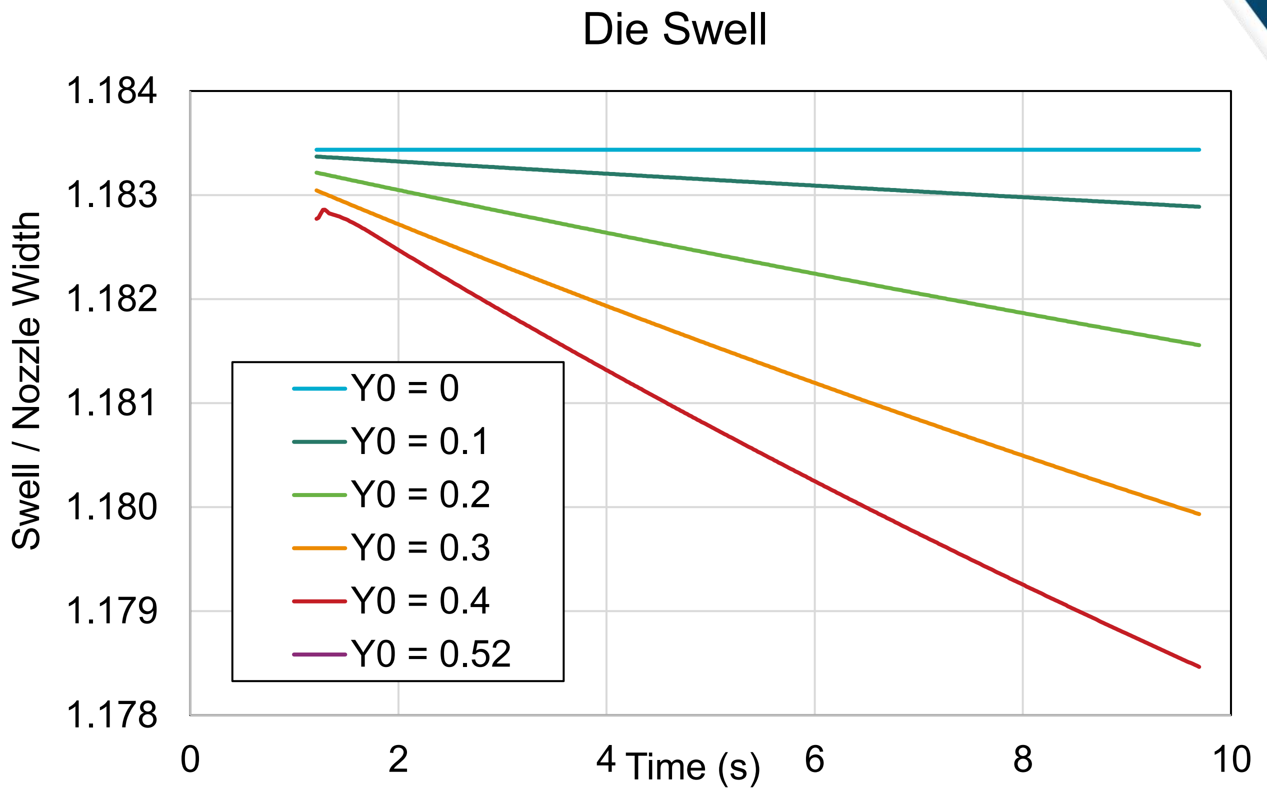


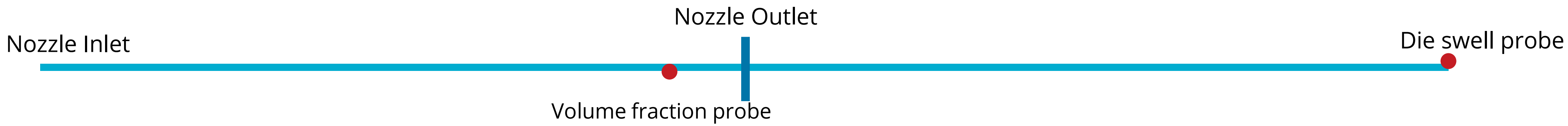


CONCENTRATION STUDY

Sweep over concentrations of Alumina 3:1 (7.39 μm)



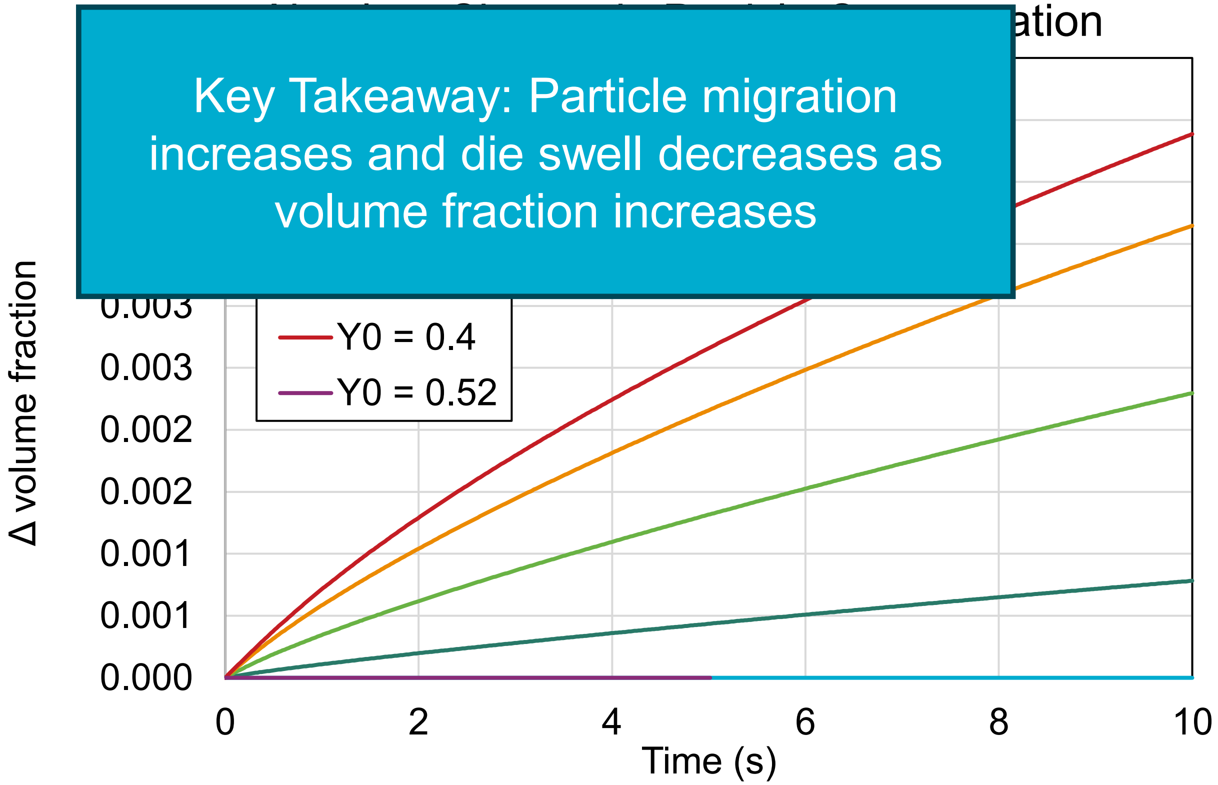


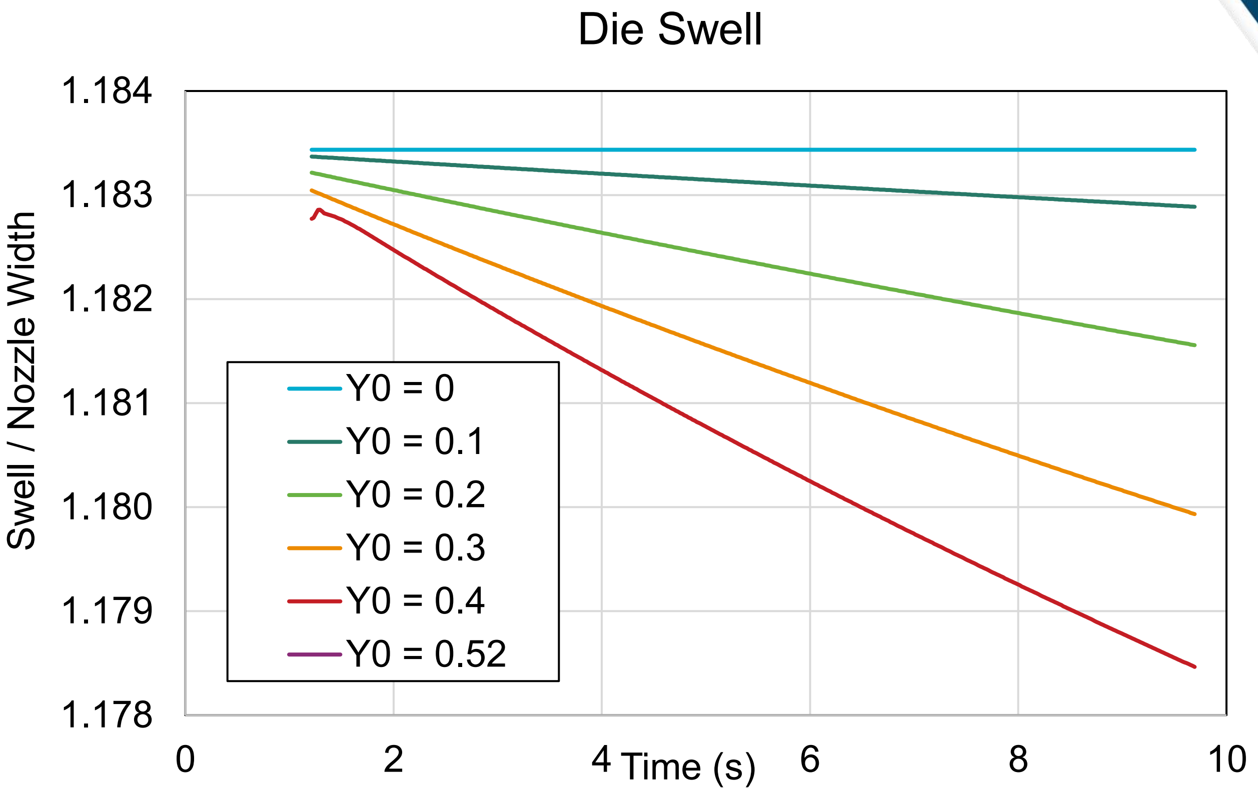


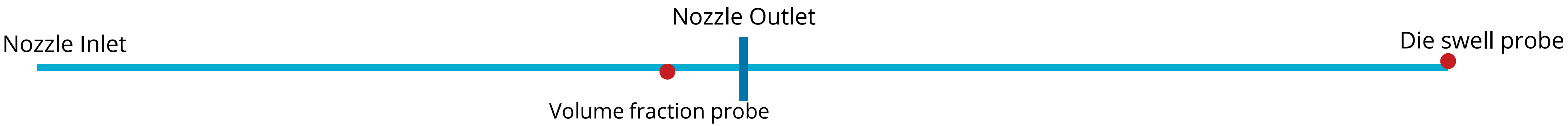
CONCENTRATION STUDY

Sweep over concentrations of Alumina 3:1 (7.39 µm)

Key Takeaway: Particle migration increases and die swell decreases as volume fraction increases







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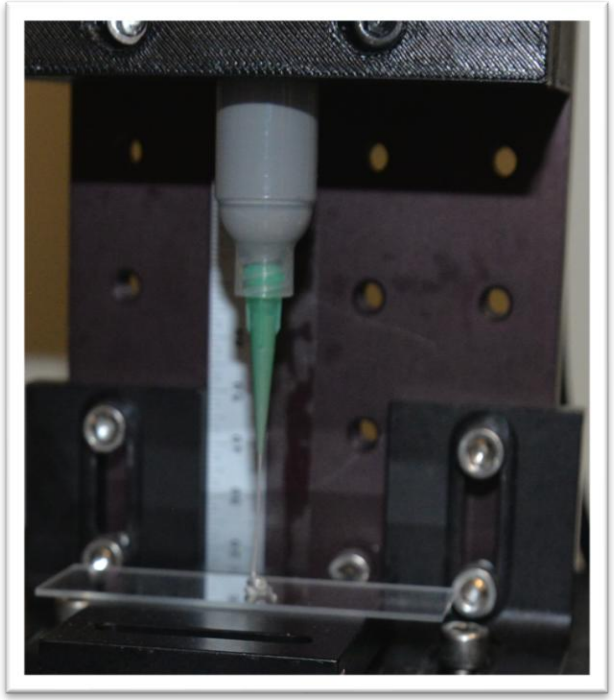
Agenda

EXTRUSION TESTING

Process:

- Fill syringe with printable material
- Use load cell to extrude material at a constant rate
- Photograph sample over time to document slumping

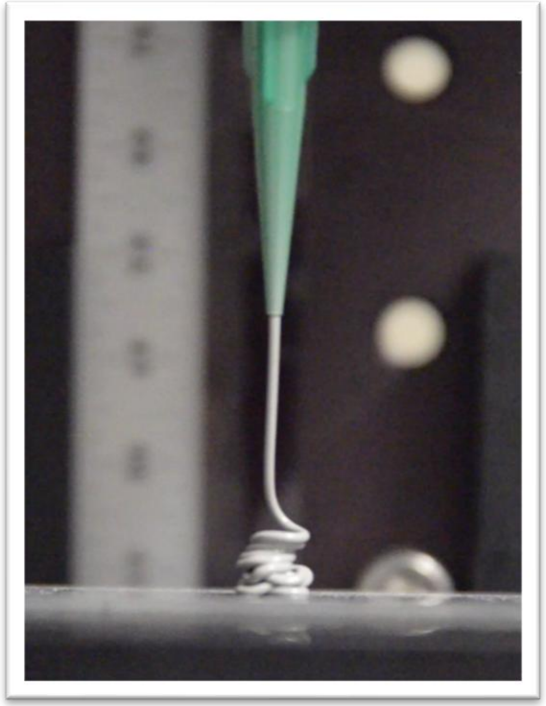
Runny



Aluminum 80:20 52% vf

Aluminum 80:20 52% vf

Extrudable



Alumina 3:1 52% vf

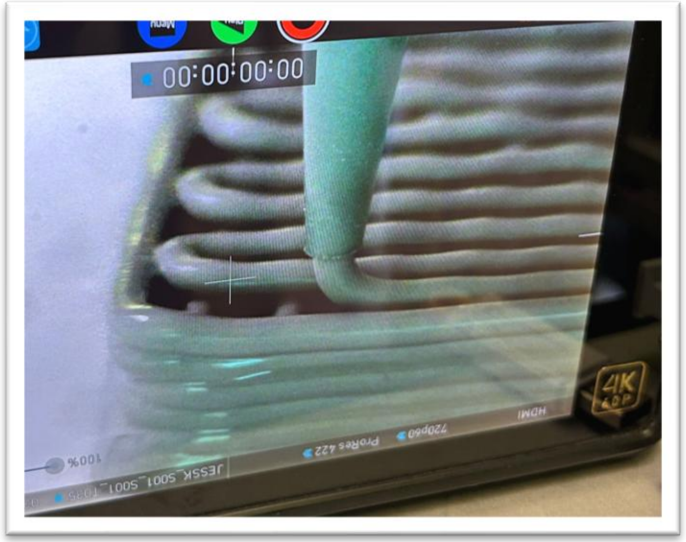
Alumina 3:1 52% vf

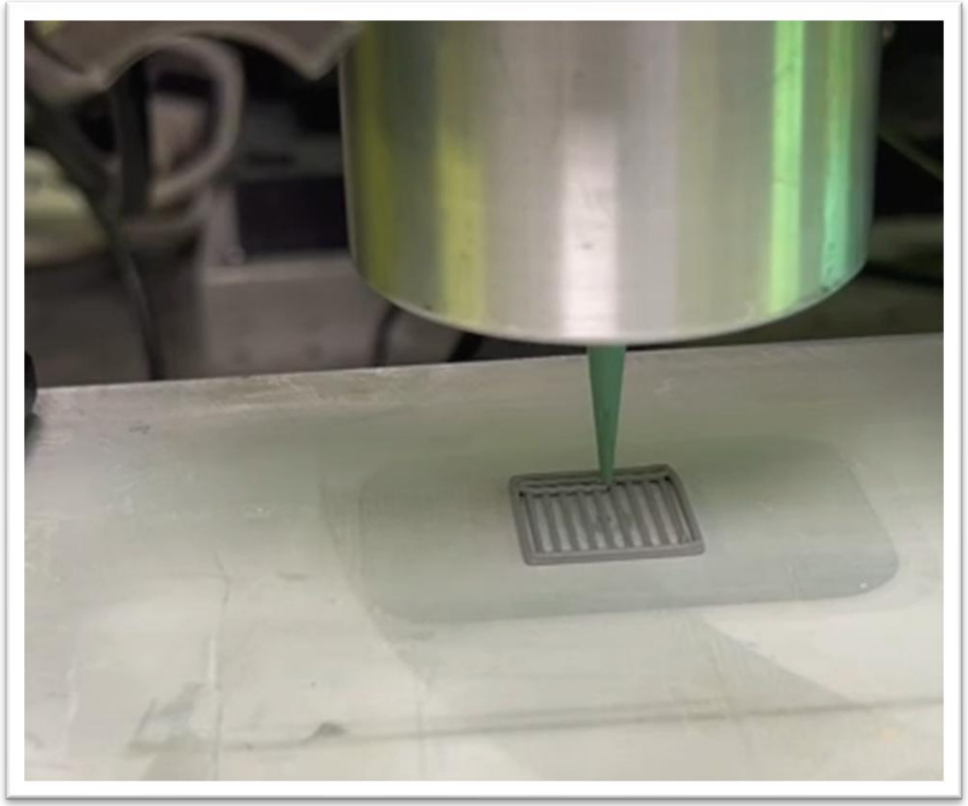
DIRECT INK WRITE PRINTING

Printing using a direct ink write printer at the AML

- Alumina 3:1 52% was jammed
- Aluminum 54% was printable, but some slumping occurred

Extrudability ≠ Printability





Aluminum 80:20 54% vf

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KEY TAKEAWAYS

Printability Experiments

- Experimental estimates still deviate from true printability range
- Lack of data and model simplifications introduce error

Particle Packing

- Experimental data can be used to calibrate frictions and simulate any ratio
- Better/More data is needed to help increase accuracy of calibration

Suspension Modeling

- Examined effects of particle size, concentration, and diffusion modeling on particle migration and die swell
- Improvements to be made to the mesh to capture area change effects

ACKNOWLEDGEMENTS

- This research was conducted at the 2026 Nonlinear Mechanics and Dynamics Research Institute hosted by Sandia National Laboratories and the University of New Mexico.
- We would like to acknowledge our project mentors: Joseph Monti, Jess Kopatz, Rekha Rao, Dan Bolintineanu, Harrison Root, and Hayden Fowler.
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