INL/CON-20-57511-Revision-0

Computationally-Aided Design of a Small-Scale Radioactive Waste Glass Melter

Alexander W Abboud, Donna Post Guillen, Mark Hall, Will Eaton, Albert Kruger, Richard Pokorny

March 2020

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Computationally-Aided Design of a Small-Scale Radioactive Waste Glass Melter

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Background

- Over 210,000 m^3 of tank waste stored at Hanford site from five decades of spent fuel reprocessing
- 177 underground tanks at Hanford with differing waste compositions across the tanks
- Contents of tanks will be retrieved, and the waste vitrified into a stable waste form by the addition of glass forming additives to the waste in Joule-heated melters
- In the near-term, low-activity waste (LAW) will be vitrified loaded into containers for disposal at the Integrated Disposal Facility

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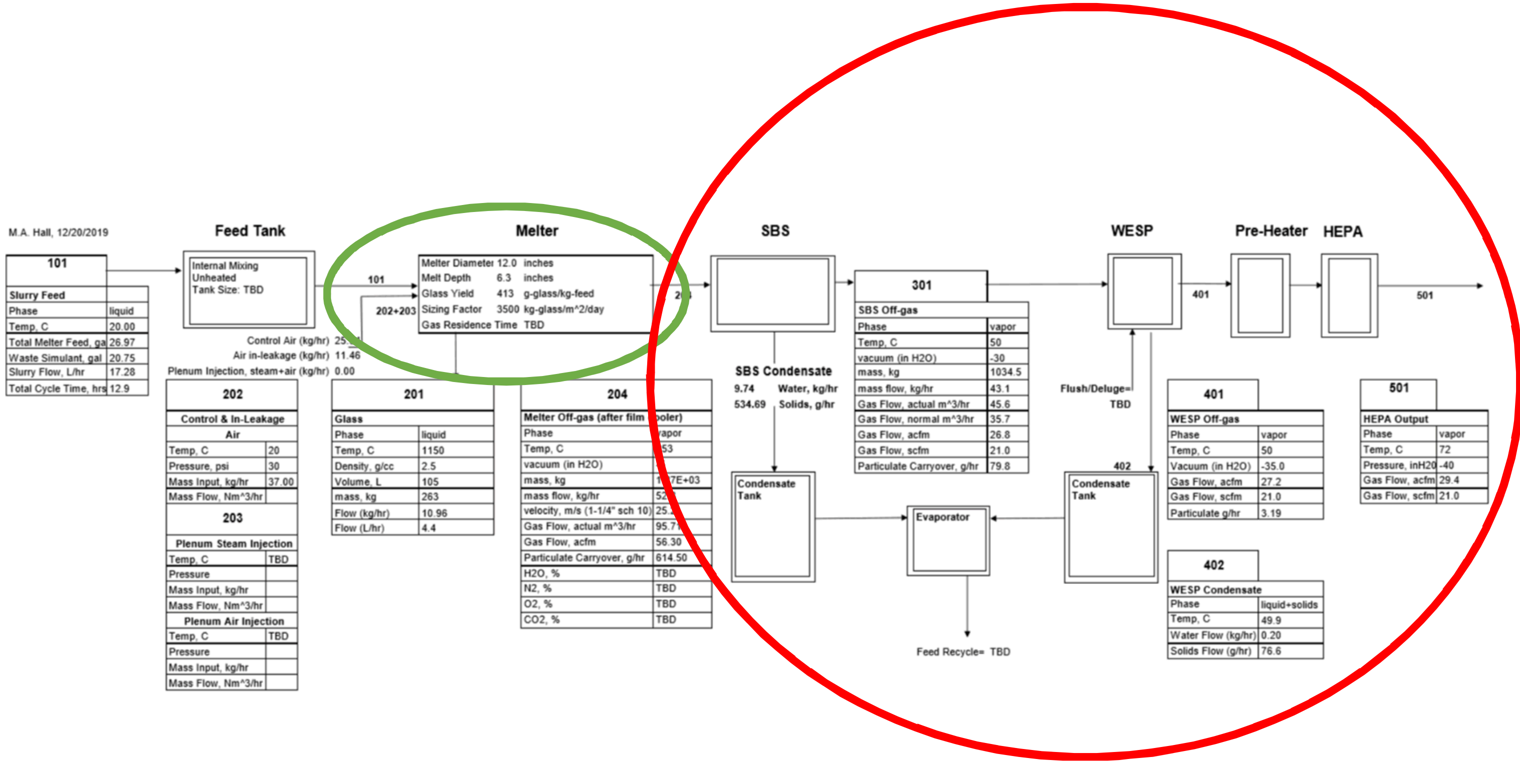
Motivation

- 6” Diameter Continuous Laboratory-Scale Melter (CLSM) was installed for testing surrogate glass formulations
- Evaluates feed-to-glass conversion well
  - Not sufficient volume to evaluate offgas system
- Goal to design a larger 12” diameter melter to produce enough offgas so that accurate chemical and performance information can be captured. Issues with:
  - Many components
  - Multiple effluent streams
  - Recycle concept
- Use experiments in combination with 3D CFD modeling to evaluate the system

Process Diagram

- Goal to test the offgas system with targets:
  - **Large off-gas production**: Volume/mass flow of offgas large enough to drive prototypic offgas components and satisfy analytical detection limits.
  - **Small volume of feed**: Availability of actual tank waste sample. Drives test cost.
  - **Short test durations:** Drives test cost

  - Test system flexibility: Turn-down/turn-up ability of all components and features.
  - Low system maintenance: System to be turned off between test runs to reduce hotel cost



Corresponding poster on experimental considerations:
"Melter Optimized for Fast Turnover, Steady State Testing"
WC Eaton (PNNL), MA Hall (PNNL), AW Abboud (INL), DP Guillen (INL), DR Dixon (PNNL), CD Lukins (PNNL), CM Stewart (PNNL), AA Kruger (DOE)

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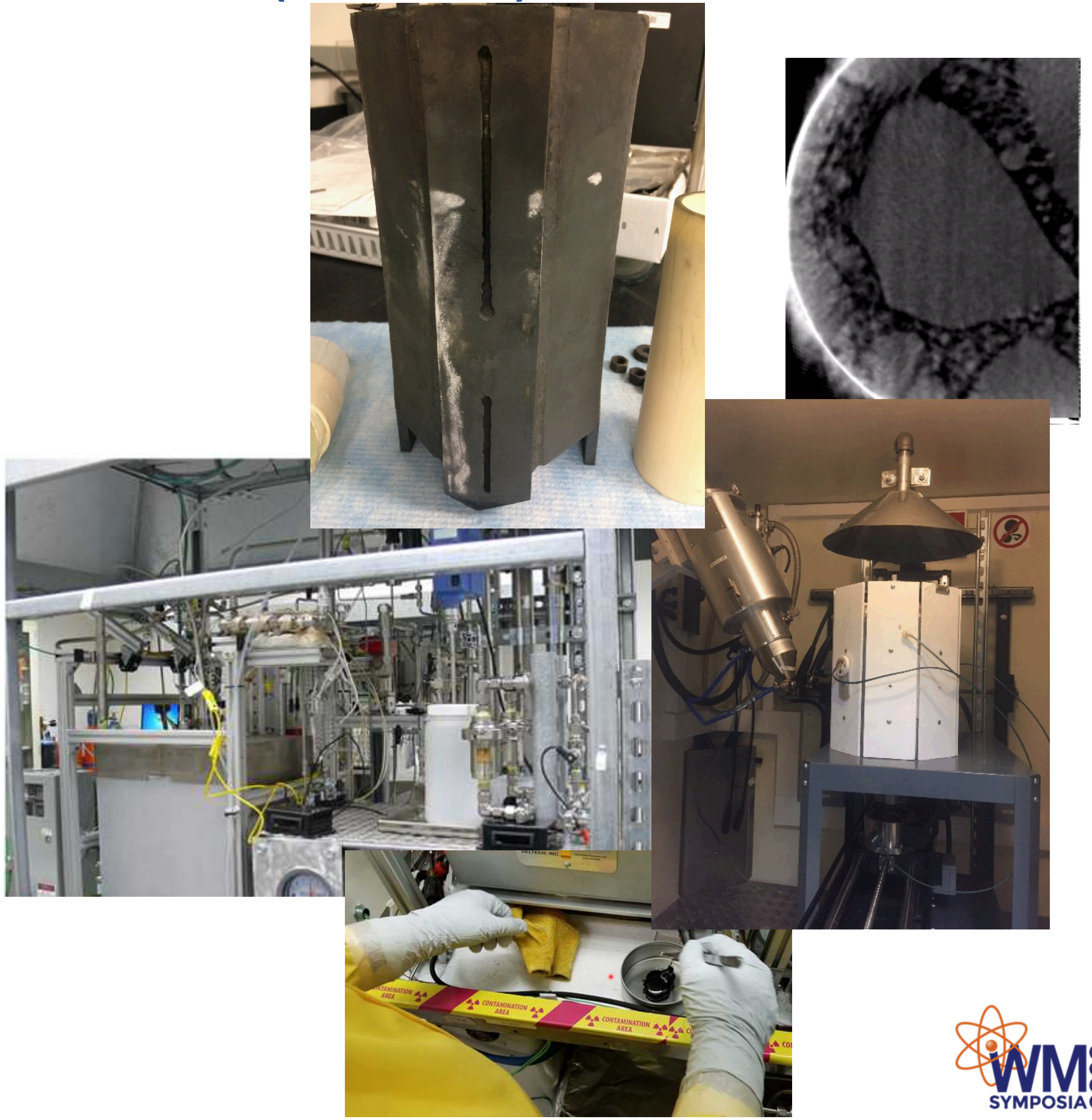
Continuous Laboratory Scale Melter (CLSM) Tests

- CLSM small-scale model testing at PNNL
- Made of Inconel for high temperature tests at 1150º C
- Heat supplied by external furnace
- Bubbler and feed tubes inserted from top
- Offgas port removes reaction gases
- CFD validation planned using X-ray tomography images of the CLSM
- 6” D melter, look to expand on this design to 12” D



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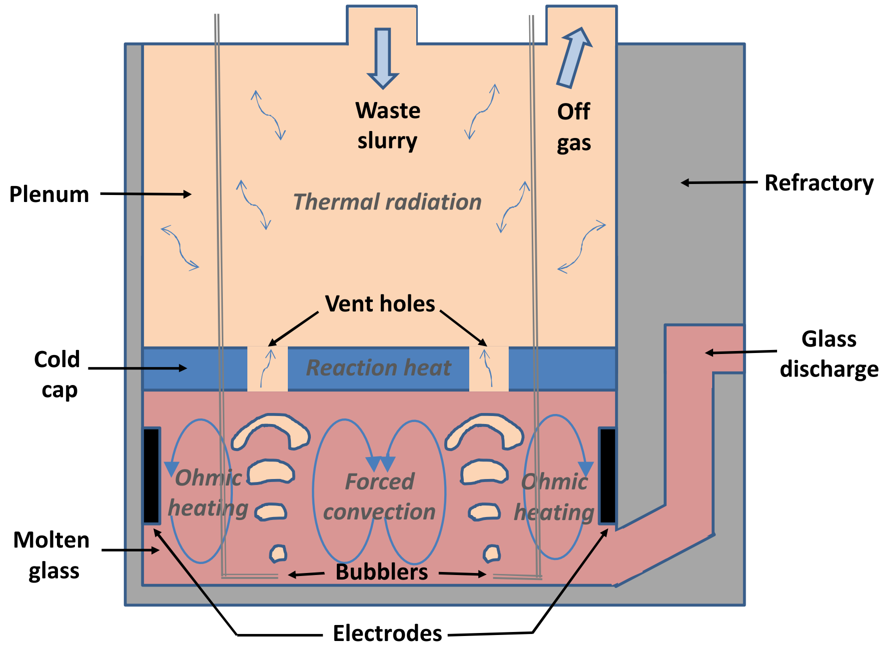
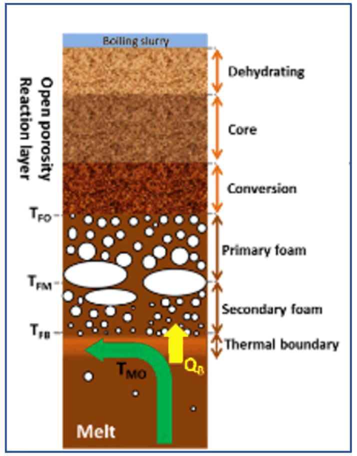
Melter Model

- A set of computational fluid dynamics and heat transfer models have been developed to complement experimental studies at various scales1
- The goal is to increase melter throughput by increasing melt rate
- To accomplish this, we must understand how changes to various parameters influence the heating provided to the cold cap, which drives the glass conversion reactions
  - As the waste slurry is fed to the melter, a cold cap that floats on molten glass is formed



Foam layer forms at the base of the cold cap resulting from chemical reactions

Forced convection bubbling from the base of the melter disrupts the foam layer and allows heat from the molten glass below into cold cap



[1]D. P. Guillen, A. W. Abboud, R. Pokorny, W. C. Eaton, D. Dixon, K. Fox, A. A. Kruger, "Development "Development of a Validation Approach for an Integrated Waste Glass Melter Model," Nucl. Technol. 203(3), pp. 244-260 (2018).

Solution Methodology

- Eulerian-Eulerian multiphase with volume of fluid (VOF)
  - Finite volume approach with 1st-order implicit time-stepping and 2nd-order spatial discretization
  - The segregated flow solver for the Navier-Stokes equations is used, which can handle constant density or mildly compressible flows with a predictor-corrector approach coupling the momentum and continuity equations.
  - A collocated variable arrangement and a Rhie-and-Chow type pressure-velocity coupling combined with a SIMPLE-type algorithm
  - Due to the low Reynolds number (~30), the laminar model is used
  - Single-component gas phase for bubbling and foaming gases
- Cold cap modeled with conjugate heat transfer into a rigid solid
  - Energy equation yields the temperature profile within the cold cap
  - Fitted parameters for density/conductivity/specific heat based on experimental data of typical "A0" feed
  - Apply constant heat sink for batch to glass transition reactions

VOF model single grid velocity/properties based on volume fraction (α) of air/glass

$$\rho = \sum_i \rho_i \alpha_i$$

$$\mu = \sum_i \mu_i \alpha_i$$

$$C_p = \sum_i \frac{C_{p,i} \rho_i \alpha_i}{\rho}$$

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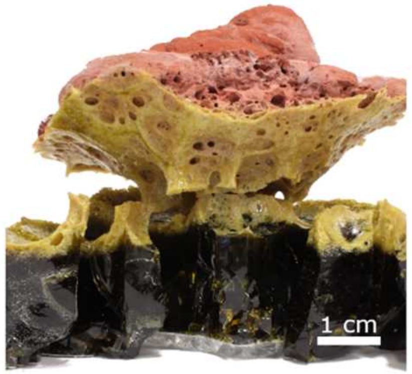
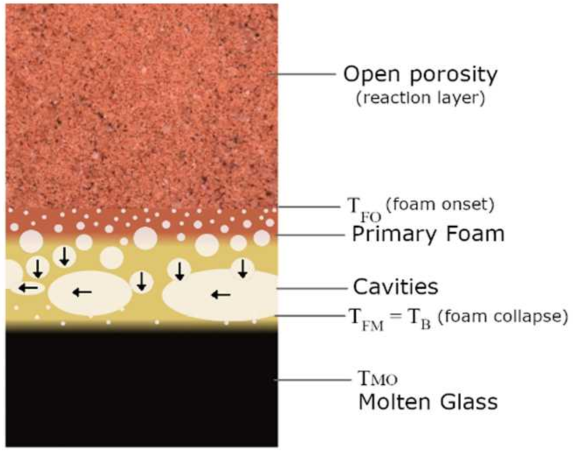
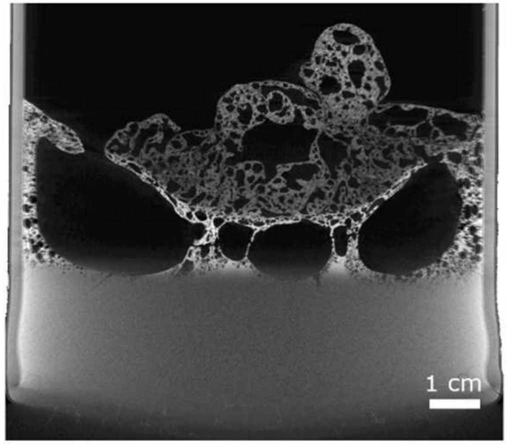
Bubbles in Foam Layer

- X-ray-tomography images of simulated melter feeds show gas bubbles that form between the cold cap and molten glass[1]
- The thickness of these bubbles is estimated at ~7 mm[2,3]



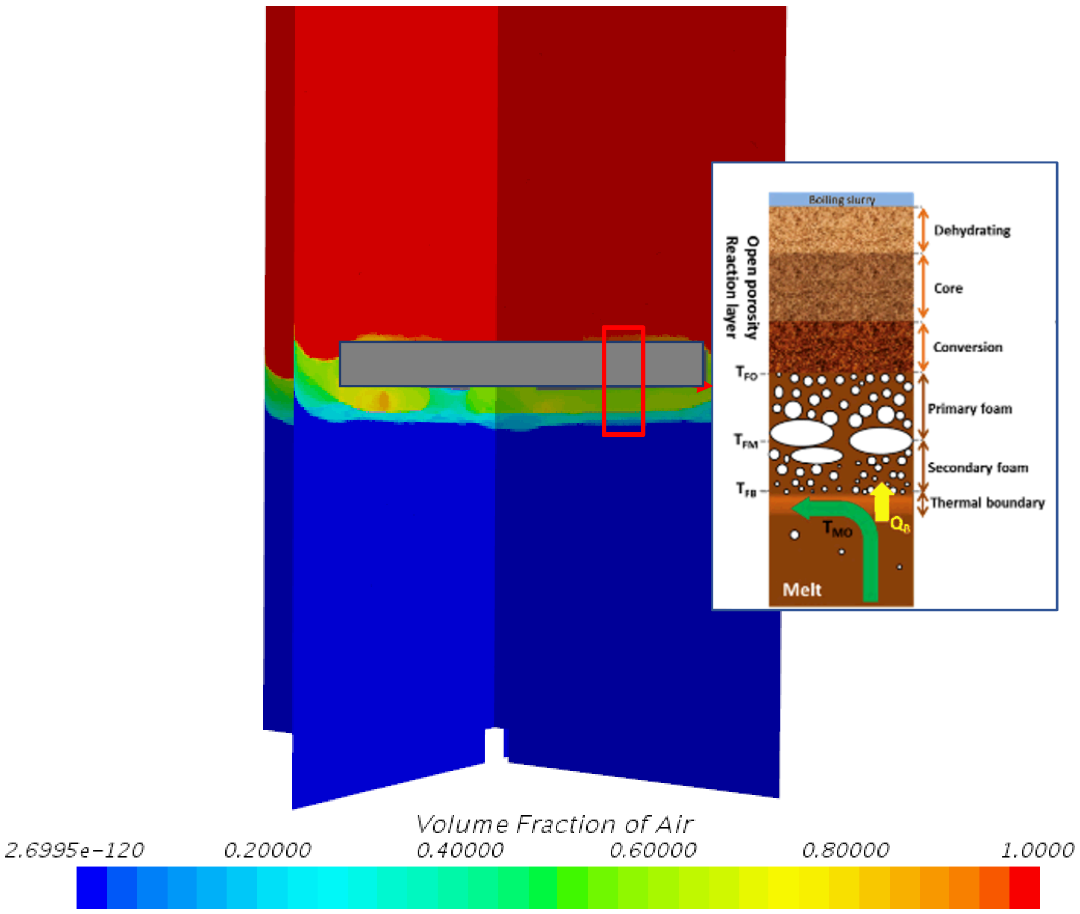




[1]*S.A Luksic, R. Pokorny, J. George, P. Hrma, T. Varga, L.R. Reno, A.C. Buchko, A.A. Kruger "In-situ characterization of foam morphology during melting of simulation waste glass using x-ray computed tomography," Ceramics International, 2020.*
[2]*R. Pokorny, P. Hrma, Mathematical Modeling of Cold Cap, Journal of Nuclear Materials 429, 245-256, 2012*
[3]*R. Pokorny, Z.J. Hilliard, D.R. Dixon, M.J. Schweiger, D.P. Guillen, A.A. Kruger and P. Hrma. "One dimensional cold cap model for melters with bubblers," Journal of American Ceramic Society, 98(10), 3112-3118, 2015.*

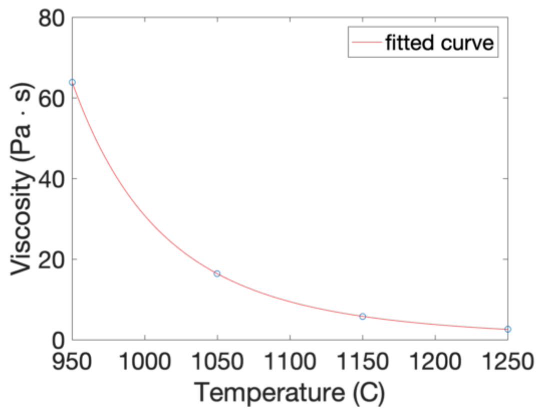
Foam Layer under Cold Cap

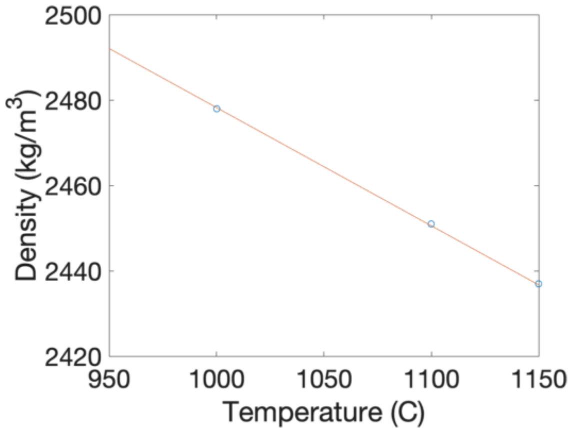
- Foaming is due to the evolution of reaction gases during the batch-to-glass conversion in the cold cap
- Model cold cap as rigid solid 4.15 mm (0.164 in.) thick with gas volumetric source in a 6.35 mm (0.25 in.) thick layer below cold cap to simulate foaming



Modeling Parameters

- AP-105 glass properties
  - Viscosity 5.8 [Pa s] at 1150 C (variable) [1]
  - Heat Capacity 1303 [J/kg K] [1]
  - Thermal Conductivity 6.1 [W/m K] [1]
  - Surface Tension 0.29 [N/m]
    - (based on composition from 1)
- QB = -131,000 [W/m^2]
- Base case Bubbling 101 [L/m^2 min]
- Solid cold cap, slip boundary condition
- Molten glass at 1150º C
- Floor at 1150º C
- Side walls Qw = -QB





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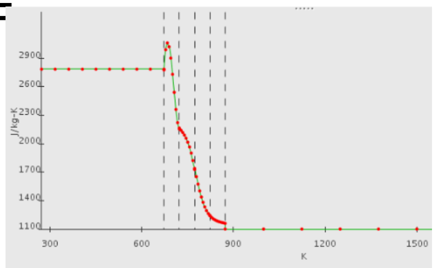
[1]Matlack, KS, Abramowitz H, Muller, IS, Joseph, I, Pegg, IL. "Final Report: Support for DF LAW Flowsheet Development Report", VSL-17R4250, Vitreous State Laboratory, Catholic University of America, 2017.

Model Description (cont.)

- Initial LAW cases in 6”D CLSM with bubbling rate
  - 0, 1/4x, 1/2x, Base, 2x, 4x

- Cold cap material properties[1,2]
  - ρ_{cc} = 1500 kg/m^3
  - $k_{CC} = \begin{cases} 0.311 - 1.06 \times 10^{-4}\, T, & \text{if } T \leq 700°\text{C} \\ -6.9164 + 0.0102\, T, & \text{if } T \leq 800°\text{C} \\ 0.5\ \text{W}/(\text{m} \cdot \text{K}), & \text{otherwise} \end{cases}$
  - Piecewise polynomial $C_{p,CC}$ =



[1]Pokorny, R., Rice, J.A., Schweiger, M.J., et al., 2013. Determination of temperature dependent heat conductivity and thermal diffusivity of waste glass melter feed. J. Am. Ceram. Soc. 96 (6), 1891–1898.
[2]Rice, J.A., Pokorny, R., Schweiger, M.J., et al., 2014. Determination of heat conductivity and thermal diffusivity of waste glass melter feed: extension to high temperatures. J. Am. Ceram. Soc. 97 (6), 1952–1958.

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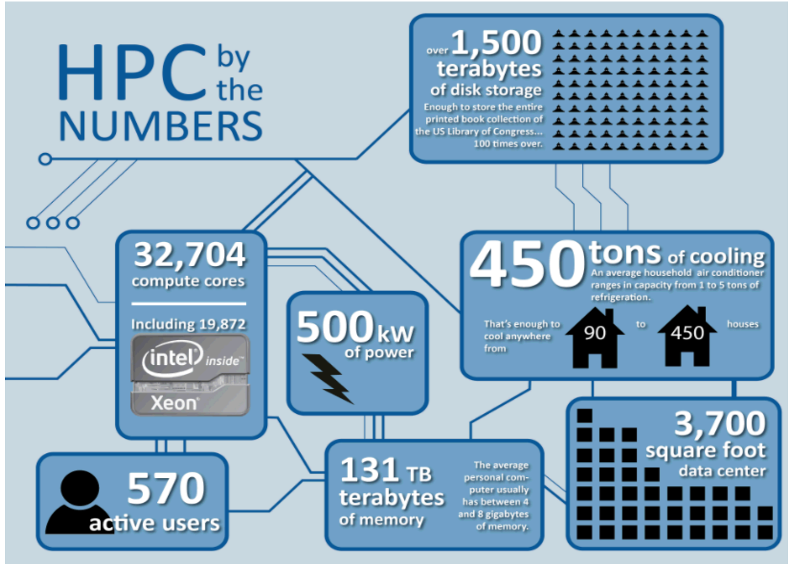
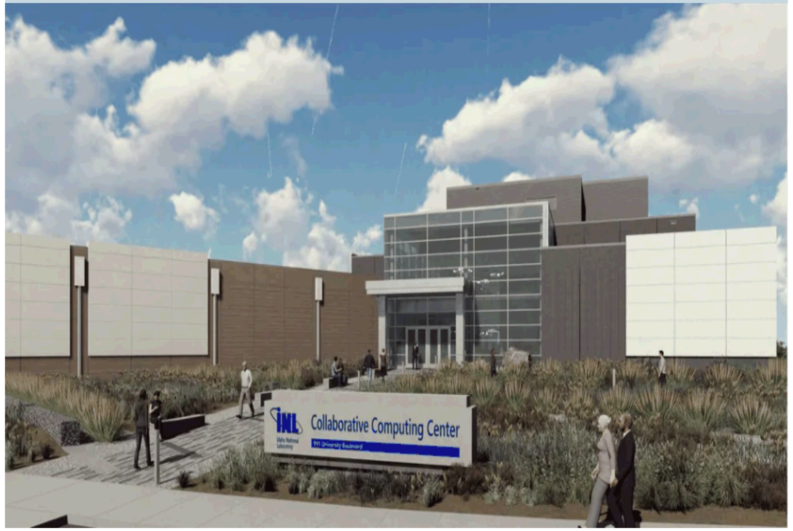
Methodology

- CFD simulations ran with STAR-CCM+ v14.04.011-R8 on 34992-core SGI ICE X distributed memory cluster with 121 TB total memory
  - FDR InfiniBand Network (56 Gbit/s), Single-Plane Enhanced Hypercube Topology
  - SUSE Linux Enterprise Server 11 Service Pack 4 operating system
  - LINPACK: 1087.58 Tflops
  - Simulation ran on 720 cores requiring 72 h of CPU time for 10s of physical time

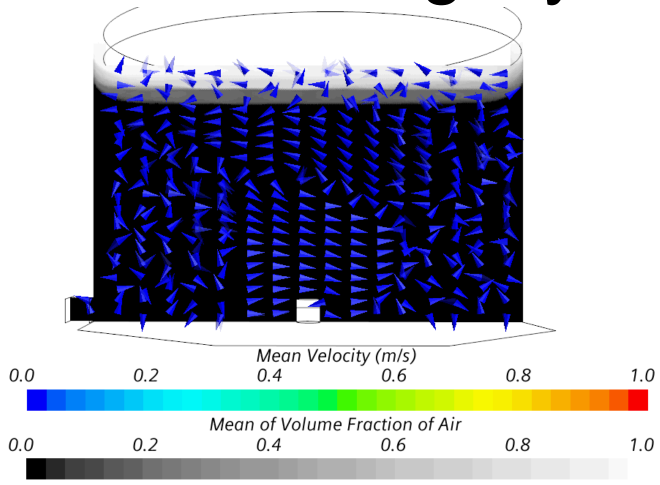




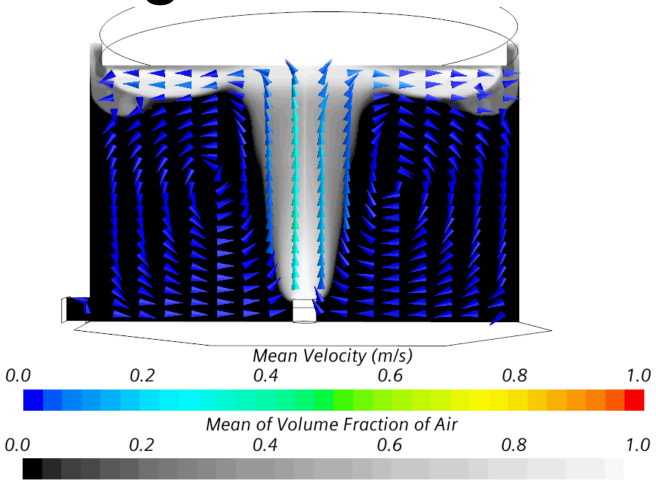
Averaged Velocity/Volume Fraction Profile

- Very weak circulation in no flow, increases velocity in central, and cavity layer increases slightly with increasing flow rate

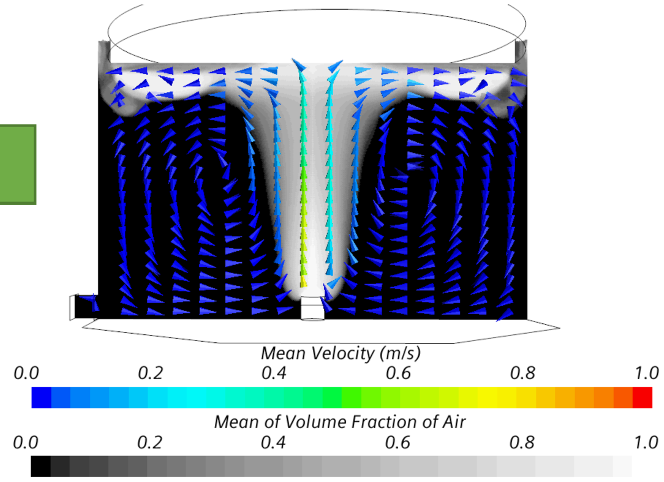
No Flow



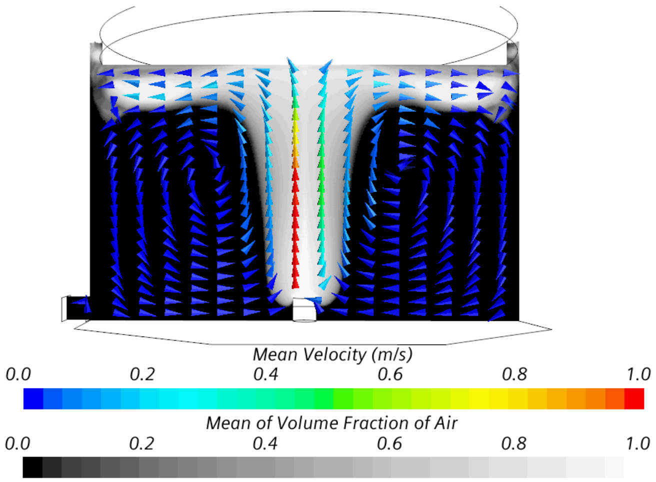
1/4x



1/2x



1x



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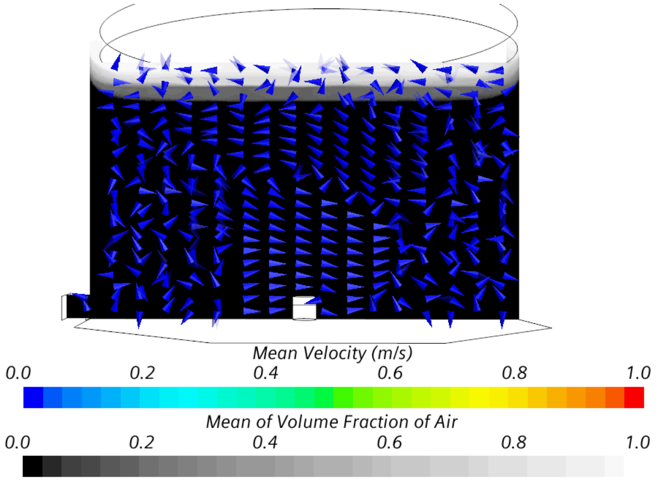
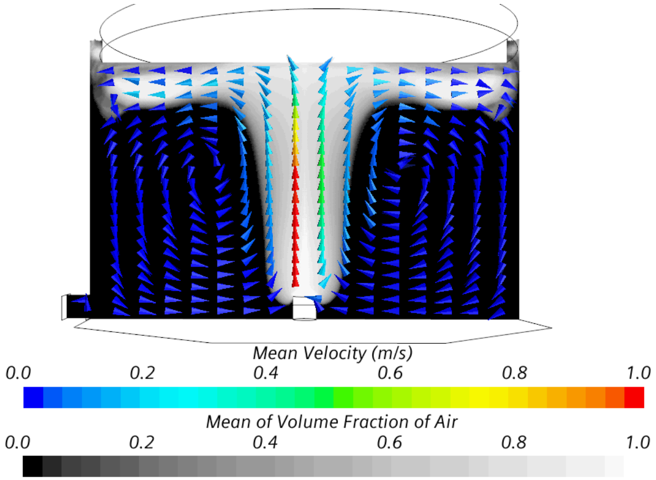
Averaged Velocity/Volume Fraction Profile

- Very weak circulation in no flow, increases velocity in central, and cavity layer increases substantially at high flow rate

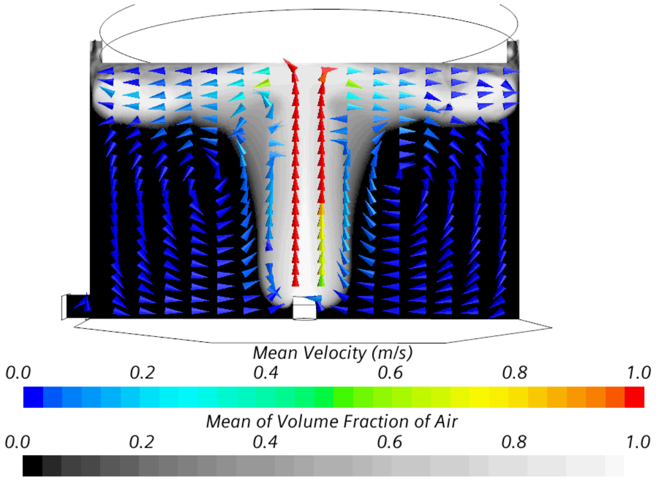
No Flow



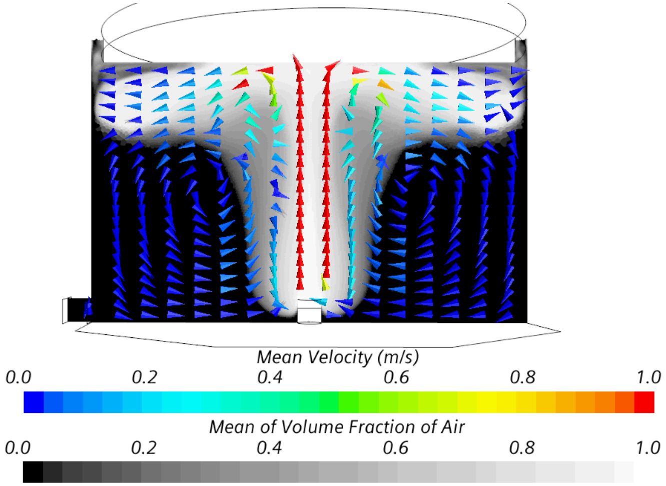
1x



2x



4x



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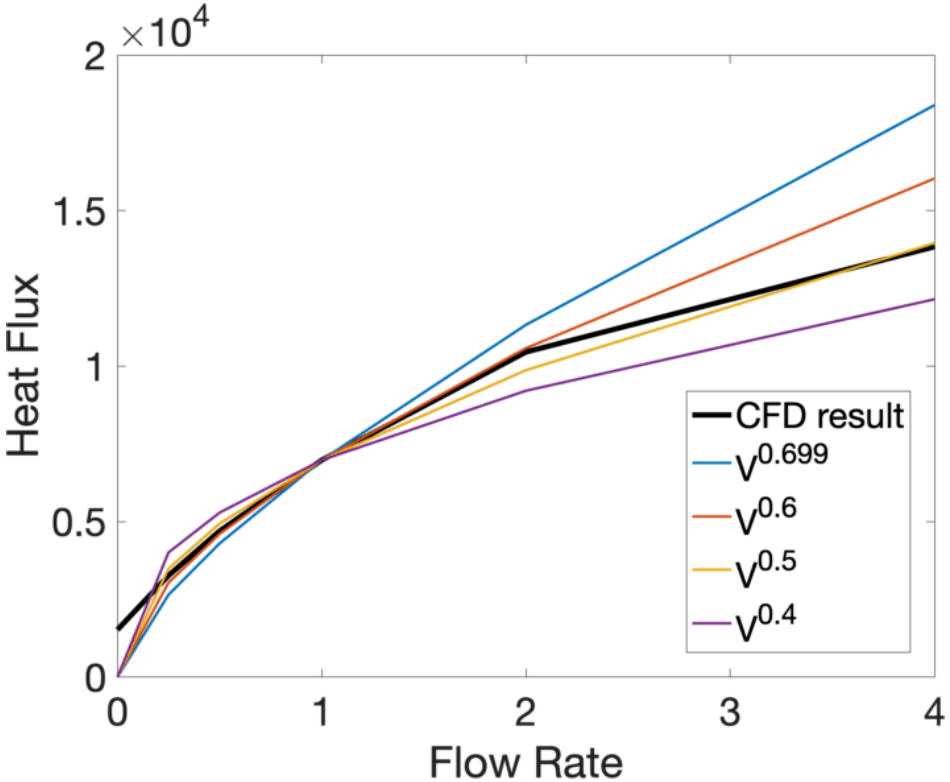
Heat Flux vs Melt Rate

- Align with bubbling rate correlation at various exponents
  - $V^{0.5}$ fits the best

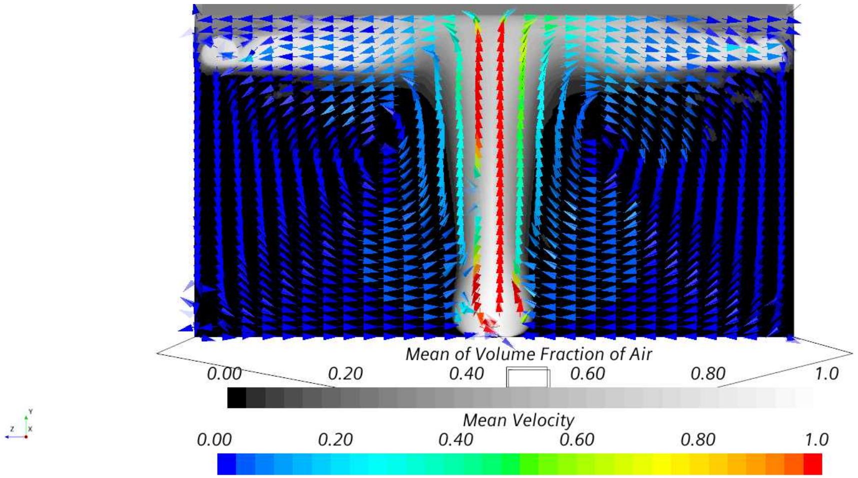
- Assume all heat flux is used for melting

Flow	Total Flux (W)
0	1525
1/4x	3268
1/2x	4697
Base	6979
2x	10455
4x	13840

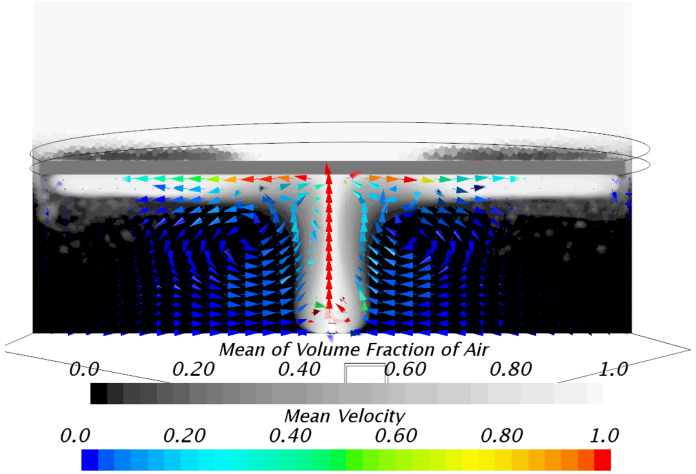


3” Deep Melter

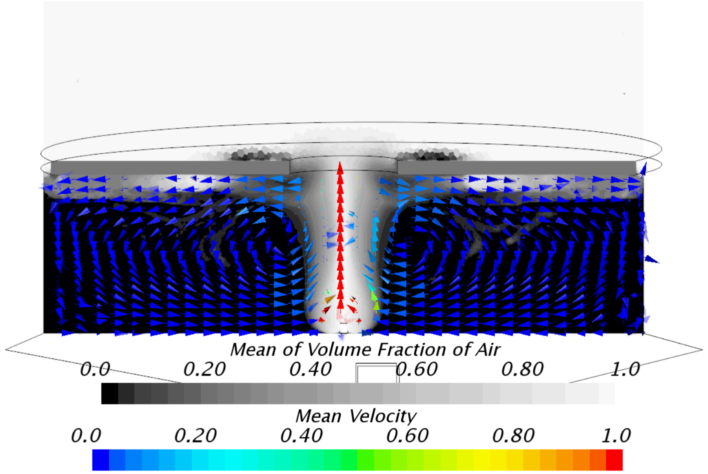
- Simple 1st test for decreasing melting volume to reach steady state
- Very poor glass circulation and heat flux, decrease in cavity Reynolds number
  - Expect decreased melt processing rate
  - Not pursued further



Base 6” H



3” H No vent hole



3” H Vent hole

Summary of Geometric Cases

12-inch octagonal melter with LAW glass

- 6-inch deep melt pool:
  1. Base case for reference
- 6-inch deep melt pool with 4x increased bubbling split between 4 bubblers
  1. Base geometry
  2. Cone
  3. Donut
  4. Cross
  5. Spacer
  6. Spacer – with 3” bubbler spacing
  7. Column
  8. Tapered Column

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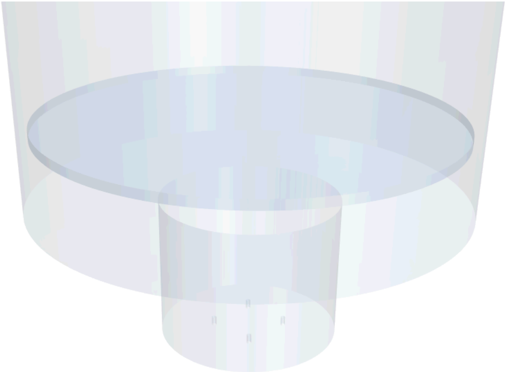
Geometry – 3-3.5” cutouts

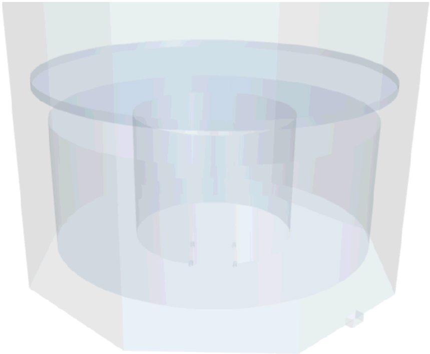

Base & Base 4x4

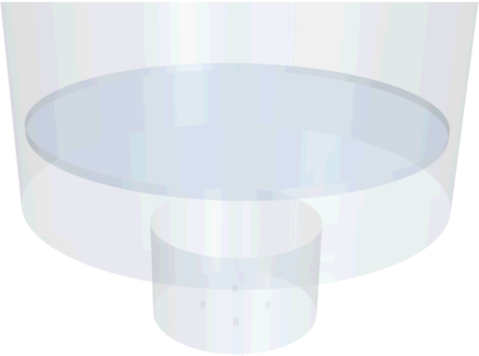

Cone


Spacer & 3” spacer


Column


Cross


Donut


Tapered Column

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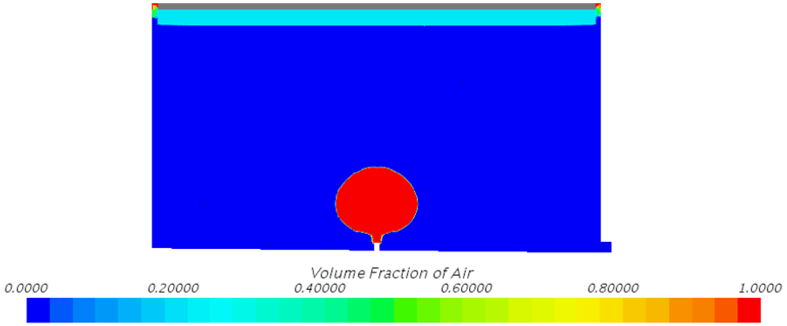
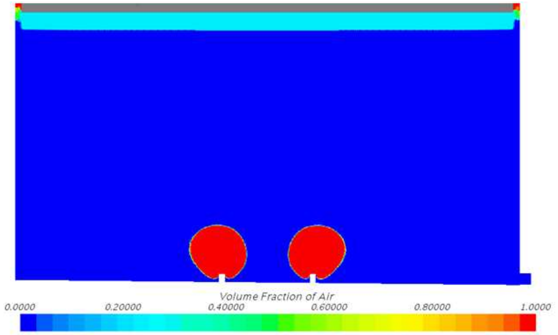
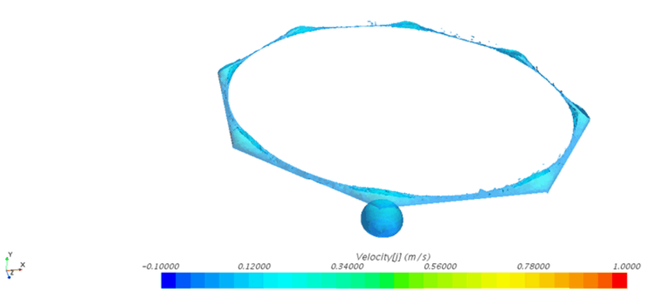
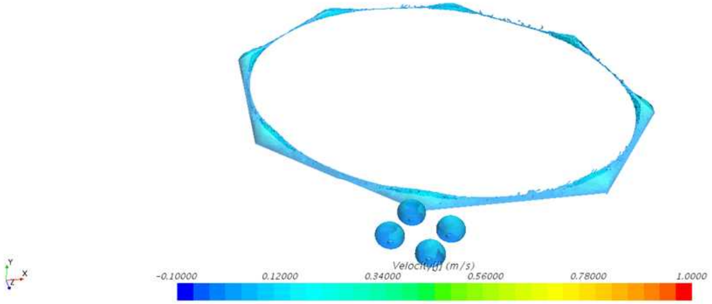
Bubbling

- Bubbling builds up cavity layer, gas escapes around corner openings

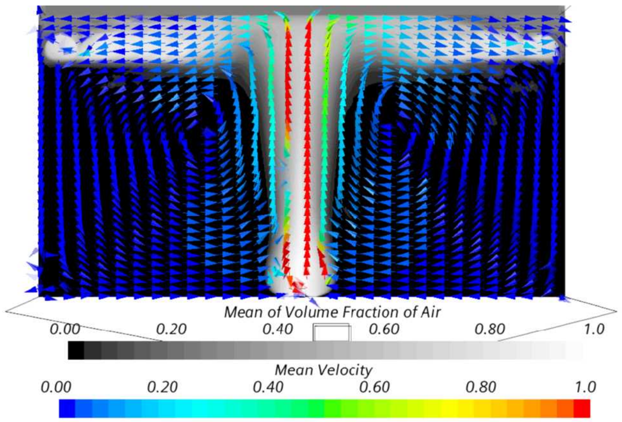




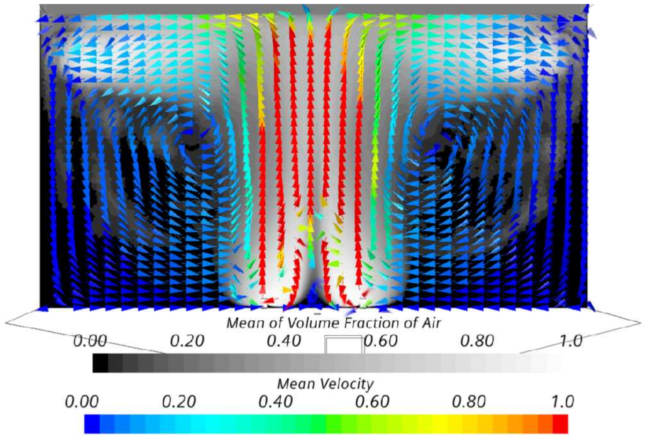




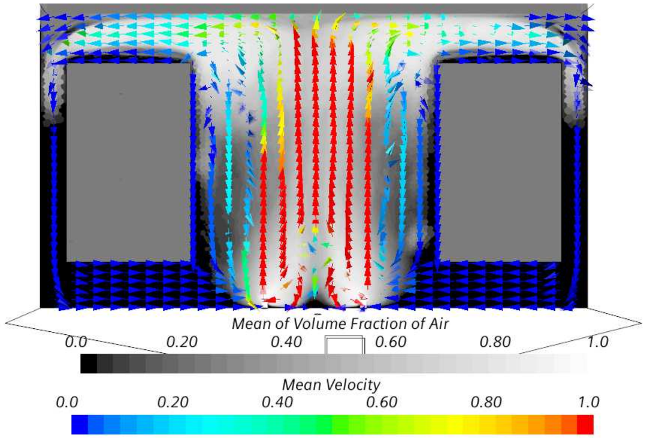
Flow Field



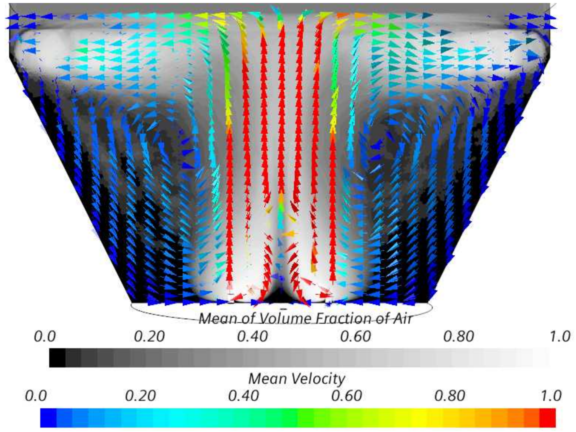
Base



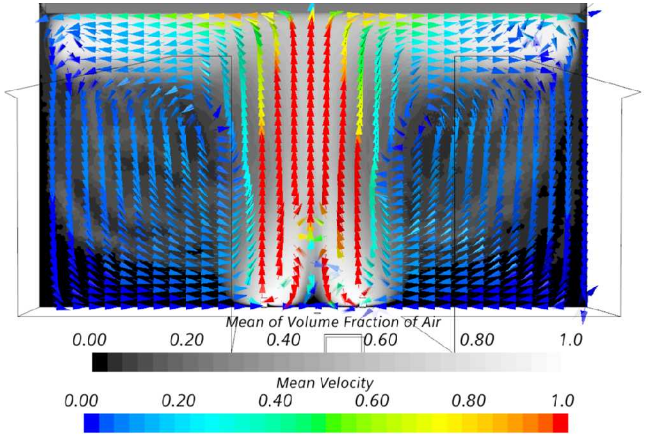
Base 4x4



Donut

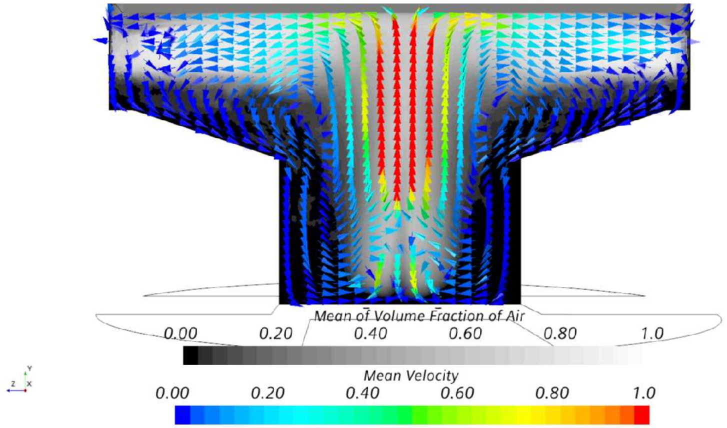


Cone

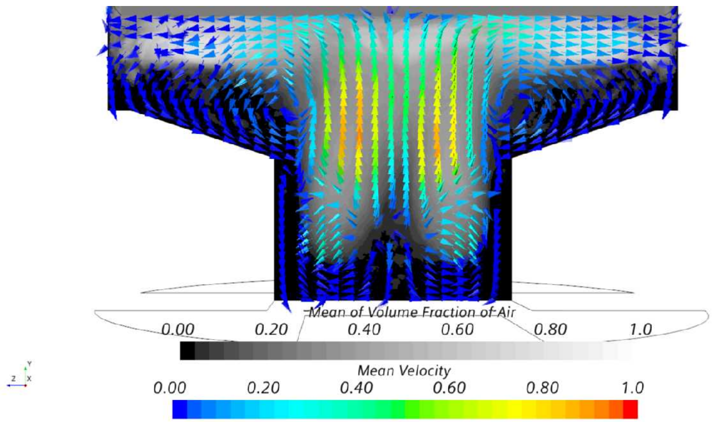


Cross

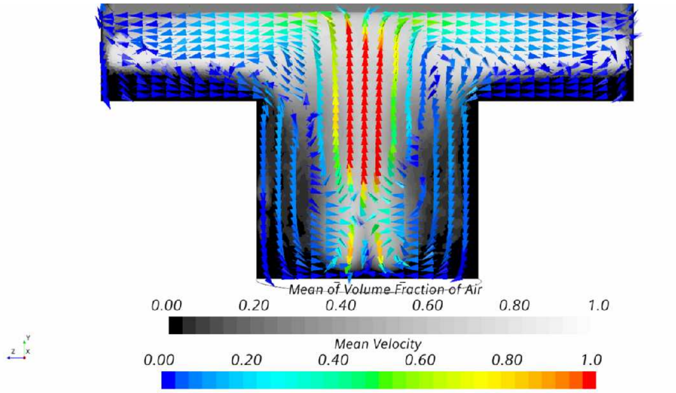
Flow Field



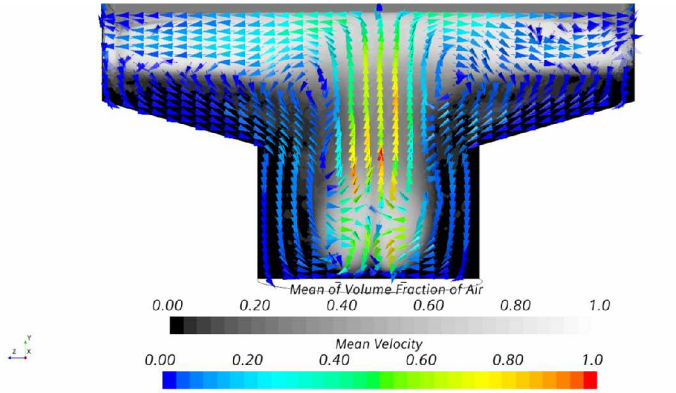
Spacer



Spacer – 3”



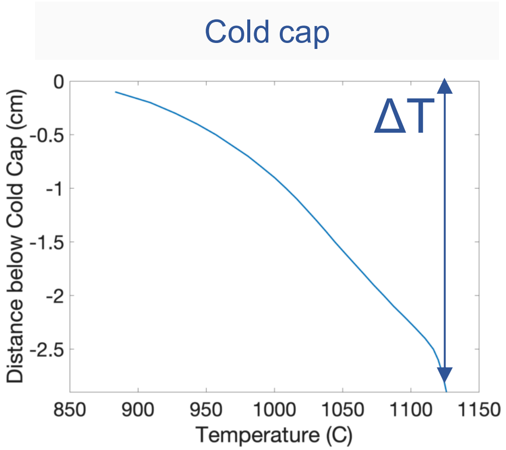
Column

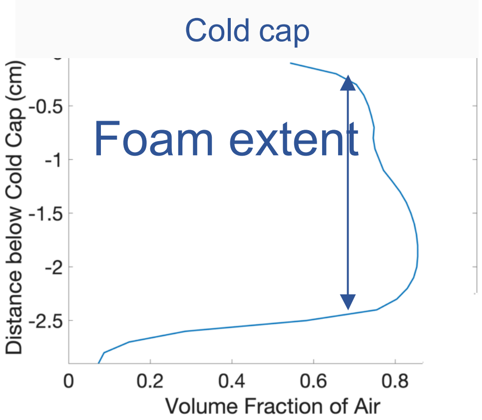


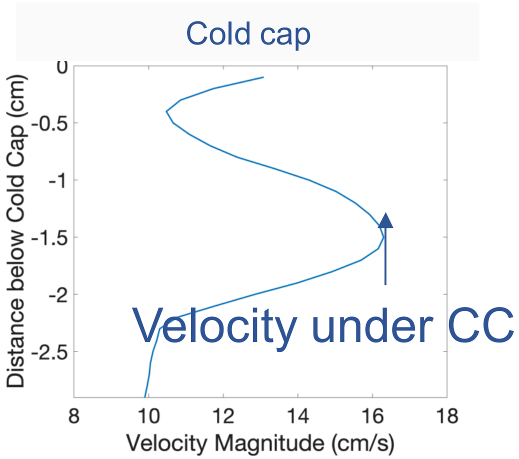
Tapered Column

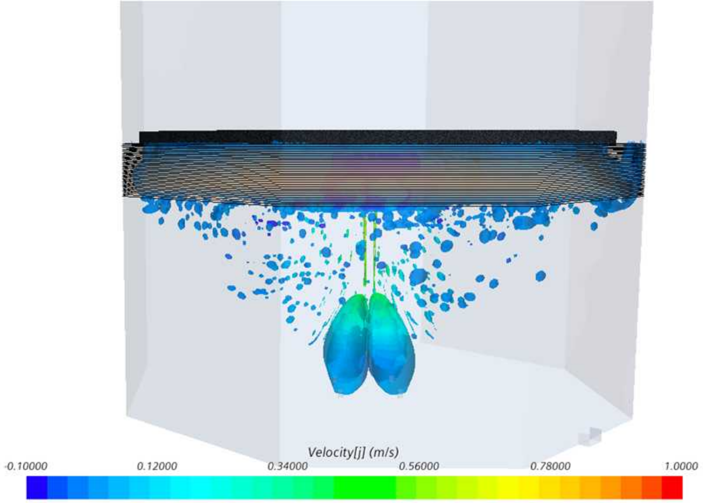
Example Case

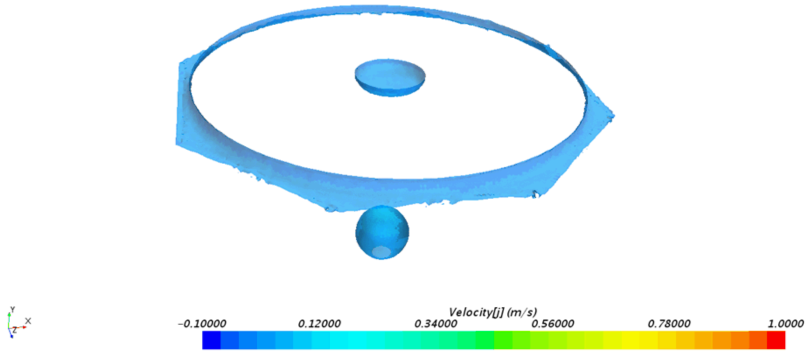
- Temperature, velocity and volume fraction of air under cold cap
- Simulations ran for 10s
- Data time-averaged over last 2s
- Data below cold cap spatially averaged in 1mm intervals





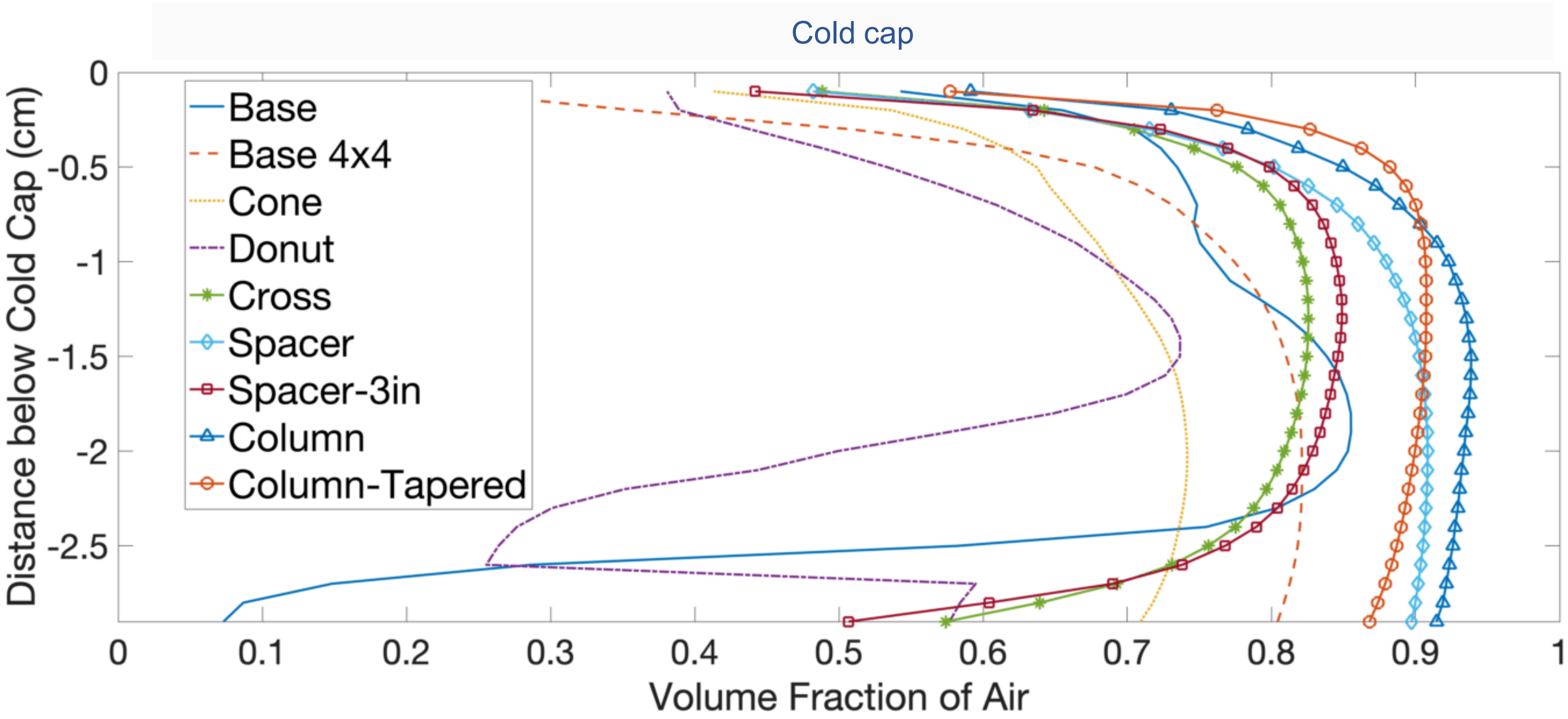






Volume Fraction Profile

- Time/Spatial averaged volume fraction, denotes cavity extent
- Column/spacer trap most air, donut/cone least



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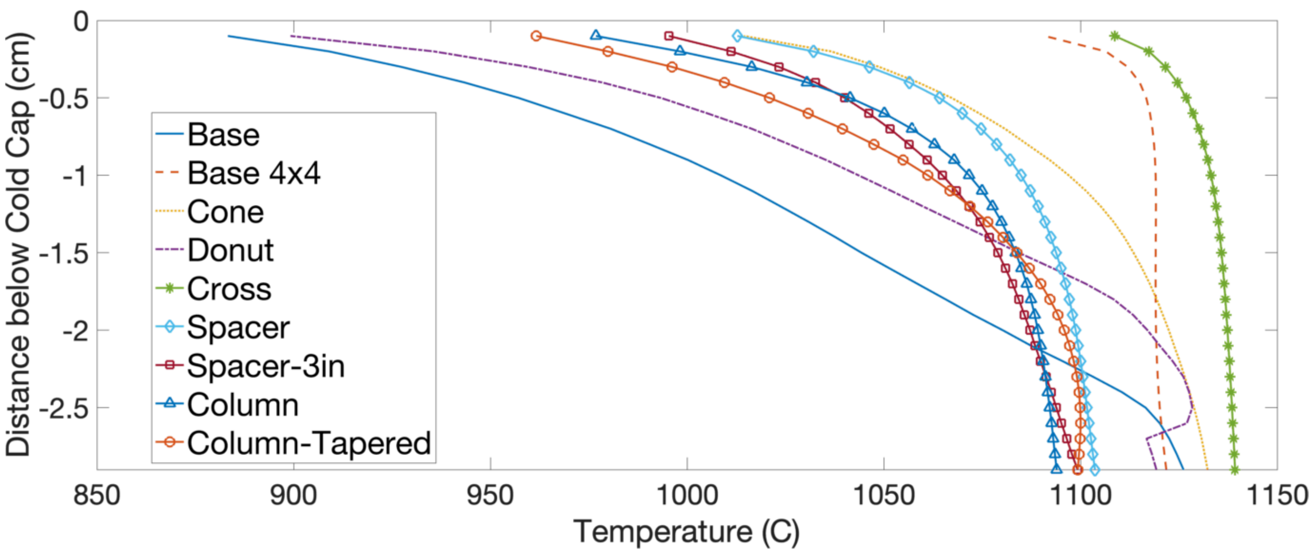
Temperature Profile

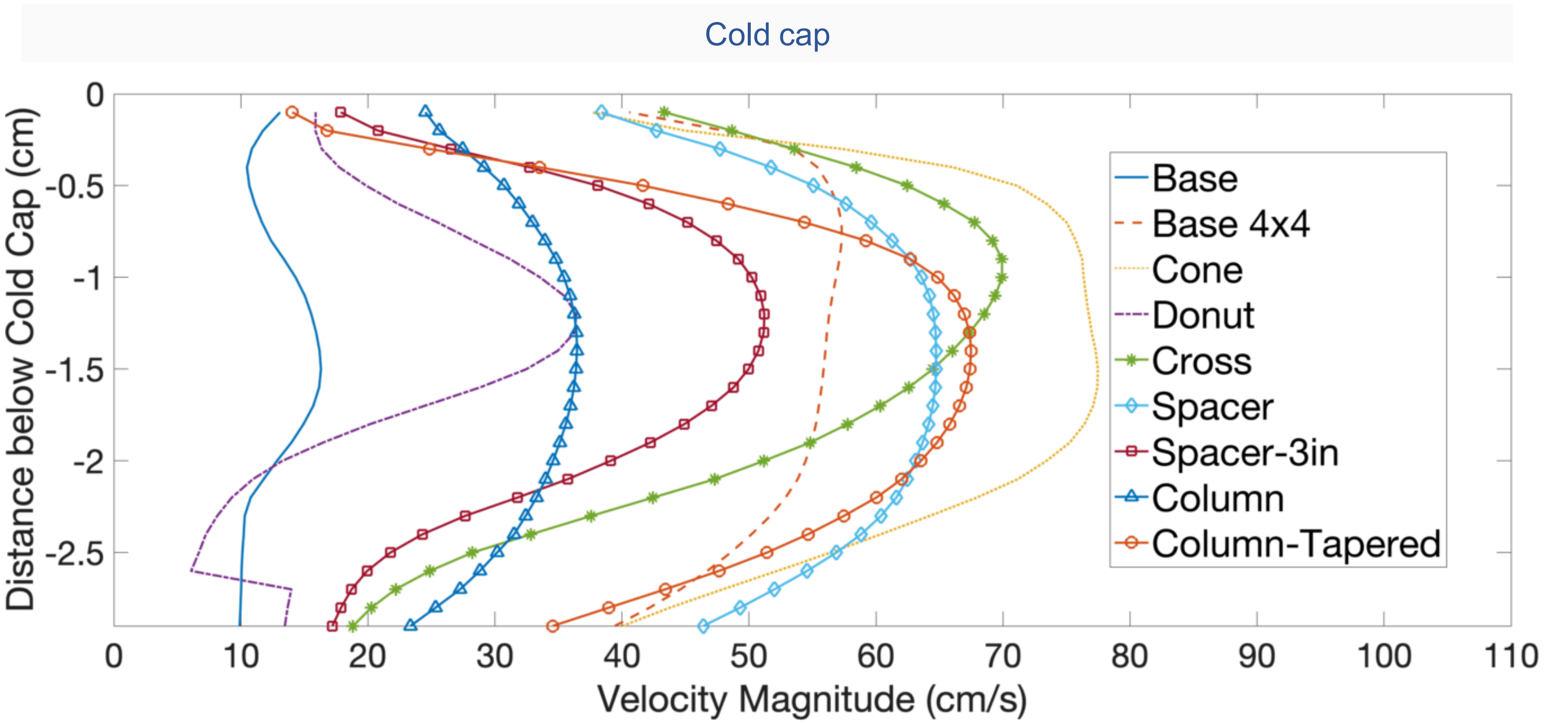
- Shallower ΔT profile in larger height
- Proximity to heat flux boundary shows highest temperatures in cross and base 4x4
- Base 1x and donut lowest temperatures

Cold cap



Velocity Profile

- Highest peak with Cone geometry
- Cross/Cone/Tapered Column similar
- Spacer-3in/Donut perform poorly



Melt Rate Implications

- Assume a 6"H melter with 101 L/m²/min maintains 1500 kg/m²/day process rate
- Assume process rate scales as $v^{0.5}$ ($Re^{0.5}$), and gas composition is still representative at higher processing rate

	Time-&-Spatial-Averaged in Cavity Layer (m/s)	Rate (kg/m²/day)
Base	0.126	1500 (assumed)
Base-4x4	0.526	3066
Cone	0.663	3441
Donut	0.205	1914
Cross	0.519	3045
Spacer	0.581	3222
Spacer-3"	0.366	2555
Column	0.321	2395
Tapered Column	0.529	3073

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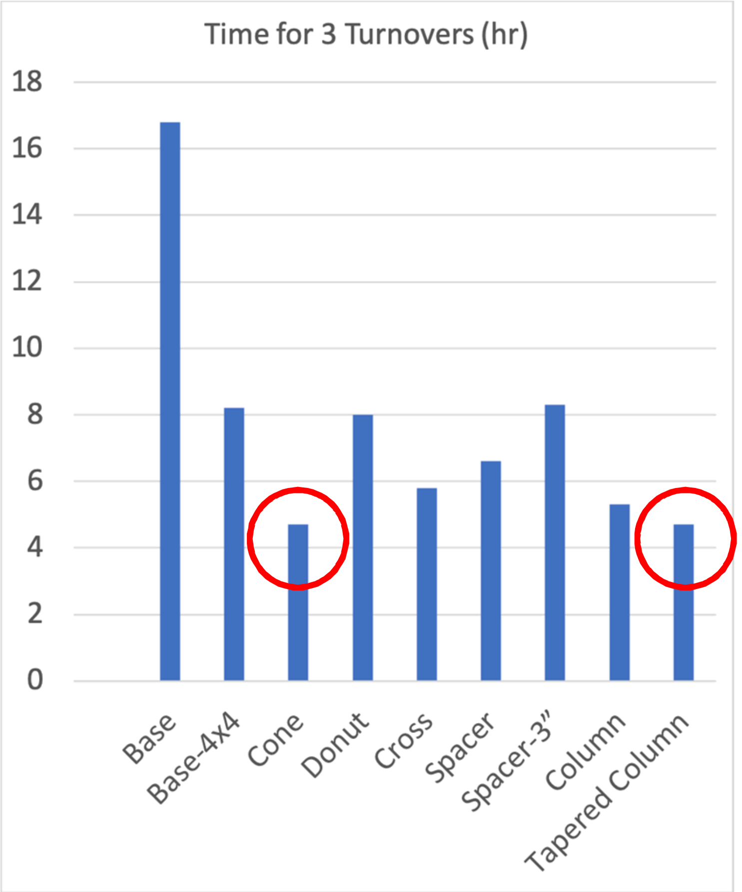
Melt Rate Implications

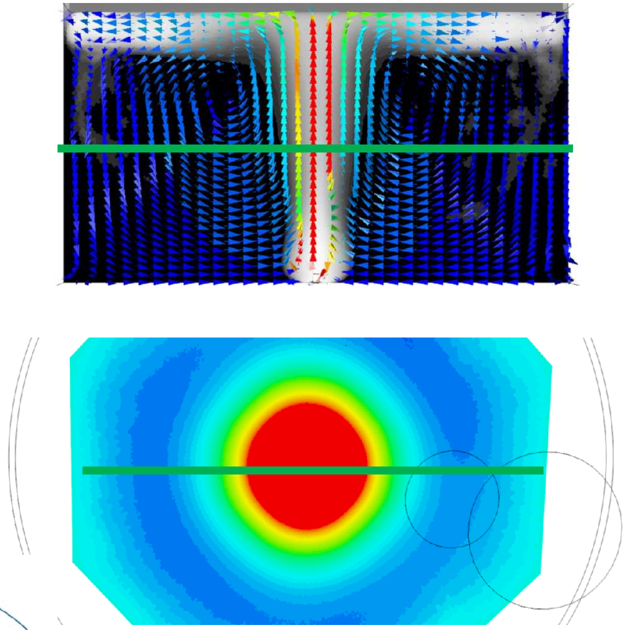
- Based on SA=0.06566 m^2 (12” D octagonal)

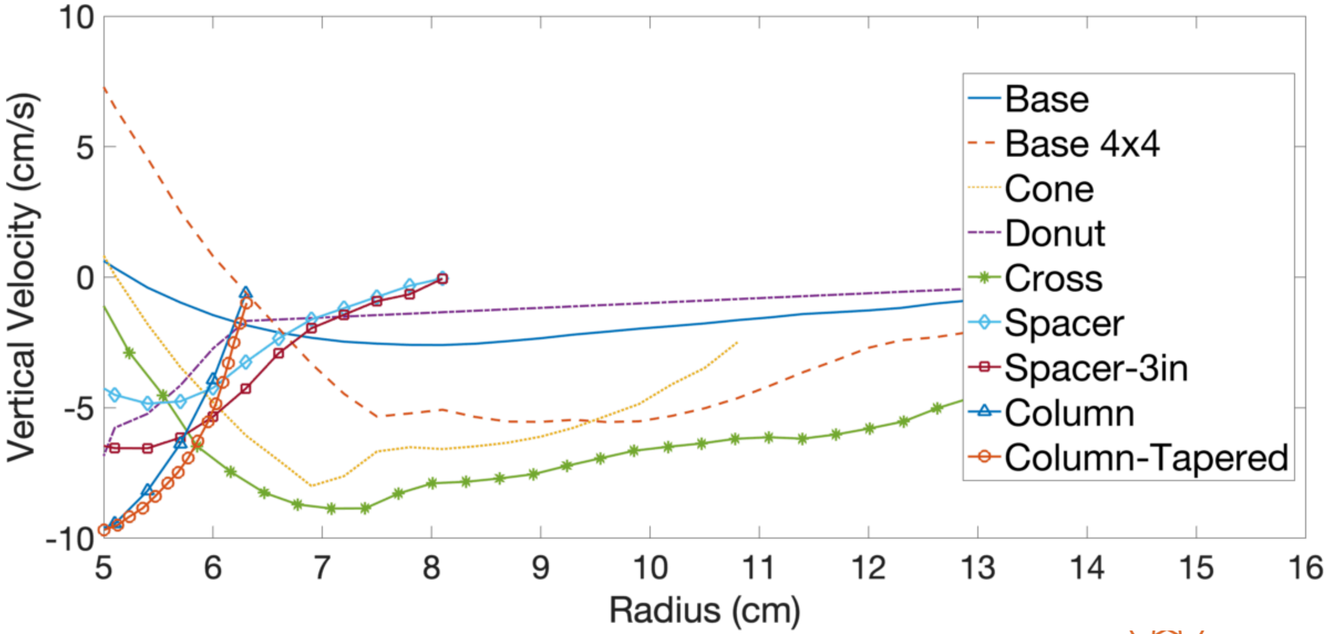
	Rate ($kg/m^2/day$)	6” Depth Glass Volume (L)	Time for 3 Turnovers (hr)
Base	1500 (assumed)	10	16.8
Base-4x4	3066	10	8.2
Cone	3441	6.4	4.7
Donut	1914	6.1	8.0
Cross	3045	7	5.8
Spacer	3222	8.4	6.6
Spacer-3”	2555	8.4	8.3
Column	2395	5.0	5.3
Tapered Column	3073	5.7	4.7



Recirculation

- Time-averaged data across center of melter – plot focus in outer region
- Cross and Cone geometry show best overall recirculation
- Column and Tapered Column show about the same order of magnitude in the same recirculating region





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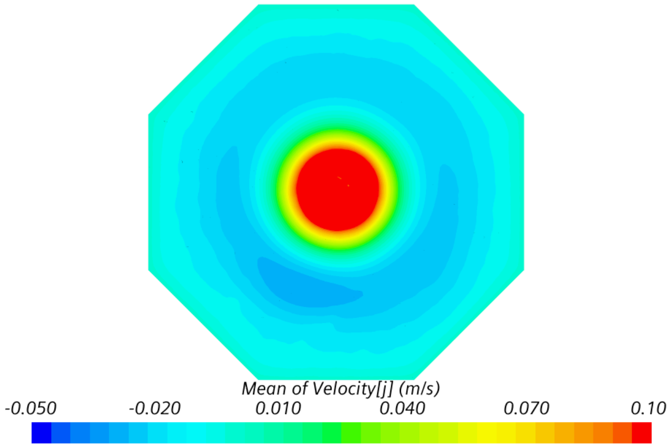
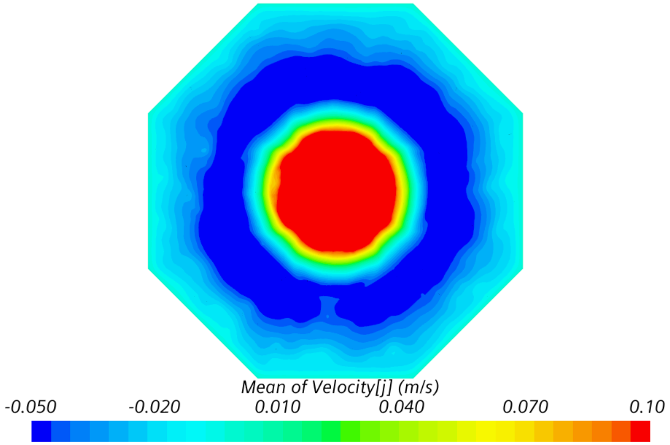
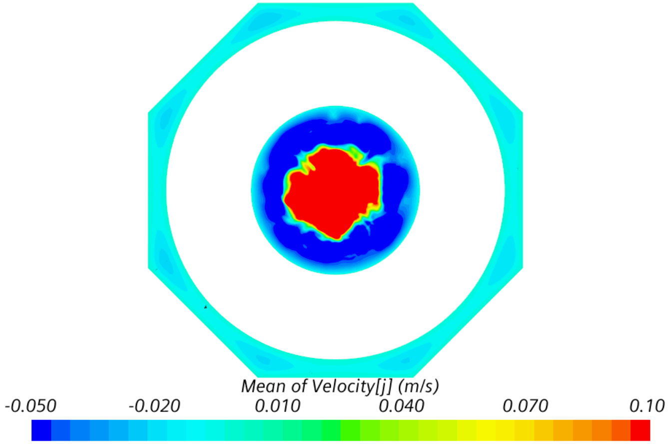
Recirculation – Mid Plane



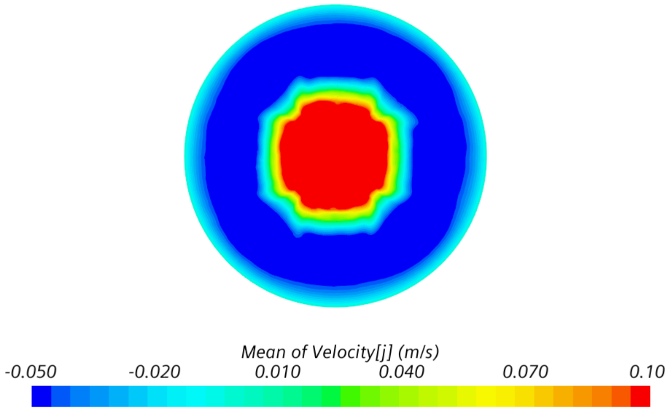
Base



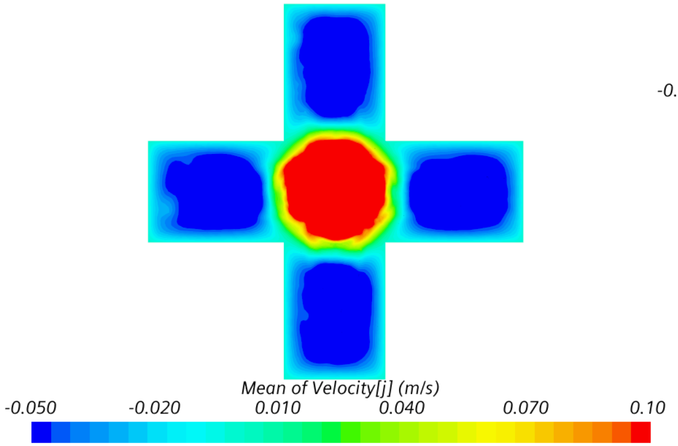
Base 4x4



Donut



Cone



Cross

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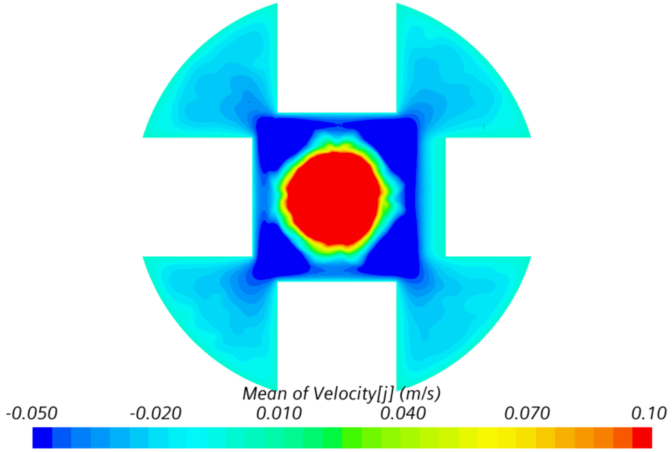
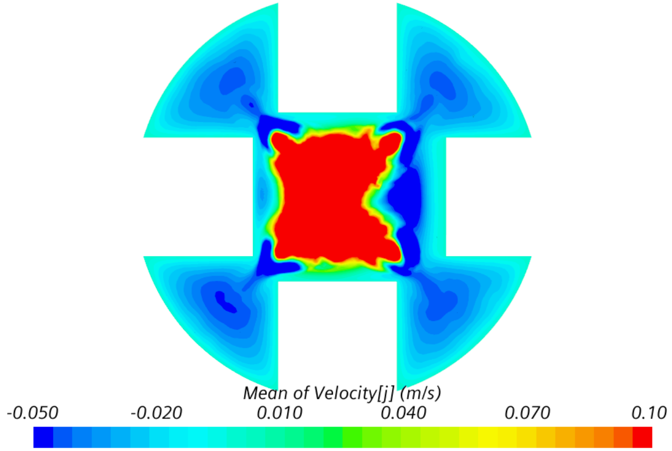
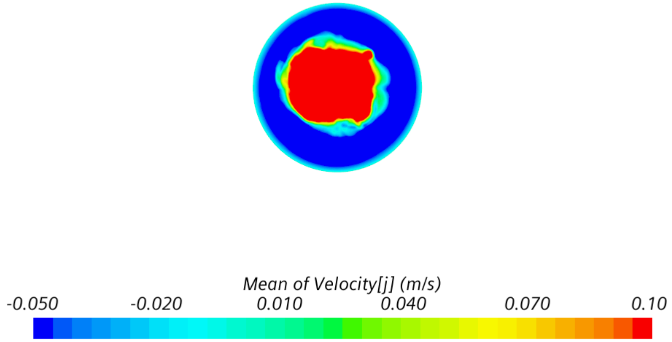
Recirculation – Mid Plane



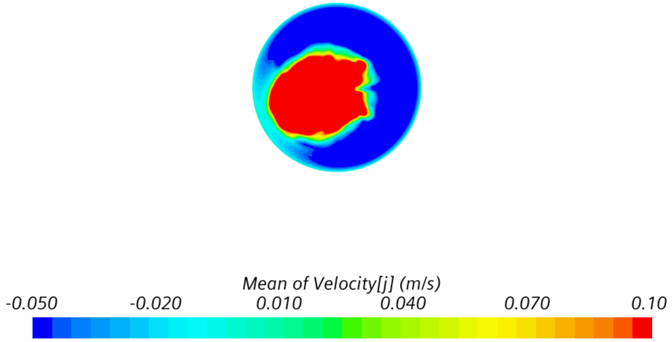
Spacer



Spacer – 3”

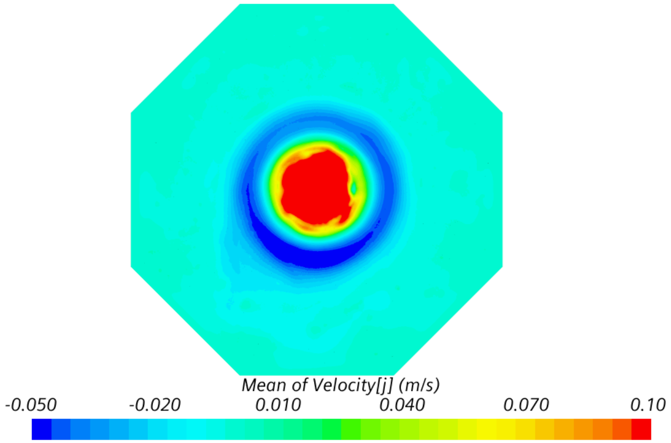


Column

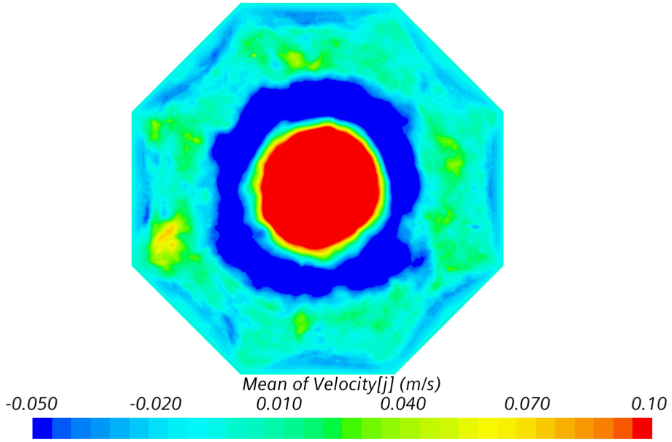


Tapered Column

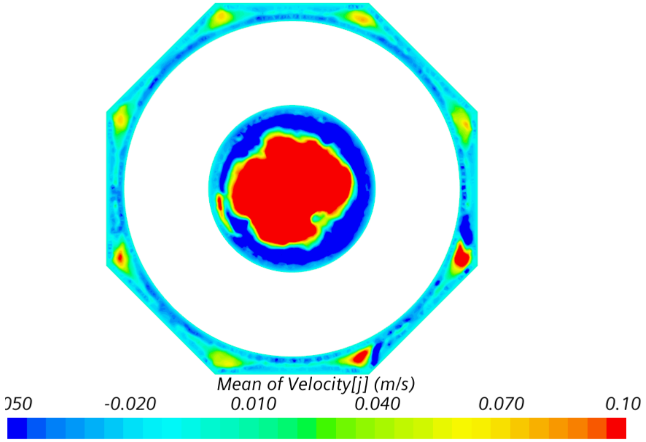
Recirculation – ¾ H (start of cavity layer)



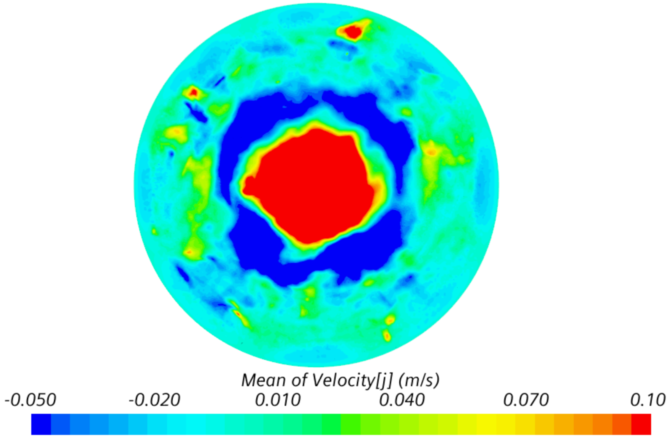
Base



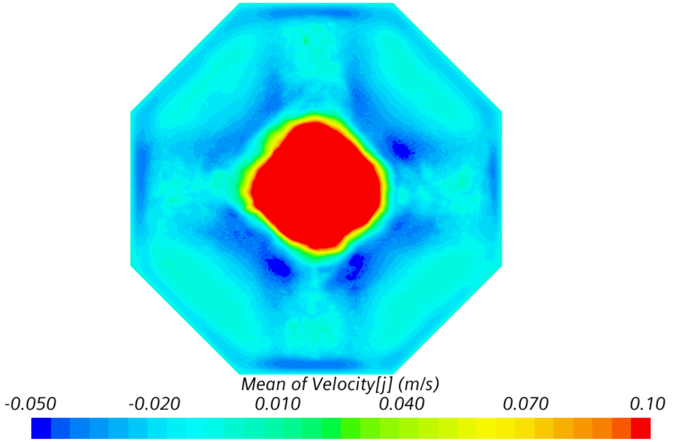
Base 4x4



Donut



Cone



Cross

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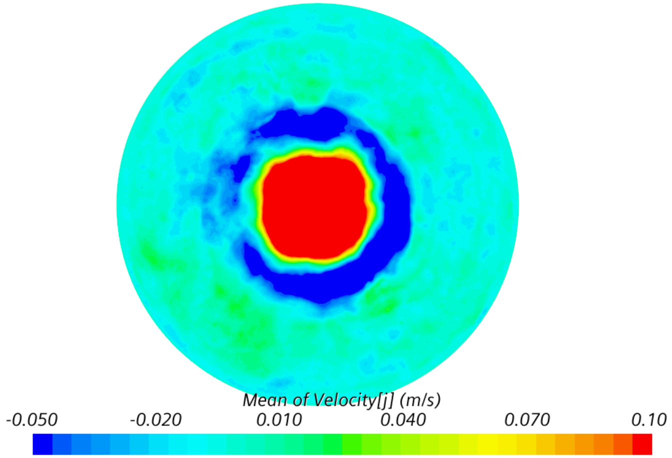
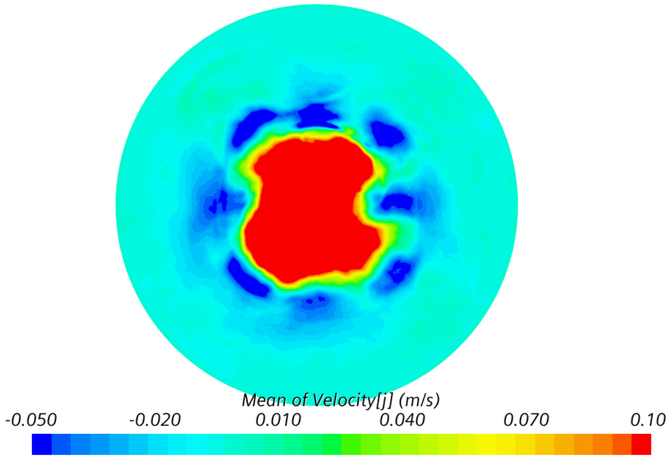
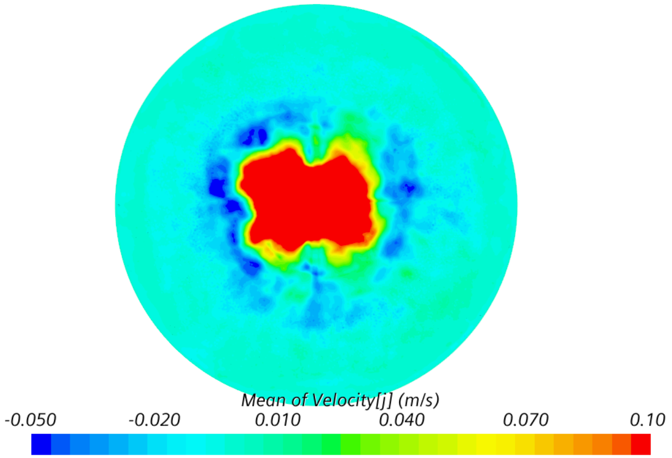
Recirculation – ¾ H - (start of cavity layer)



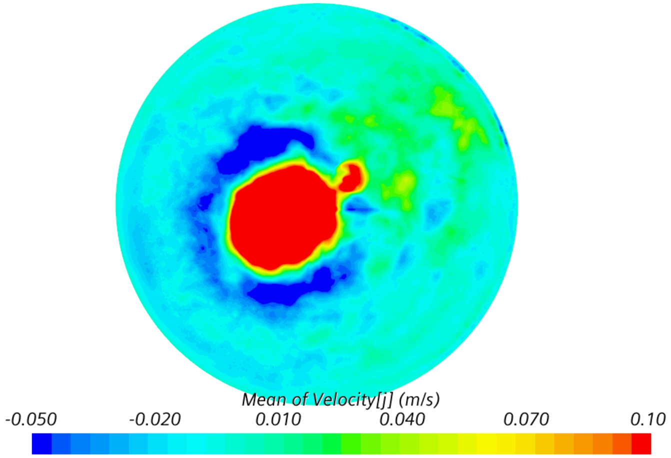
Spacer



Spacer – 3”



Column



Tapered Column

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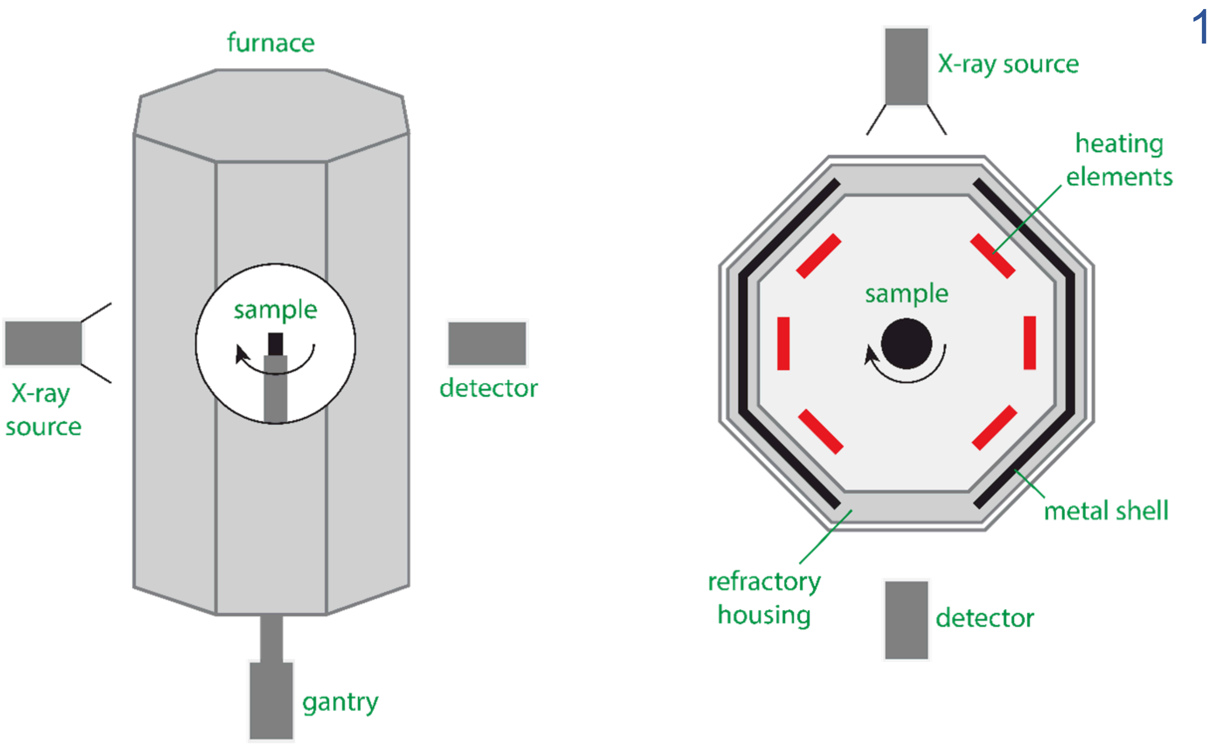
Summary

- Within estimates of melt rate, best geometries for total melt:
  - Cross, Cone, Spacer-2” bubblers, or Tapered Column
  - 7.0, 6.4, 8.4, 5.7 L respectively compared to 10 L base
- Potential for 3.5 x faster runs for experiments, with 50-60% less feed required for Cone or Tapered Column → decrease experimental cost
  - Combination of higher bubbling rates giving higher processing rate
  - Higher Reynolds number in cavity giving higher processing rate
  - Lower total melter volume
- Pursue Cone geometry further – fabrication is easier

Corresponding poster on experimental considerations:
“Melter Optimized for Fast Turnover, Steady State Testing”
WC Eaton (PNNL), MA Hall (PNNL), AW Abboud (INL), DP Guillen (INL), DR Dixon (PNNL), CD Lukins (PNNL), CM Stewart (PNNL), AA Kruger (DOE)

Proposed Validation

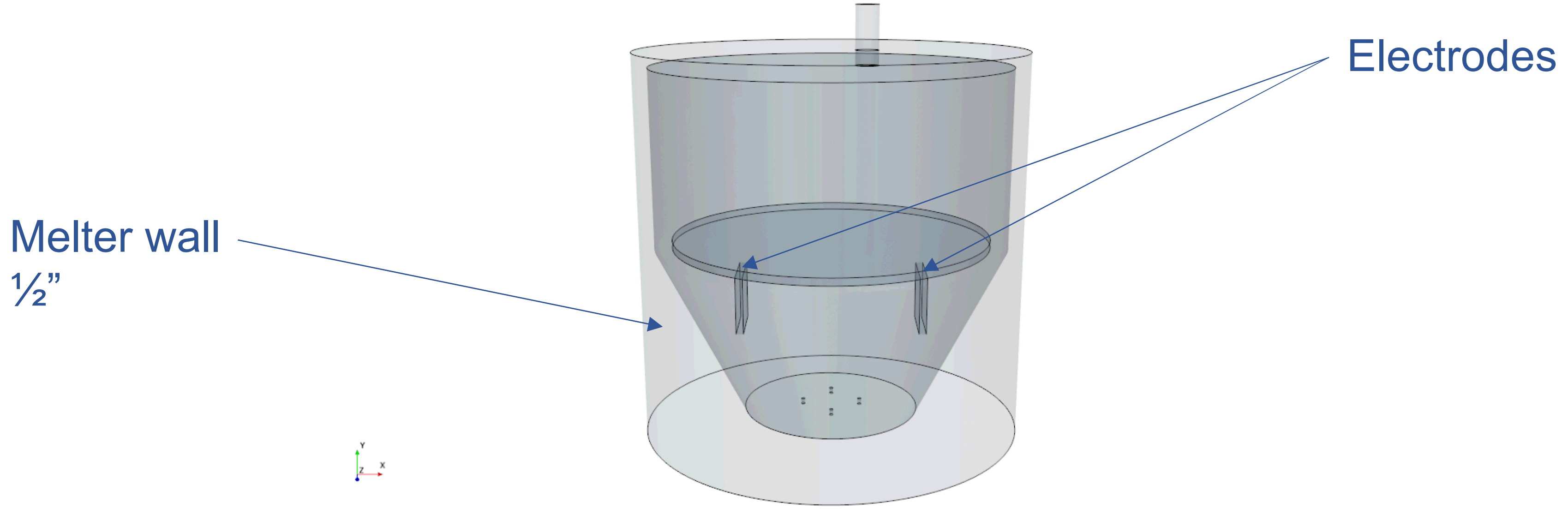
- X-ray CT CLSM for cavity layer[1]
- Use quartz melter design for model comparison of 6” D simulations with surrogate viscous fluid
- Runs at ½ x, 1 x, 2x of bubbling flow
- Low St number particles for tracers
- Camera observations of tracers
  - Based on simulations, outside of the bubbling column fluid velocity is ~1-10 cm/s, shouldn’t need too high framerate for camera



[1]S.A Luksic, R. Pokorny, J. George, P. Hrma, T. Varga, L.R. Reno, A.C. Buchko, A.A. Kruger *“In-situ characterization of foam morphology during melting of simulation waste glass using x-ray computed tomography,” Ceramics International. 2020.*

Future Work

- Perform design optimization of insert configuration with melter
- Incorporate Joule heating
  - Add Inconel 2” square electrodes centered 3” below CC, 6” spacing
  - Set Q_e to boost center glass to 1175 and 1225 ºC
  - Mesh melter walls for potential of current to travel through
  - Try a few placements to see if flow is improved



Acknowledgements

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