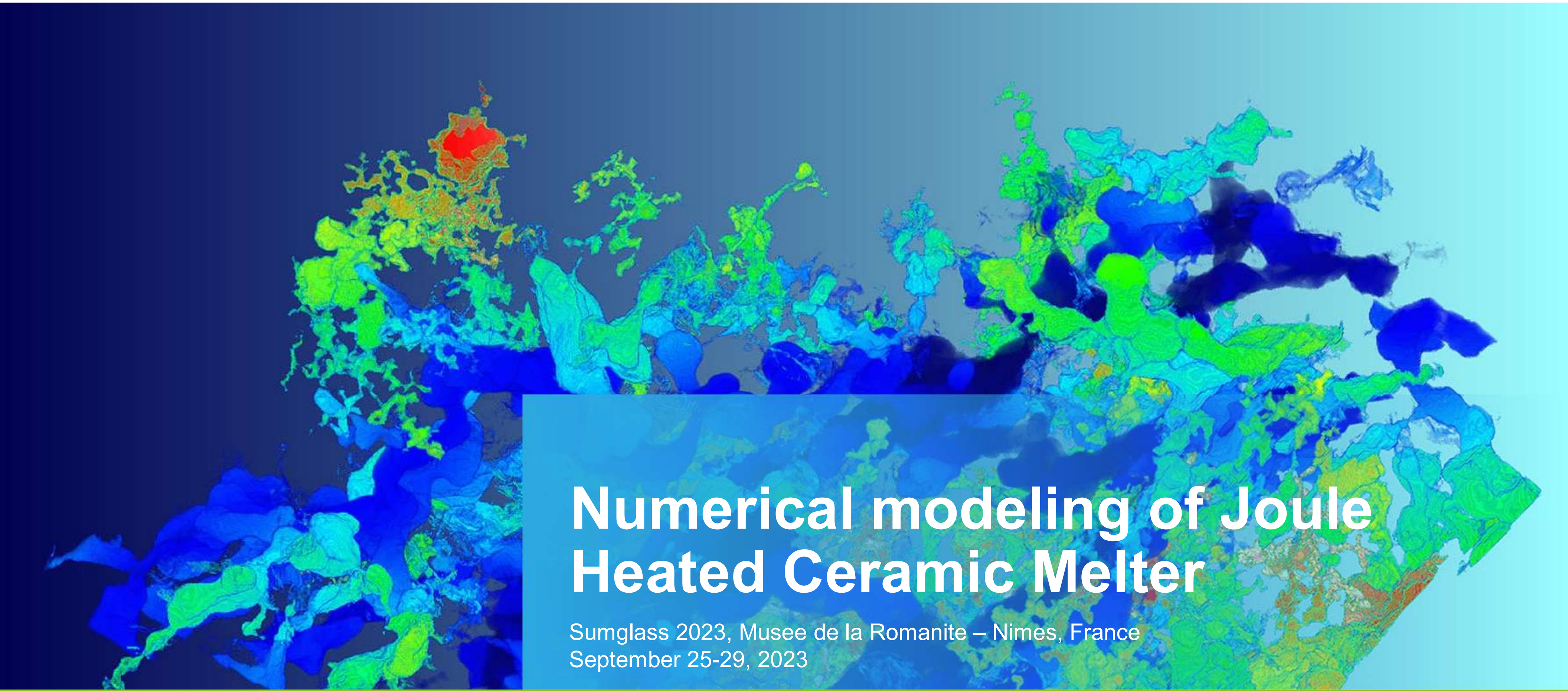

Numerical modeling of Joule Heated Ceramic Melter

Sumglass 2023, Musee de la Romanite – Nimes, France
September 25-29, 2023

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Idaho National Laboratory

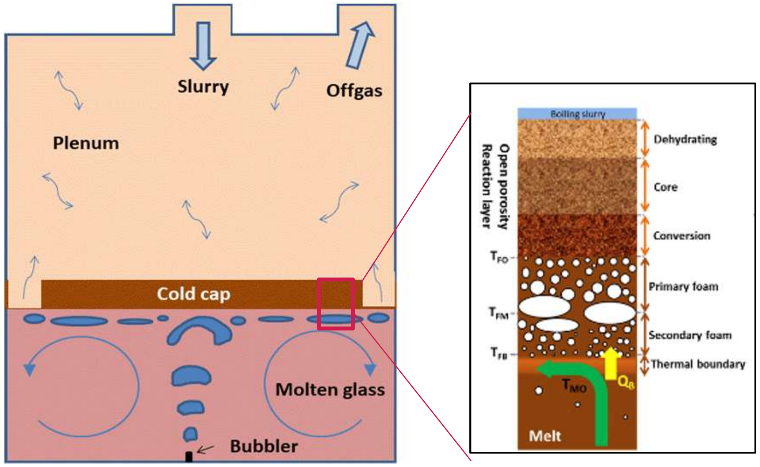
Background

Ref.: Vienna, J.D., Nuclear Waste Vitrification in the U.S.: Recent Developments and Future Options, *IJAGS*, 2010

- Over 210,000 m^3 of tank waste stored at Hanford site from five decades of spent fuel reprocessing
- Historically,177 underground tanks with differing waste compositions across the tanks
- The Waste Treatment and Immobilization Plant (WTP) is being constructed to treat the waste
- Tank waste will be retrieved, the low activity waste (LAW) fraction will be separated from the high level waste (HLW) and vitrified into a stable waste form by adding glass forming materials to the waste in Joule-heated melters, where it will be melted to form borosilicate glass that can be poured into stainless steel containers
- After the glass cools and solidifies, the containers and canisters would be sealed and decontaminated in preparation for storage or permanent disposal

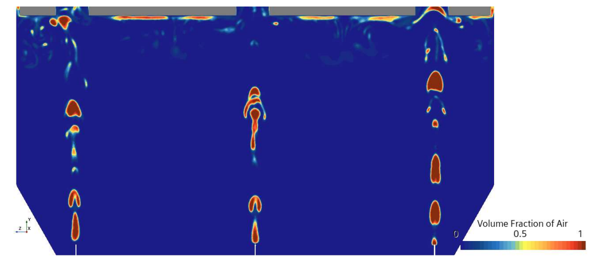
Vitrification Process

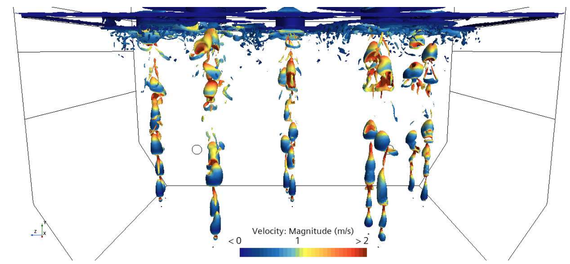
- Within the glass melters, the cold cap is where the batch-to-glass reactions occur
  - The goal is to increase melter throughput by increasing melt rate via heat transfer to the cold cap
- To accomplish this, we must understand how changes to various parameters influence the heating provided to the cold cap, which drives the glass conversion reactions
  - Tank waste is mixed with glass-forming additives to form slurry
  - As the waste slurry is fed to the melter, a cold cap that floats on molten glass is formed
  - Insulating foam layer forms at the base of the cold cap
  - Forced convection bubbling from the base of the melter brings hot glass melt to the vicinity of the cold cap, thus increasing the heat flux to the cold cap bottom, and creates vent holes



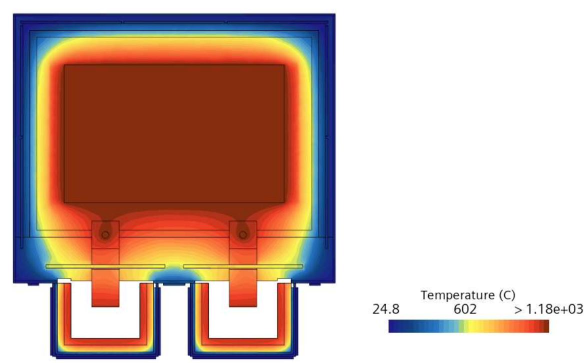
CFD Modeling in Support of Tank Waste Vitrification

- For the past two decades, INL has been providing computational fluid dynamics and heat transfer support to DOE’s Office of River Protection in the form of calculations and simulations
- CFD is a powerful complement to experimental campaigns to provide insight on the factors that influence melter throughput
- A suite of models has been developed for melters over a range of scales including laboratory-, pilot-, and full-scale to facilitate understanding of
  - Forced convection bubbling
  - Offgas generation/Emissions
  - Cold cap behavior
  - Refractory corrosion



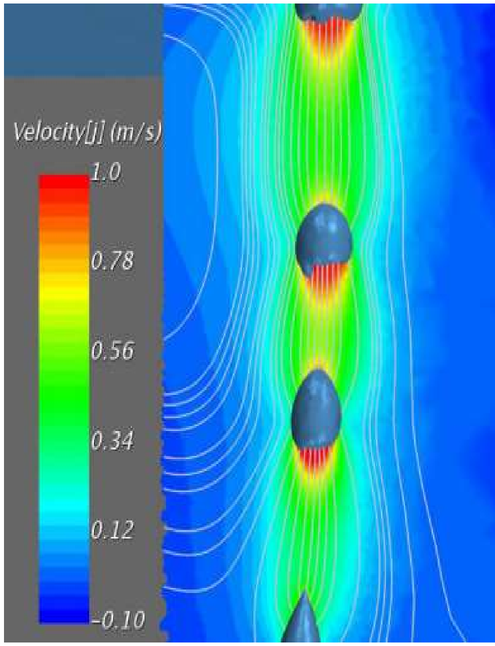


Simcenter STAR-CCM+



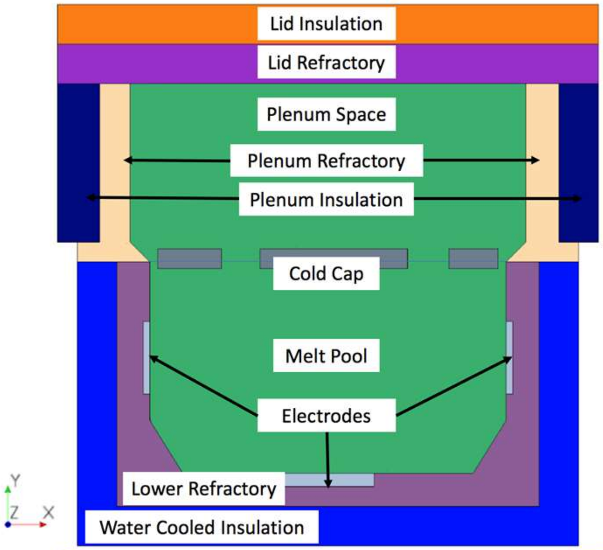
STAR-CCM+ Model Description

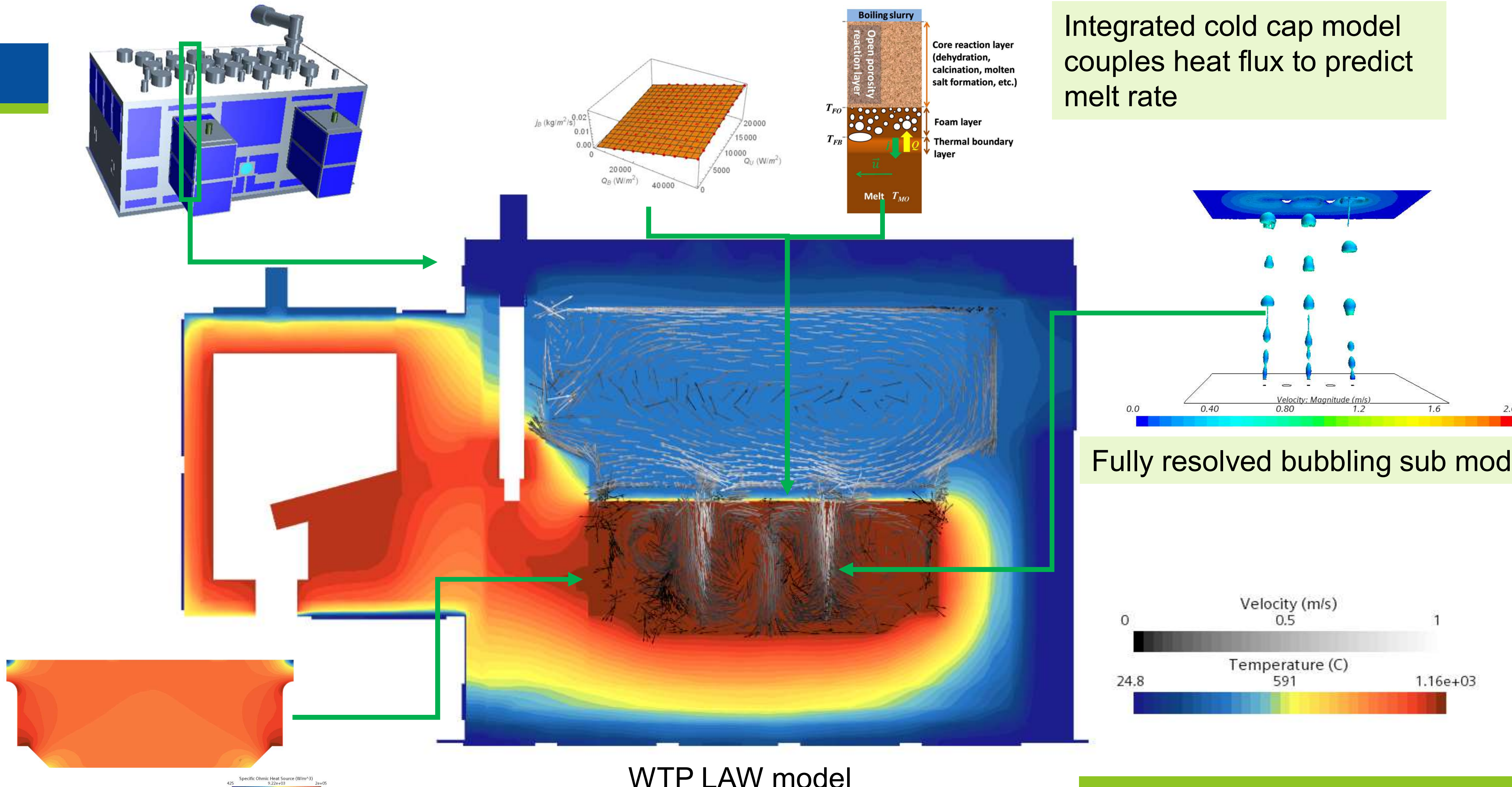
- Eulerian-Eulerian multiphase with volume of fluid (VOF)
  - Finite volume approach with 1st-order implicit time-stepping and 2nd-order spatial discretization
  - The segregated flow solver for the Navier-Stokes equations is used, which can handle constant density or mildly compressible flows with a 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
  - 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 feed
  - Apply constant heat sink for batch to glass transition reactions
- Plenum temperatures can be coupled to off-gas evolution



Melter Model

- A set of computational fluid dynamics and heat transfer models have been developed to complement experimental studies at various scales
  - The goal is to increase melter throughput by increasing melt rate via heat transfer to the cold cap
  - Better fundamental understanding of the melter operation during run-time will ensure reliable processing
- Validation of modeling the multi-physics and cold cap dynamics which occur in the Waste Treatment and Immobilization Plant (WTP) site at Hanford can provide one way to improve the control protocols
- The full-scale melter will not allow for visual observations, and the plenum temperatures can provide immediate feedback regarding the cold cap configuration





Integrated cold cap model couples heat flux to predict melt rate

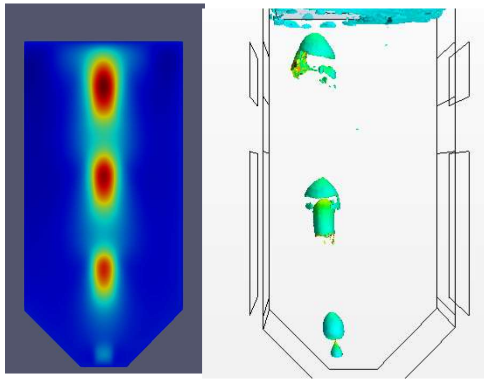
Fully resolved bubbling sub model

WTP LAW model

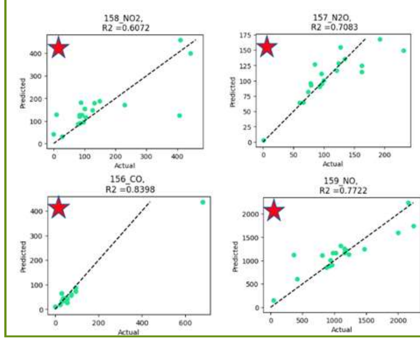
Fully resolved Joule heating of melt pool

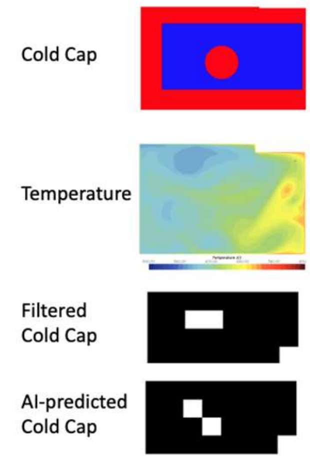
Suite of CFD models developed

Replacing expensive VOF in STAR-CCM+ with momentum source terms

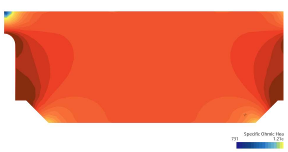


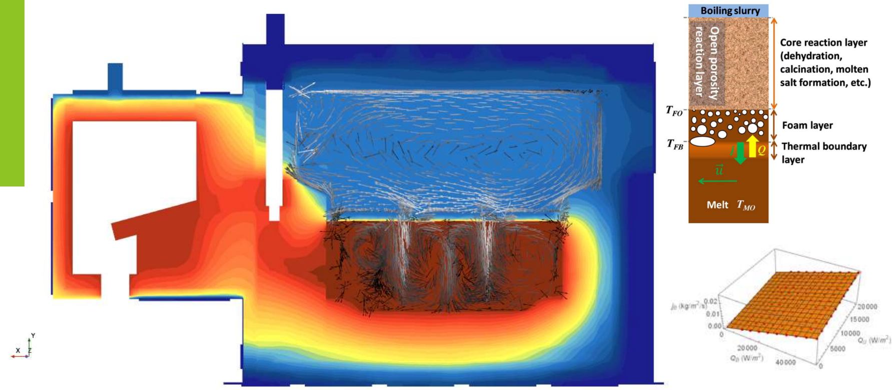
Machine learning for predictions of cold cap coverage and plenum composition



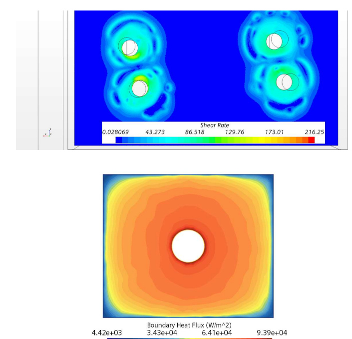


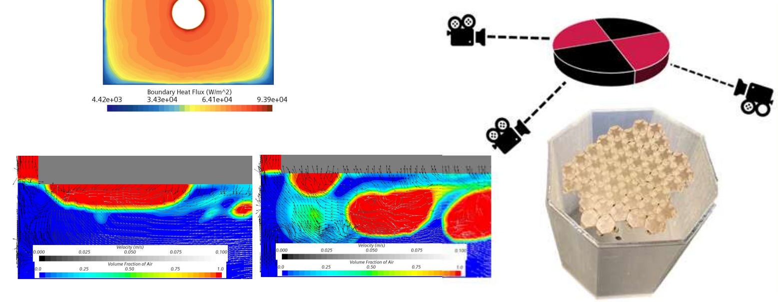
Full-scale WTP with cold cap kinetics, joule heating, and momentum source



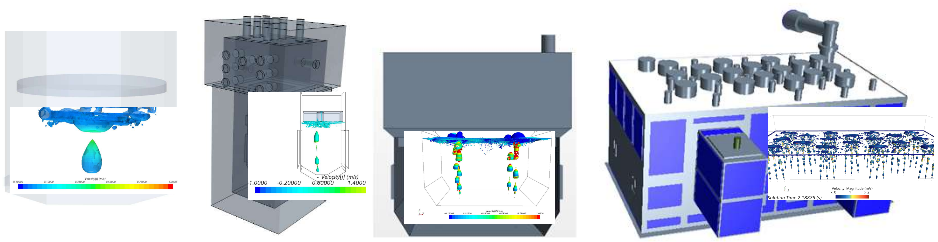


Study of cold cap dynamics: heat flux, foaming, shear, fluid-body interaction





Validation across multiple scales



~0.02 m^2 | 0.1 m^2 | 1.2 m^2 | 10 m^2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Collaborative Computing Center
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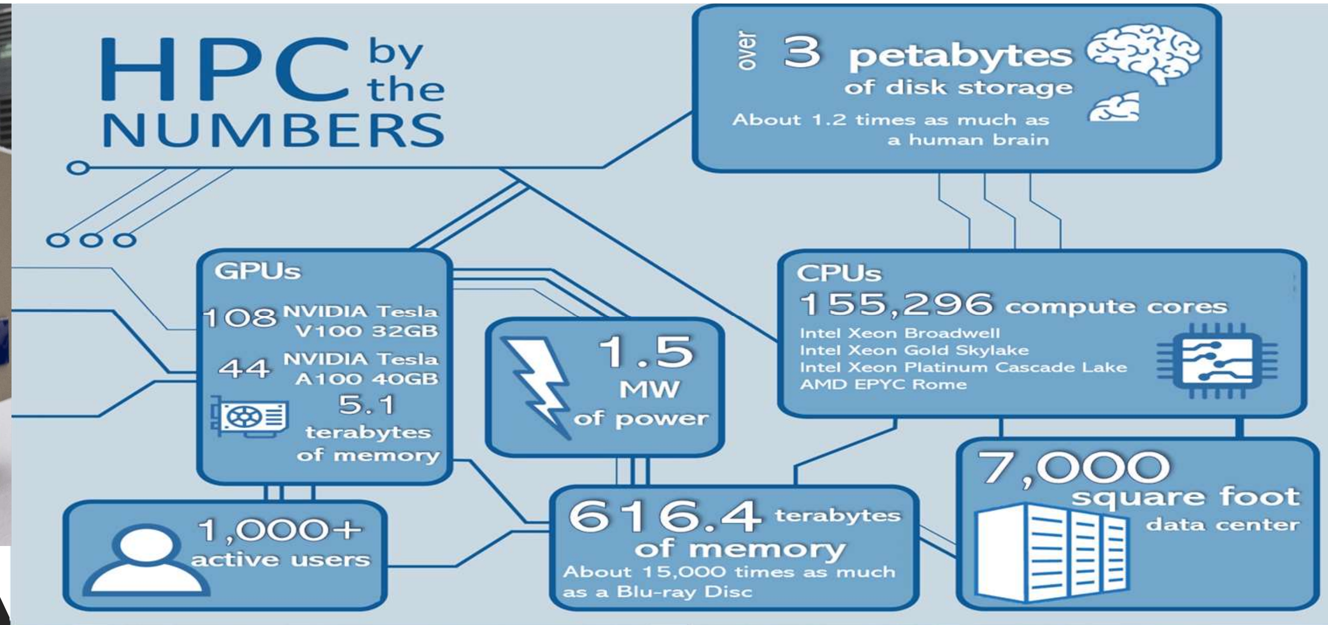
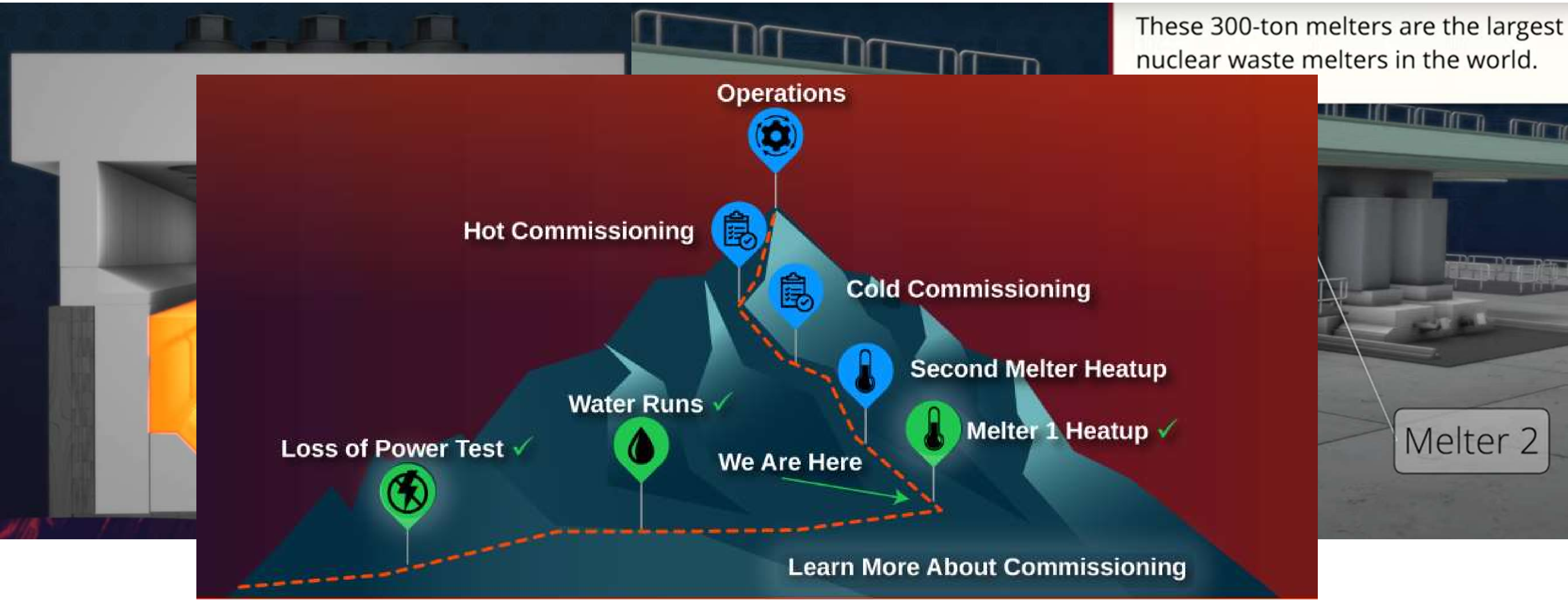

HPC by the NUMBERS
over 3 petabytes of disk storage
About 1.2 times as much as a human brain
GPUs
108 NVIDIA Tesla V100 32GB
44 NVIDIA Tesla A100 40GB
5.1 terabytes of memory
1.5 MW of power
CPUs
155,296 compute cores
Intel Xeon Broadwell
Intel Xeon Gold Skylake
Intel Xeon Platinum Cascade Lake
AMD EPYC Rome
1,000+ active users
616.4 terabytes of memory
About 15,000 times as much as a Blu-ray Disc
7,000 square foot data center

INL HPC


Sawtooth
HPE SGI 8600
~6 Petaflops Max Performance
12 11 10 9 8 7 6 5

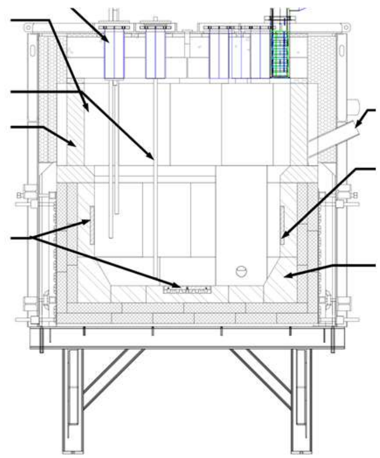
WTP LAW Melters

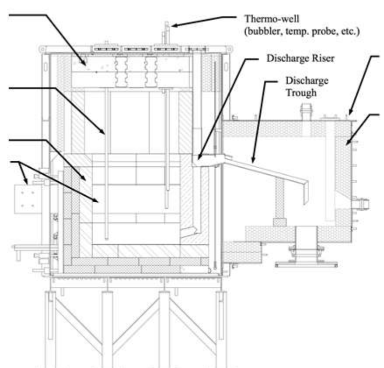


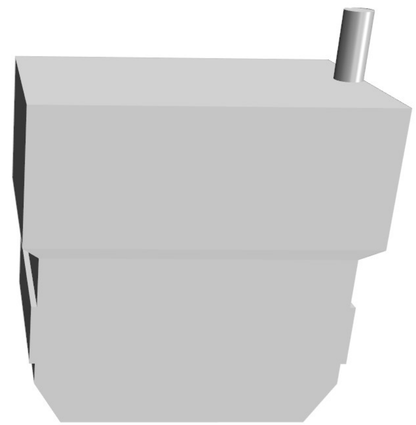
Commissioning is underway with startup anticipated in 2025

DuraMelter (DM1200) Tests

- Pilot-scale melter of the WTP facility with simulant waste glass
  - Experimental campaign conducted by Vitreous State Laboratory (VSL)
- 0.813 m pool depth with 1.2 m^2 surface area
  - Approximately 32% of the surface area, and 57% of the pool height of the WTP
- Heated with two side Inconel electrodes





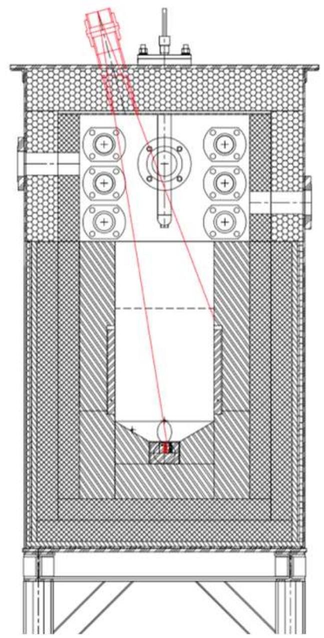


Matlack, K, Gan H, Chaudhuri M, Kot W, Gong W, Bardakci, T., et al. Final Report DM100 and DM1200 Melter Testing with High Waste Loading Glass Formulations for Hanford High-Aluminum HLW Streams, VSL-10R1690-1 Rev. 0. The Catholic University of America, Vitreous State Laboratory; 2010.

Duramelter 100 (DM100) Designs

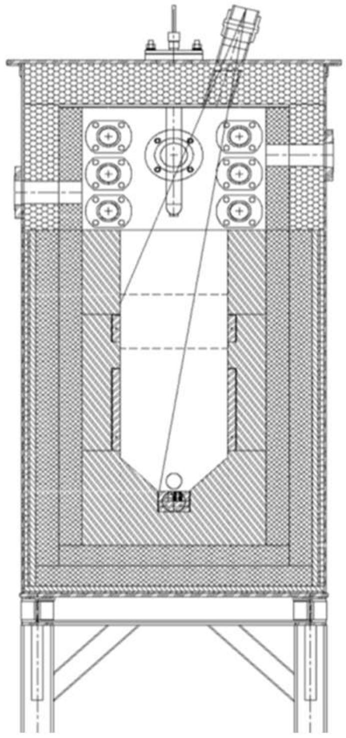
- DM100 melters were designed to examine the effects of different glass formulations and operational parameters on the waste processing rate and product quality
  - Testing of simulant feeds performed by VSL
- There are two versions of the DM100 melters with identical melt pool surface area and plenum region
  - DM100-WV
    - 19” glass depth, primarily used for LAWs
    - One set of electrodes
  - DM100-BL
    - 29” glass depth, primarily used for HLWs
    - Two sets of electrodes
- Both have outer mica plate insulation, rather than water cooling jackets (as used in full-scale design)

DM100-WV



Kruger, A.A., et al. VSL06R6480 DM100 Tests to Support LAW Glass Formulation Correlation Development, Catholic University of America, 2006.

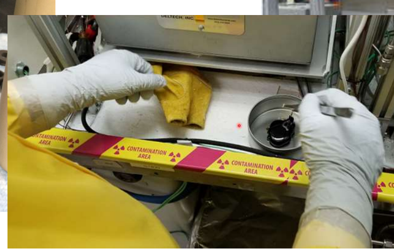
DM100-BL



Matlack, K.S., et al. VSL05R5710 DM100 HLW Simulant Validation Tests with C106/AY102 Feeds, Catholic University of America, 2005.

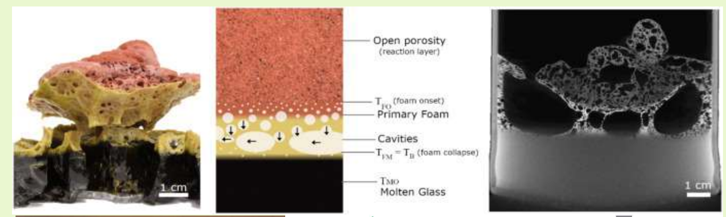
Continuous Laboratory Scale Melter (CLSM)

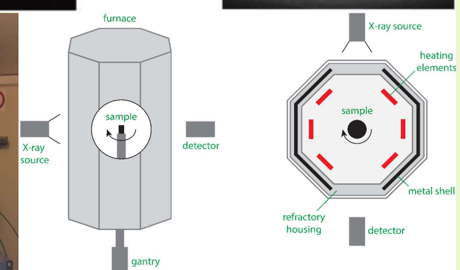
- CLSM small-scale model testing at PNNL
  - 93.5 cm^2 cold cap surface area, 6.35 cm glass depth
- Made of Inconel for high temperature tests at 1150°C
- Heat supplied by external furnace
- Bubbler and feed tubes inserted from top
- Offgas port removes reaction gases
- Two systems are in service processing simulated and actual tank waste



CFD validation planned using X-ray tomography images of the CLSM

3-D characterization of bulk volume, bubble size, and distribution over a range of temperatures during batch-to-glass conversion

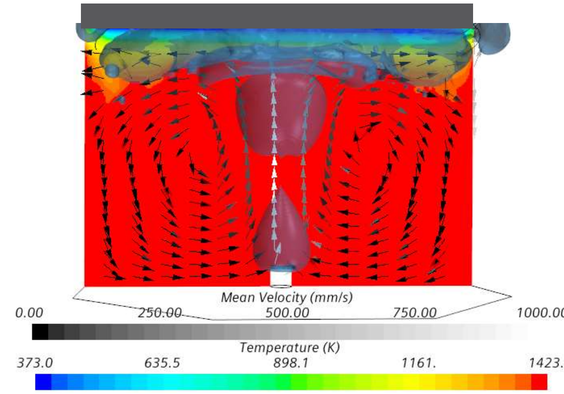


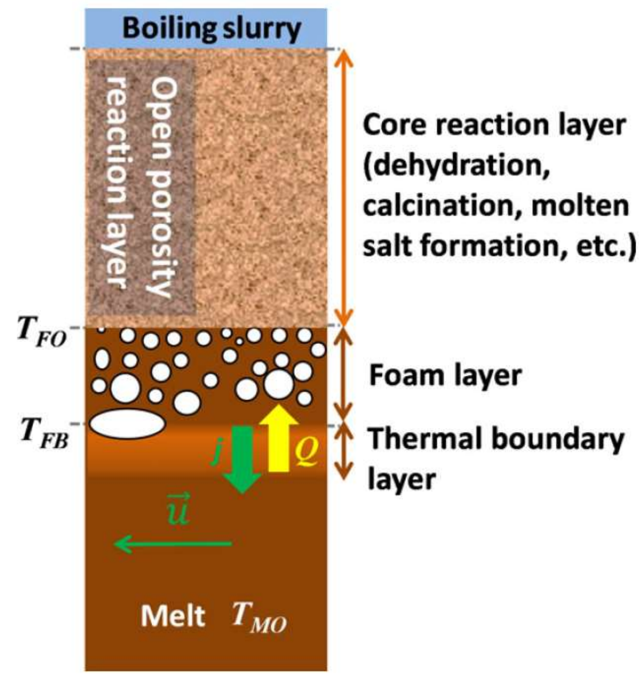


Luksic, Steven A., et al. "In situ characterization of foam morphology during melting of simulated waste glass using x-ray computed tomography." *Ceramics International* 46.11 (2020): 17176-17185.

Cold Cap Representation

- Cold cap submodel integrated into melter model solves coupled kinetic and thermal equations
  - Kinetic equation predicts the conversion profile within cold cap
  - Energy equation yields the temperature profile within the cold cap
- Resolve bubbling, velocity profiles, cavity layer immediately below cold cap
- Updated cold cap representation will allow for changing boundary conditions based on heat flux to predict melting

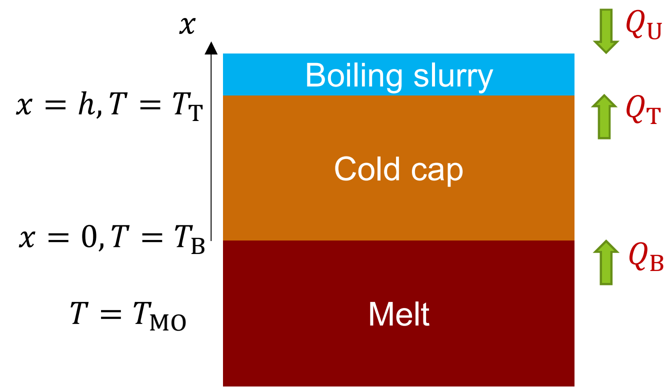


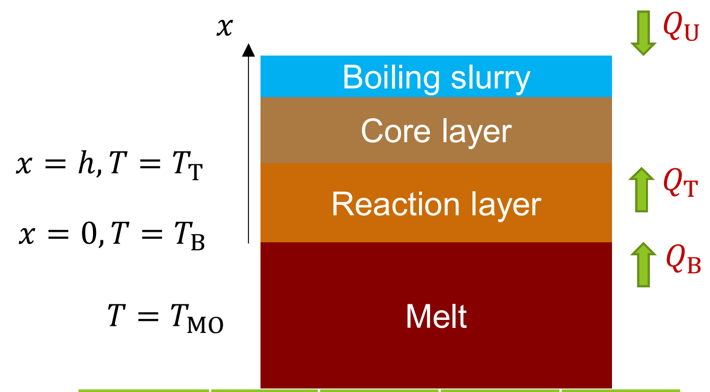


Abboud, A. W., Guillen, D. P., Hrma, P., Kruger, A. A., Klouzek, J., & Pokorny, R. (2021). Heat transfer from glass melt to cold cap: Computational fluid dynamics study of cavities beneath cold cap. *International Journal of Applied Glass Science*, *12*(2), 233-244.

Cold Cap Structure

- Boiling slurry typically does not cover the entire top surface of the cold cap.
- Thicker cold cap can temporarily build up on portion of the cold cap where new slurry is fed. The melting rate depends conditions inside the reaction layer and not on conditions in the overall cold cap.
- Core layer has elevated temperature.
- About 50% of heat is consumed by water evaporation.
- Core layer is expected to be transient, so there is still heat coming to core layer from reaction layer. Boundary of core and reaction layer is defined by temperature.
- Explored two options:
  - No core layer, temperature of top surface 100°C
  - Core layer with elevated temperature 400°C

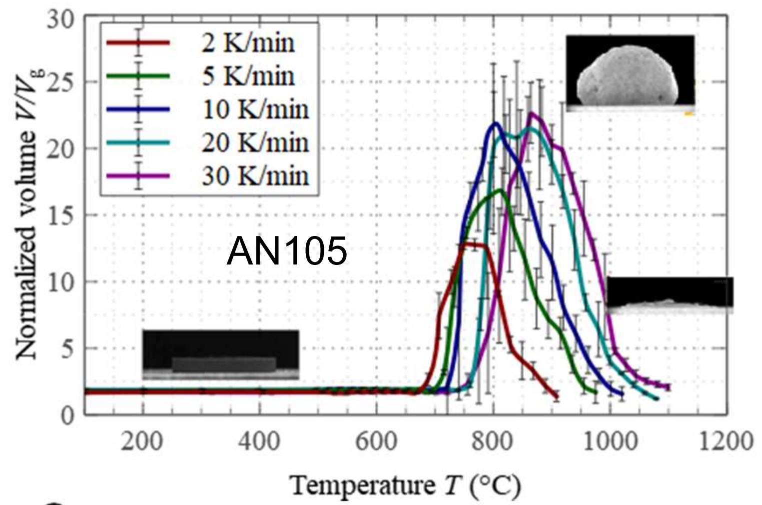


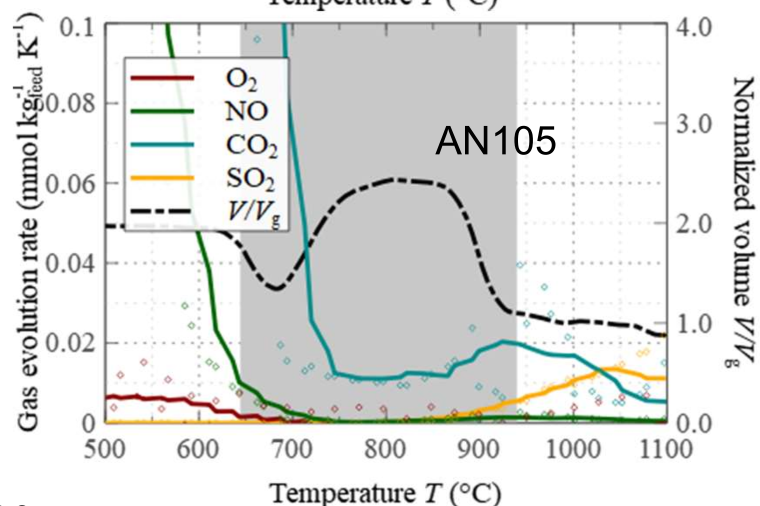


Feed	ΔH_W (J/g)	ΔH_R (J/g)	ΔH_S (J/g)	ΔH (J/g)
AI19	3677	1087	1155	5919
NGFe2	3339	582	1155	5076
AN105	1805	-223	1155	2737
AZ102	1669	227	1155	3216

Estimate Temperature at Cold Cap Bottom

- Initial estimate of this temperature is based on FET and EGA and it can be associated with a value dissolved silica fraction
- Unlike in the laboratory, the cold cap in an operational melter will experience a highly non-linear temperature history. This is considered by:
  - Estimating temperature profile inside the cold cap using 1D heat transfer model
  - Developing conversion kinetics model based on dissolved silica fraction that can be used for any temperature history
- Reduced model must be developed to enable fast evaluation in CFD code by parameterizing model results for Q_U and Q_B.



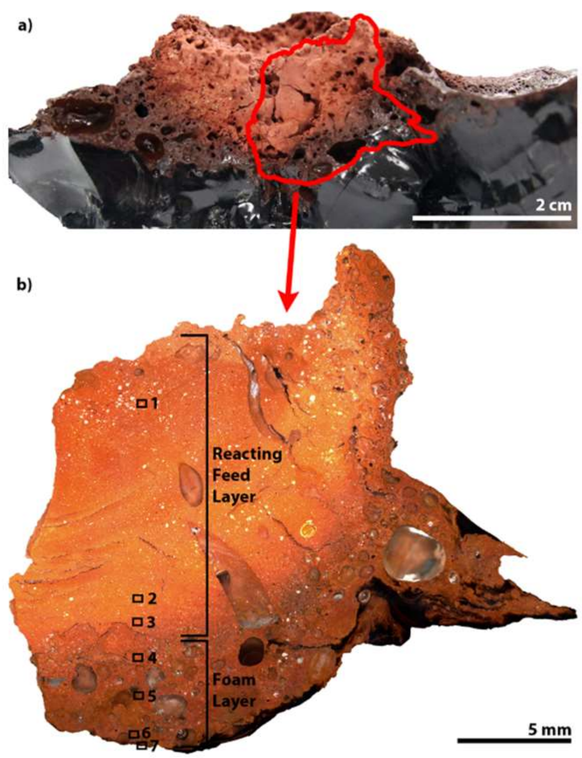


Hujova, M., Pokorny, R., Klouzek, J., Lee, S., Traverso, J. J., Schweiger, M. J., ... & Hrma, P. (2018). Foaming during nuclear waste melter feeds conversion to glass: Application of evolved gas analysis. *International Journal of Applied Glass Science*, *9*(4), 487-498.

Lee, S., VanderVeer, B. J., Hrma, P., Hilliard, Z. J., Heilman-Moore, J. S., Bonham, C. C., ... & Kruger, A. A. (2017). Effects of heating rate, quartz particle size, viscosity, and form of glass additives on high-level waste melter feed volume expansion. *Journal of the American Ceramic Society*, *100*(2), 583-591.

Cold Cap Model

- Cold cap model solves coupled kinetic and thermal equations
  - Kinetic equation predicts the conversion profile within cold cap
  - Energy equation yields the temperature profile within the cold cap
- Developed for four feeds so far
  - Two LAW feeds
    - AN105
    - AZ102
  - Two HLW feeds
    - NGFe2
    - AI19
- Additional models for AP105 and AP107 in process



Conversion Kinetics

- Conversion kinetics model is based on XRD data of silica dissolved fraction
- To obtain dissolution rate, data is first fitted to an empirical continuous function

$$f = 1 - c_0 \exp\left(\left(\frac{T}{T_0(1+\Phi/\Phi_0)}\right)^{p_0}\right) - (1-c_0)\exp\left(\left(\frac{T}{T_1(1+\Phi/\Phi_1)}\right)^{p_1}\right)$$

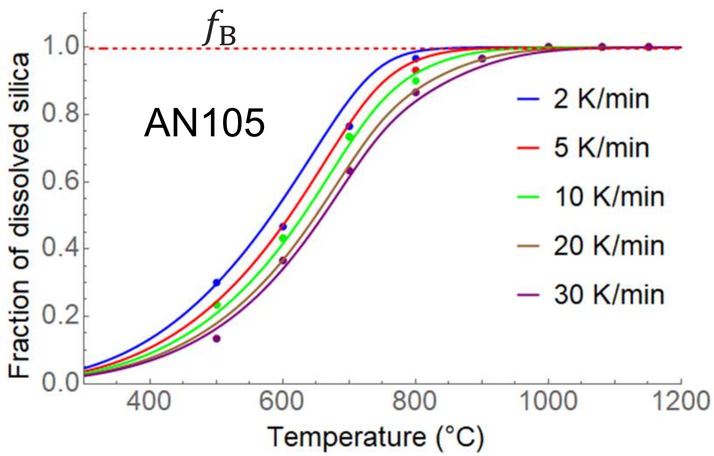
- When multiple steps are used, each peak is fitted separately to Sestak-Berggren model

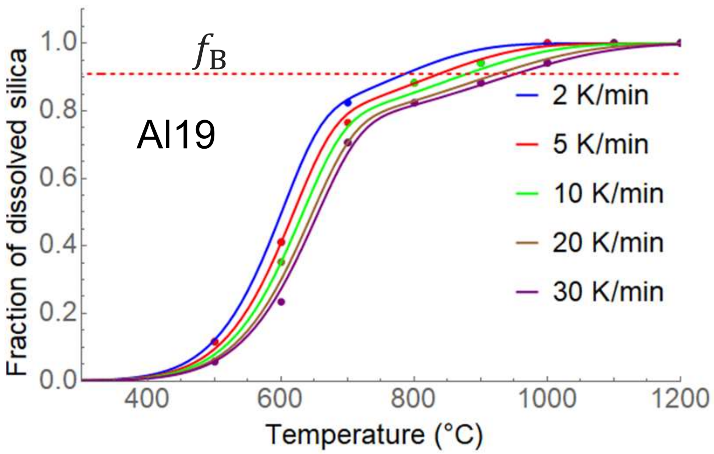
$$\frac{df_i}{dt} = A_i f_i^m (1-f_i)^n \exp\left(-\frac{E_i}{RT}\right)$$

- Complete kinetic model is then given by

$$\frac{df}{dt} = c_0 \frac{df_0}{dt} + (1-c_0)\frac{df_1}{dt}$$

- Boundary condition at batch-melt interface $f\big|_{x=0} = f_B$





Cold Cap Model – Temperature Profile

- Assumes 1D heat and mass transfer
- Cold cap top covered with boiling slurry
- Local steady-state heat balance of cold cap

$$\left(j_b c_{p,b} - j_g c_{p,g}\right)\frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right)$$

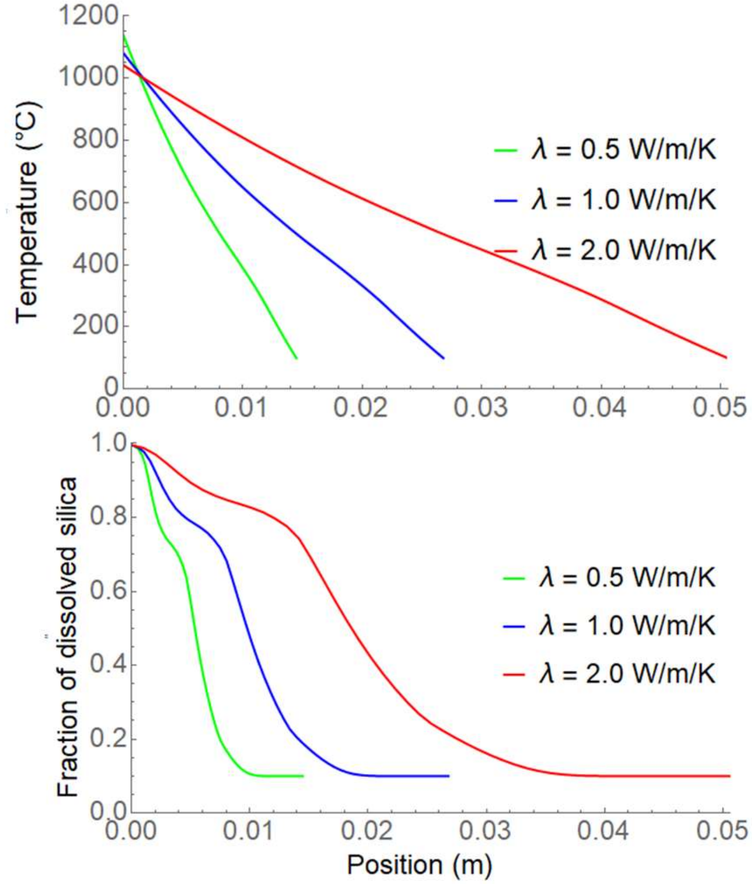
- Subject to boundary conditions

$$T(x=0) = T_{\mathrm{B}} \qquad -\lambda \frac{dT}{dx}(x=0) = Q_{\mathrm{B}}$$

$$T(x=h) = T_{\mathrm{T}} \qquad -\lambda \frac{dT}{dx}(x=h) = Q_{\mathrm{T}}$$

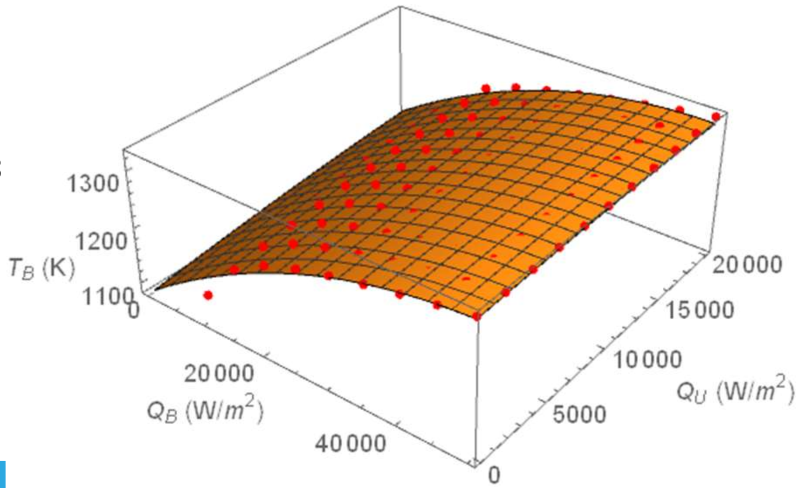
- The melt rate is given by

$$j\Delta H = Q_{\mathrm{B}} + Q_{\mathrm{U}}$$

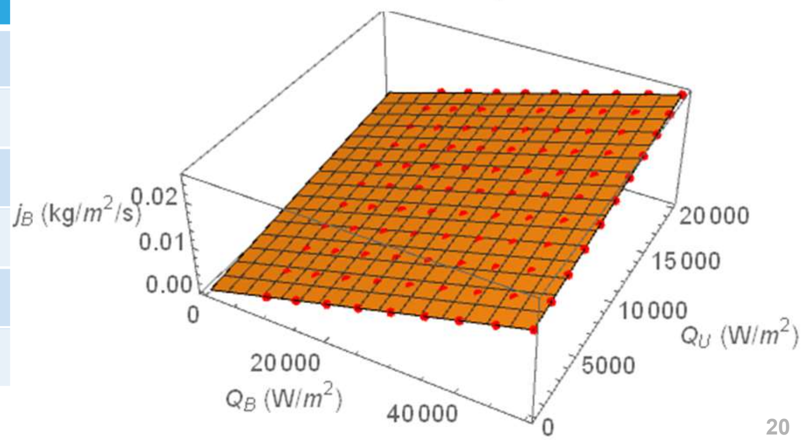


Response Surface → AN105

- Polynomial fit for fast evaluation in CFD code
- Cold cap bottom temperature
  - $T_B = p_{00} + p_{01}Q_U + p_{10}Q_B + p_{02}Q_U^2 + p_{11}Q_U Q_B + p_{20}Q_B^2$
- Local melting rate and gas mass flux given by
  - $j_B = q_{00} + q_{01}Q_U + q_{10}Q_B + q_{02}Q_U^2 + q_{11}Q_U Q_B + q_{20}Q_B^2$
  - $j_G = r_{00} + r_{01}Q_U + r_{10}Q_B + r_{02}Q_U^2 + r_{11}Q_U Q_B + r_{20}Q_B^2$



Index	p	q	r
00	1.086×10^{3}	1.087×10^{-17}	4.29×10^{-19}
01	3.575×10^{-3}	3.653×10^{-7}	9.118×10^{-8}
10	8.444×10^{-3}	3.653×10^{-7}	9.118×10^{-8}
02	-4.652×10^{-8}	-3.534×10^{-27}	-2.965×10^{-27}
11	-4.433×10^{-8}	6.678×10^{-29}	-1.394×10^{-27}
20	-7.909×10^{-8}	-4.673×10^{-28}	-3.865×10^{-28}



Effect of Vent Holes in Cold Cap

Without bubbling

- Hot glass travels upward along walls and downward in the center, driven by buoyancy, resulting from temperature gradients
- Cold cap shape does not affect cavity layer

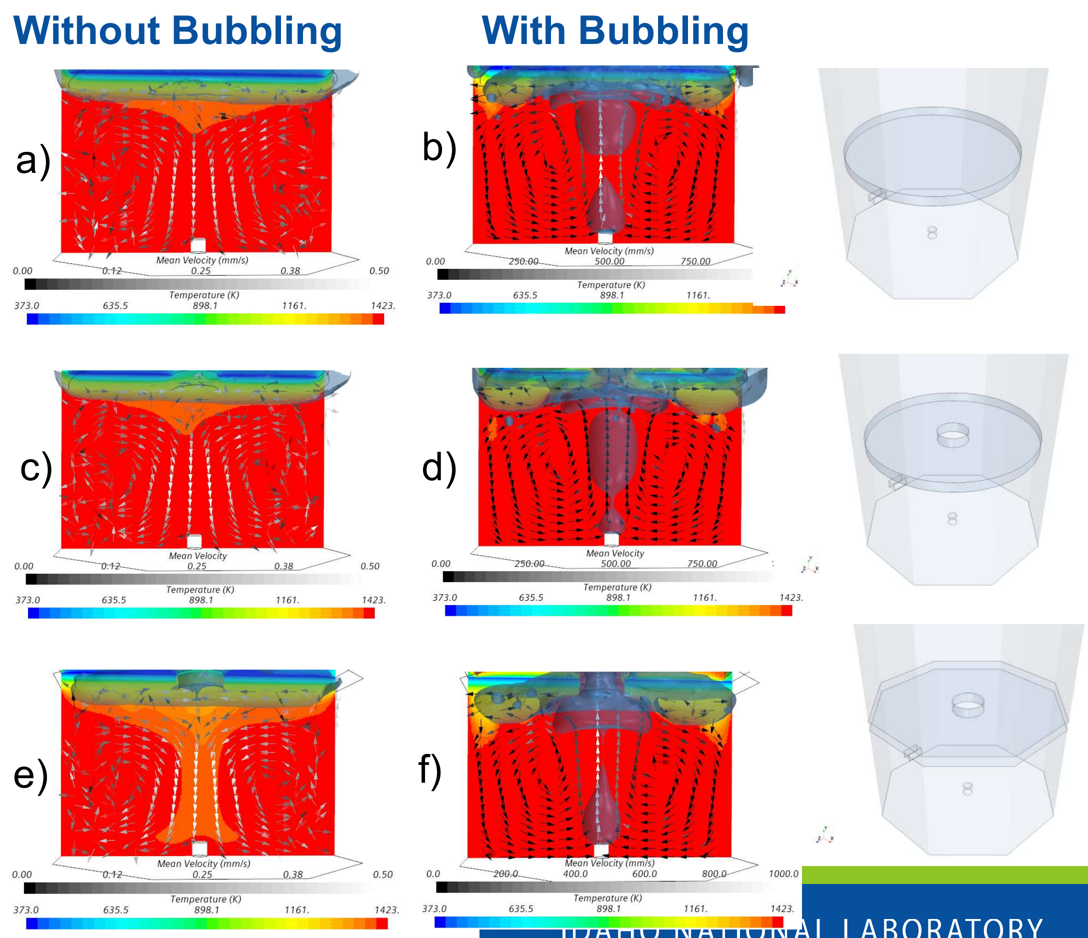
With bubbling

- Velocities are several orders of magnitude higher and circulation pattern reverses as the molten glass is dragged upward by bubbles in the center
- Cold cap shape affects cavity layer

b) Rising bubbles flatten as they hit the solid cold cap and move to the sides where they escape

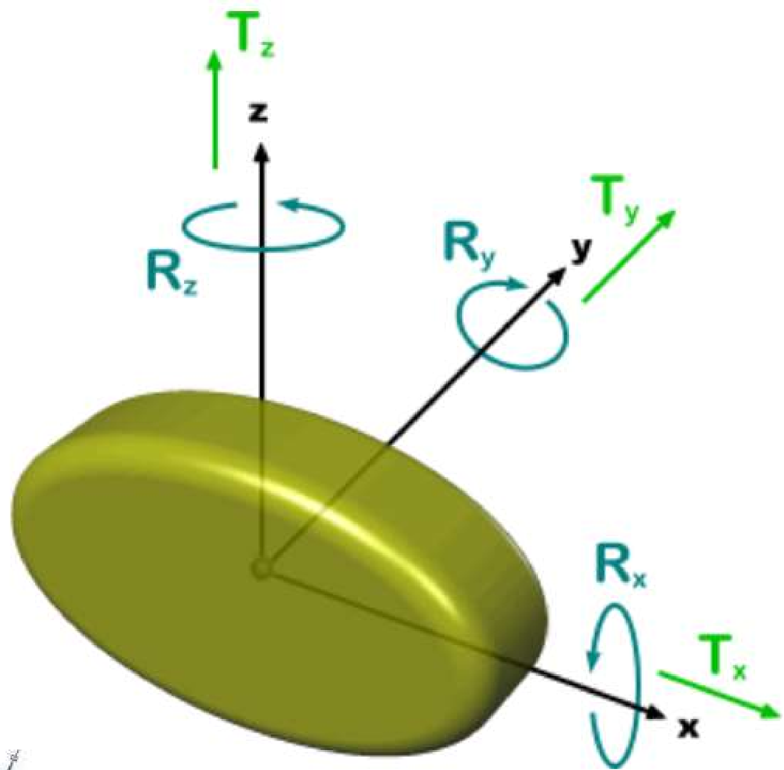
d) A lot of bubbling gas escapes directly through a vent hole, thus contributing less to the horizontal movement below the cold cap

f) For bridged case, significant gas buildup occurs below cold cap as the gas is forced to move against the melt flow toward the central vent hole



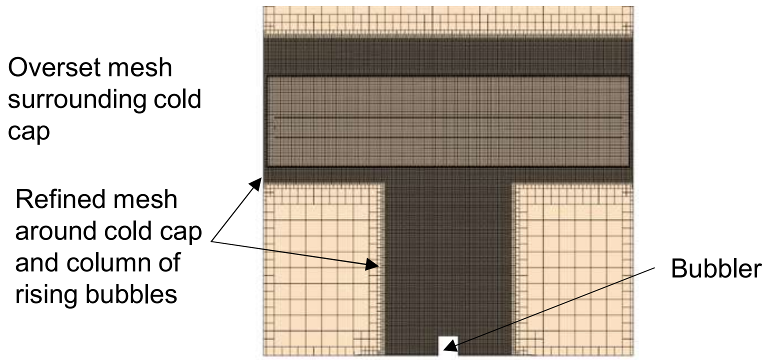
CFD Multiphase Framework with DFBI

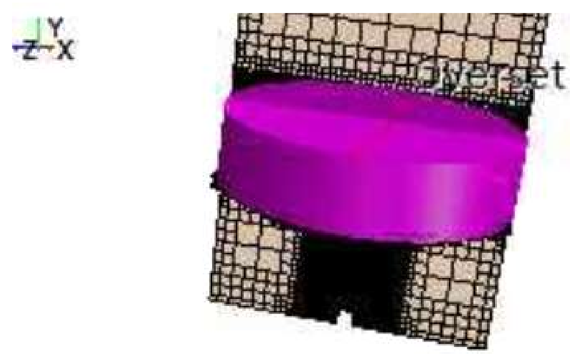
- STAR-CCM+ v15.06.008
  - Eulerian-Eulerian multiphase volume of fluid (VOF) approach
  - High-resolution interface capturing scheme used to maintain sharp interfaces
  - Solid cold cap with conjugate heat transfer
- Dynamic Fluid-Body Interaction (DFBI) models coupling between a fluid and a rigid body
  - The rigid body moves in response to the fluid forces and moments at the coupled boundary
  - A 3D rigid body that is free to rotate and translate in all directions has 6 degrees of freedom

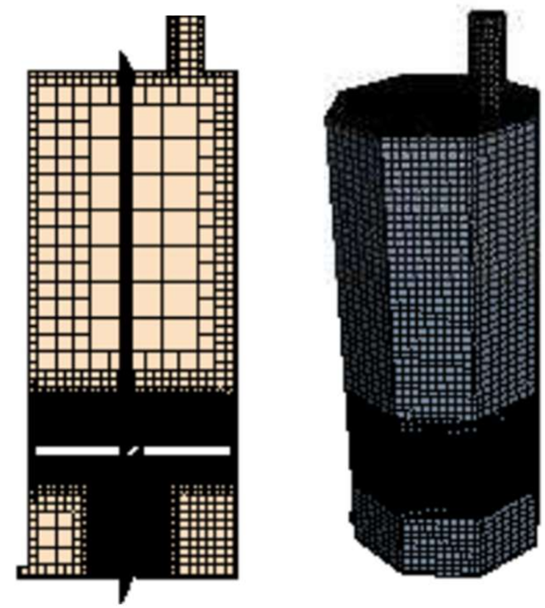


DFBI Mechanics

- An overset mesh is required for the DFBI simulations
- Overset mesh region
  - Base size = 0.001 m
- Automated mesh
  - Base size = 0.005 m
- Motion allowed in y-direction
- Refined mesh in column of rising bubbles and around cold cap
- Interpolation of overset and background meshes increase computational time by >2x
  - Coarse mesh: 5 days of physical time for 15s on 120 CPUs
  - Fine mesh: 7 days of physical time for 5 s on 960 CPUs







D.P. Guillen, A.W. Abboud, Heat Transfer Enhancement due to Cold Cap Motion from Bubbling in a Waste Glass Melter, *Journal of Energy Resources Technology*, 2023.

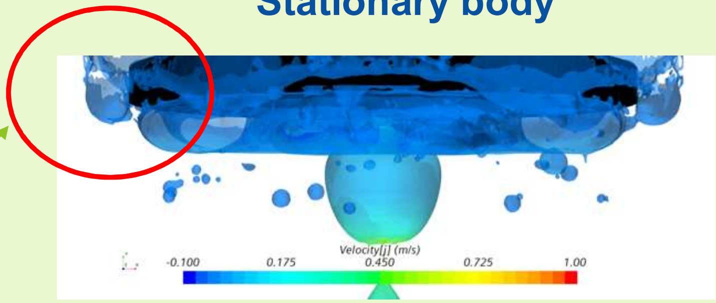
Gas Isosurfaces

- Instantaneous cavity layer
  - 0.5 gas volume fraction
- Color variation of the isosurface indicates gas velocity

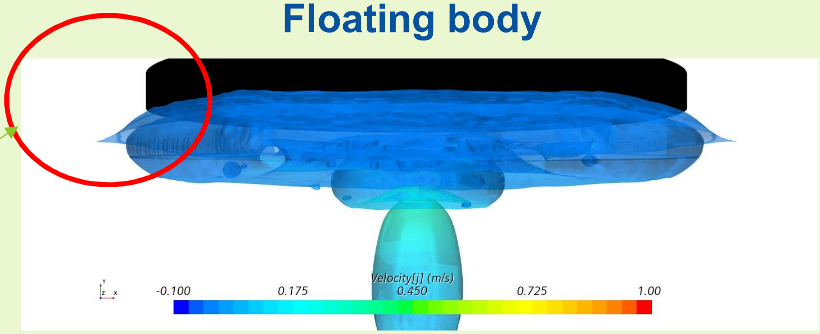
- With fixed cold cap some glass can get pushed to level of cold cap top height

- With DFBI cold cap is raised as gas builds up, glass isn't pushed around the sides

Stationary body



Floating body



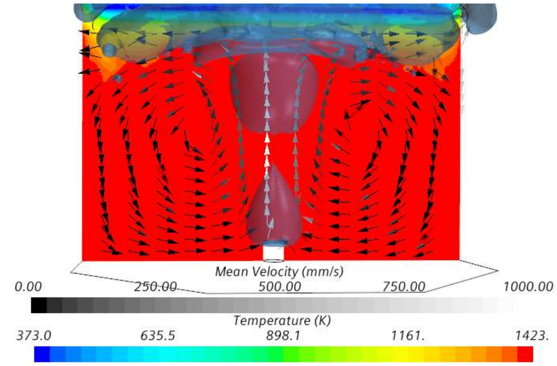
Time-averaged Temperature Contours, Velocity Vectors and Gas Phase Volume Fractions

- Images show a superposition of time-averaged temperature, velocity vectors and gas volume fractions in the melt pool and cavity layer beneath the cold cap

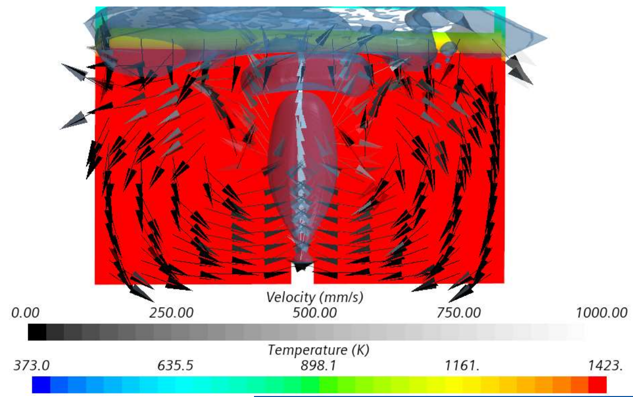
- Overall recirculation pattern within the melt pool remain very similar between cases

- Rising bubbles flatten as they hit the solid cold cap and move to the sides where they escape

Fixed cold cap

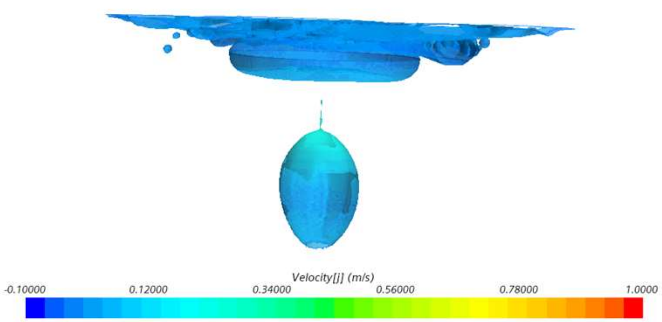


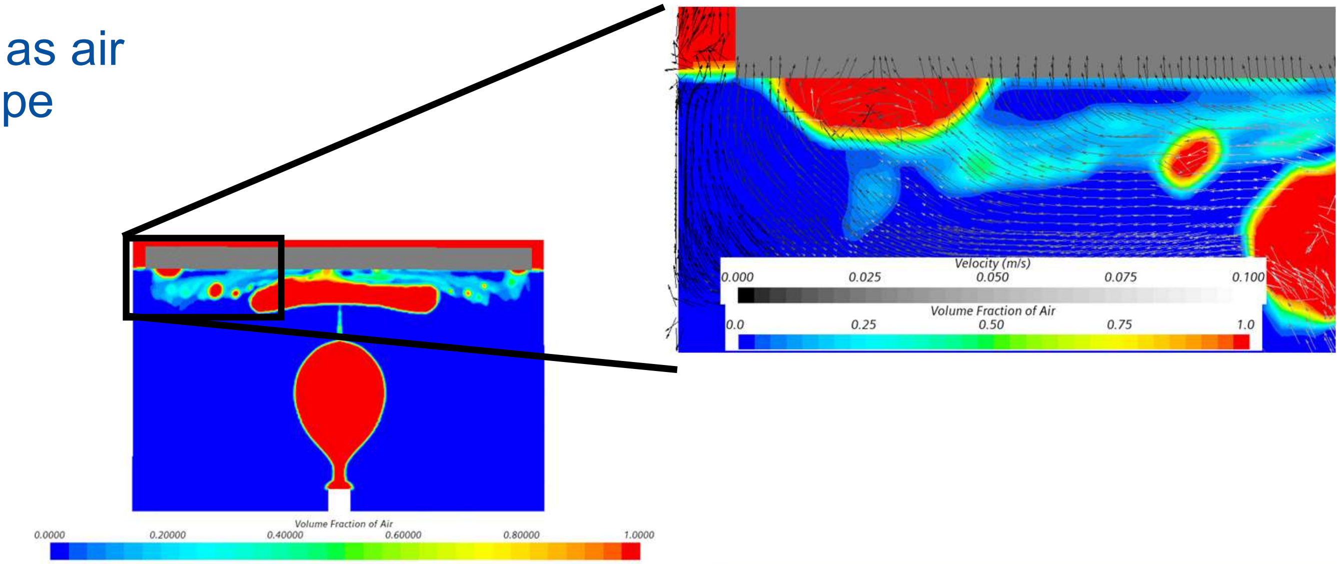
DFBI cold cap



Cold Cap Motion Resulting from Bubbling at Base of Melter

- Bubbles flow from the bubbler nozzle into the cavity and the height of the cold cap oscillates upwards
- Cold cap oscillates down as air bubbles periodically escape around edges

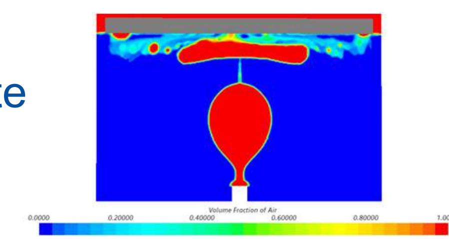


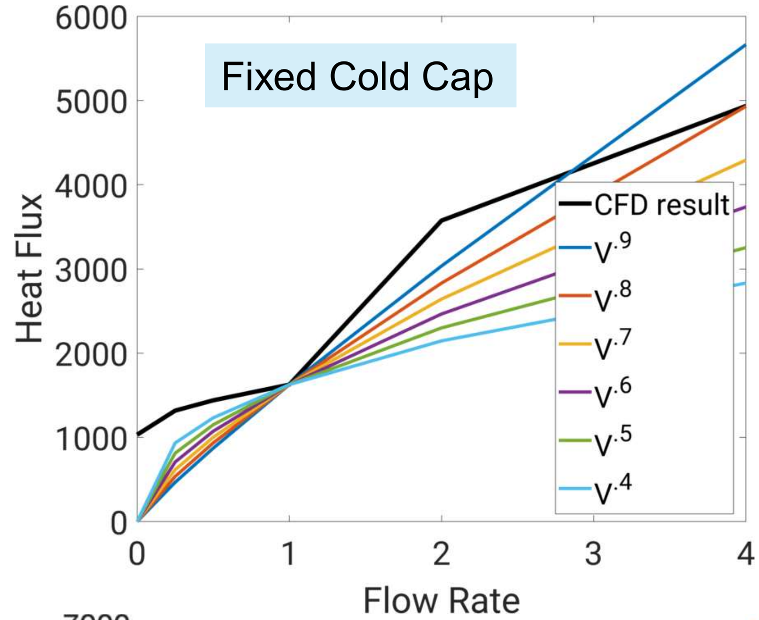


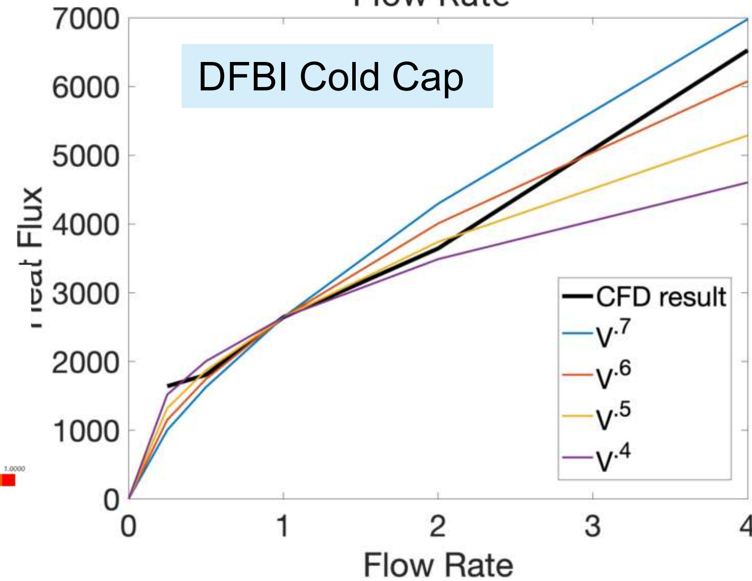
A.W. Abboud, D.P. Guillen, P. Hrma, A.A. Kruger, J. Klouzek, R. Pokorny, Heat Transfer from Glass Melt to Cold Cap: Computational Fluid Dynamics Study of Cavities Beneath Cold Cap, *International Journal of Glass Science*, 12(2), 233-244, 2021. https://doi.org/10.1111/ijag.15863

Moving vs. Static Cold Cap

- Heat flux to the cold cap as a function of forced convection bubbling can be expressed as $Q \sim v^{\gamma}$
- CFD simulations with the Dynamic Floating Body Interaction (DFBI) model show that DFBI cold cap has higher total flux than fixed cold cap, but lower slope
  - Fixed γ ~0.8, DFBI γ ~ 0.6
  - But ~25% higher at 4x bubbling rate
- This heat transfer augmentation effect due to cold cap motion can be implemented into full-scale WTP melter model
  - Use a function fitted to oscillation for movement
  - Apply heat transfer enhancement factor
- Experimental data will be used to validate CFD model and extend its applicability
  - Cold cap interaction with bubbles

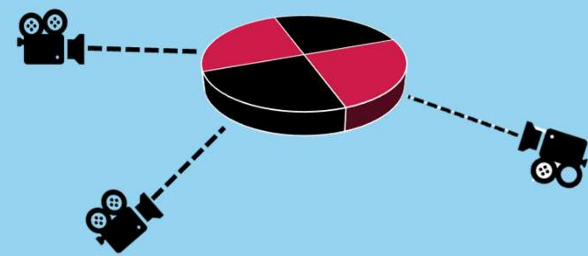


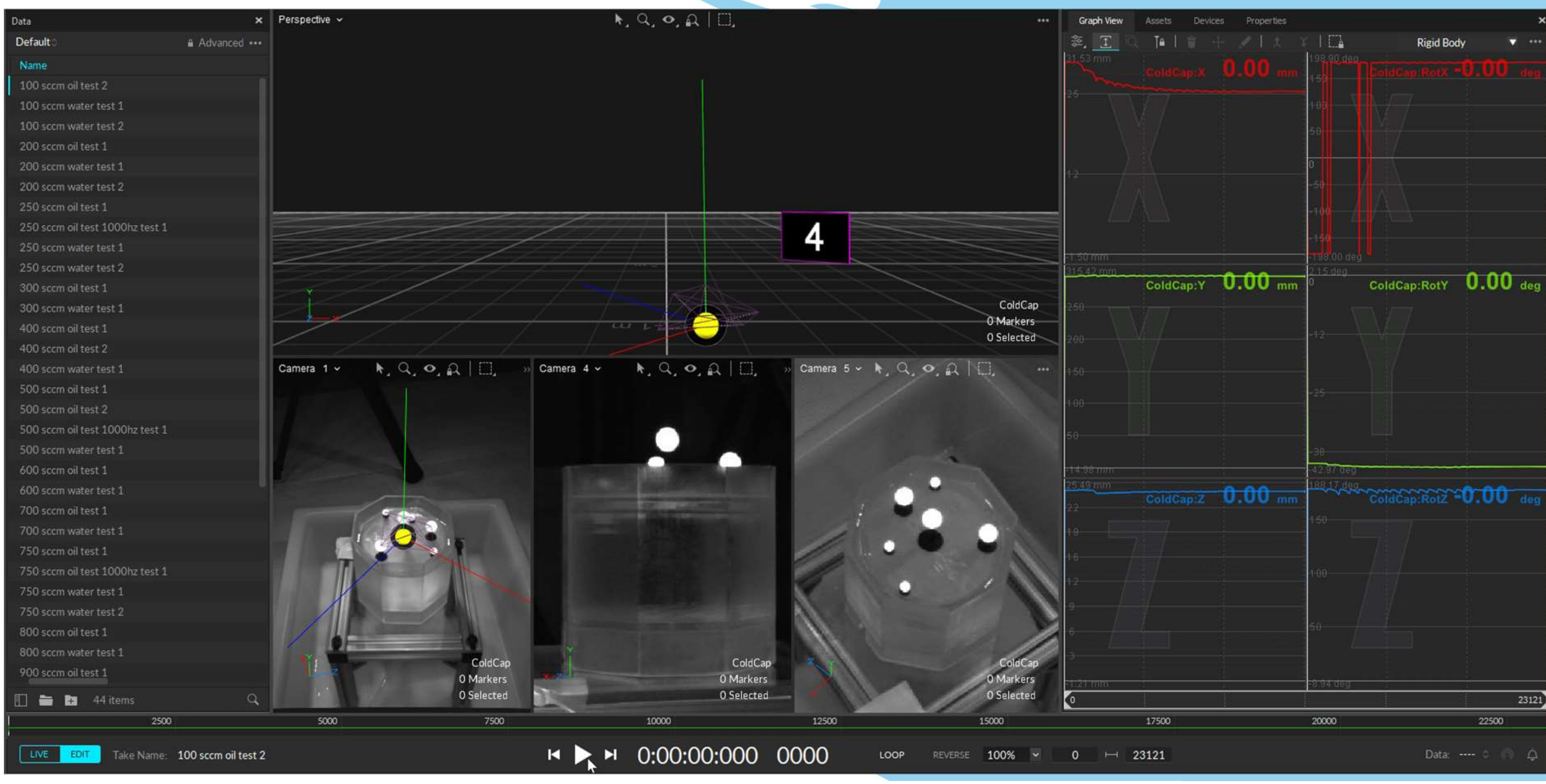




Transparent Melter Test

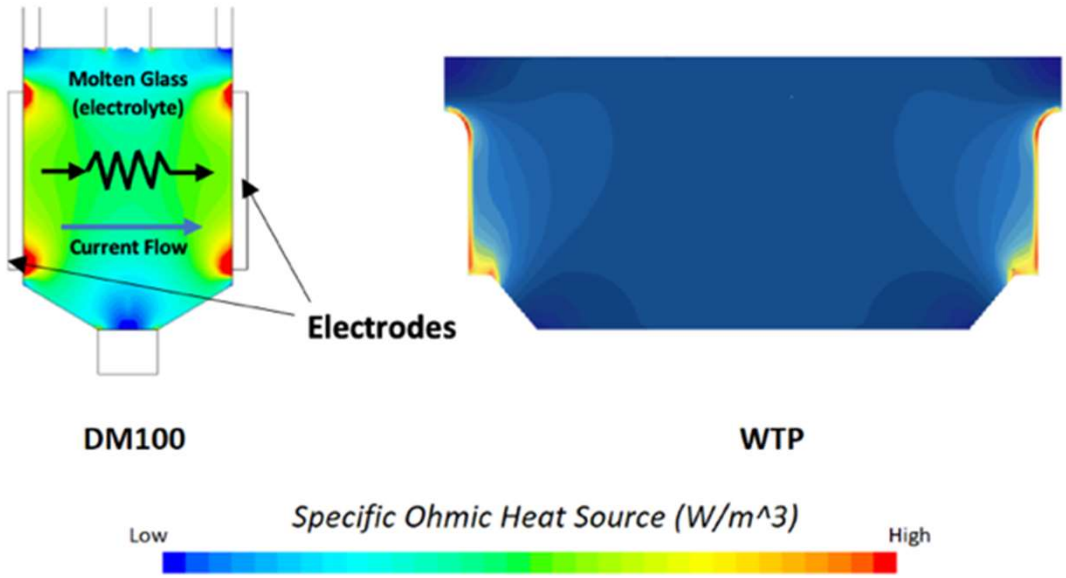
- Obtain data on cold cap motion resulting from forced convection bubbling to validate CFD model



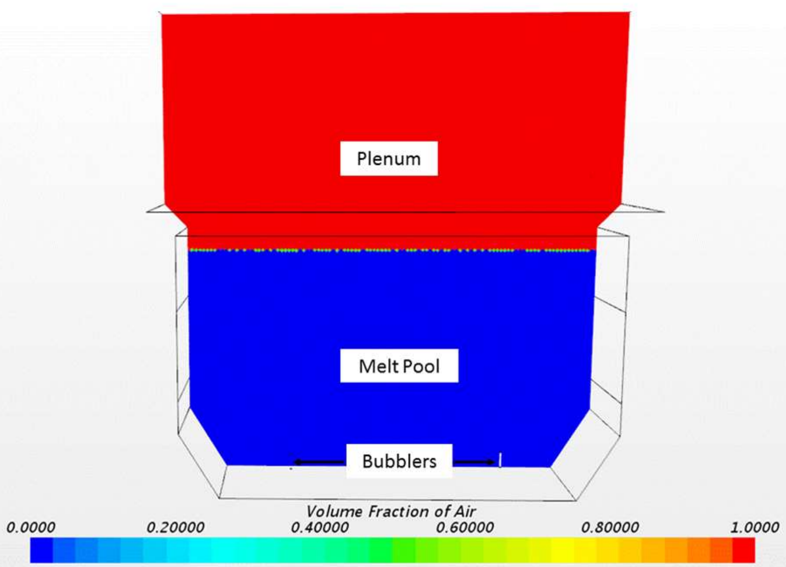


Incorporation of Joule Heating

- Joule heating is accomplished by passing alternating current directly through the molten waste glass by opposing electrodes
- The energy consumed to push the current through the melt is absorbed as heat
- This heat is transferred to the cold cap to facilitate the batch-to-glass reactions

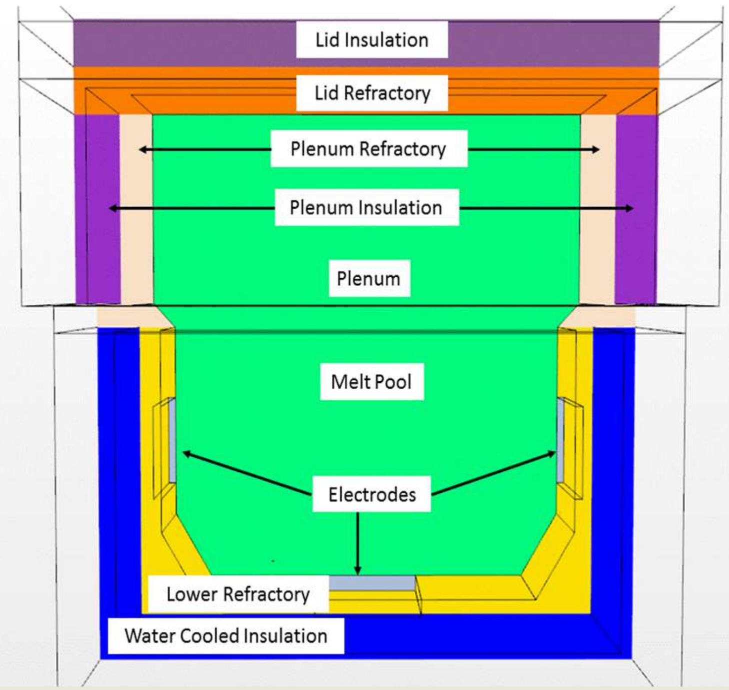


High-Fidelity vs. Simplified Model



High-fidelity model for studying bubbling and foaming

Guillen, D.P, Cambareri, J., Abboud, A.W., Bolotnov, I., Numerical Comparison of Bubbling in a Waste Glass Melter, Annals of Nuclear Energy, 2018



Simplified model to validate heat transfer

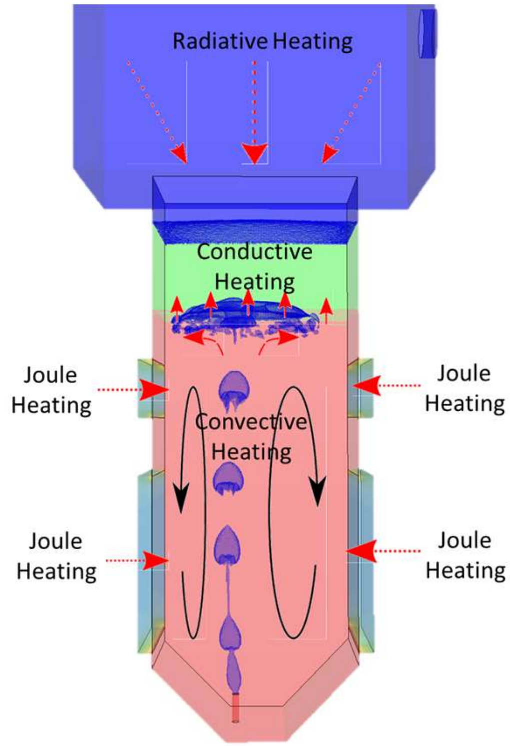
Abboud, A.W. and Guillen, D.P., A Methodology to Reduce the Computational Cost of Transient Multiphysics Simulations for Waste Vitrification, Computers & Chemical Engineering, 2018

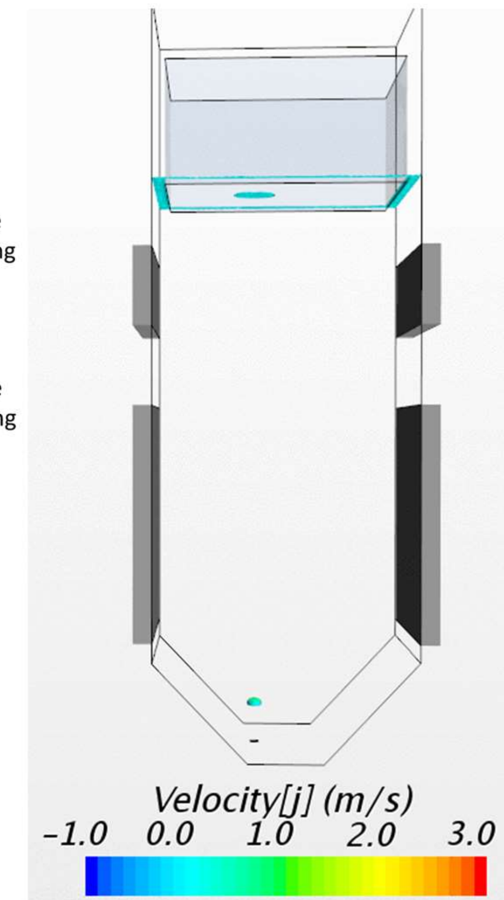
If mainly interested in plenum, can use momentum source term implementation for forced air bubbling at different bubbling rates and glass viscosity

The fully resolved bubbling model enables the implementation of physics to describe foaming and gas bubble movement underneath cold cap

Momentum Source Term Approximation

- CFD simulations with fully resolving bubbling requires timesteps on the order of 1×10^{4} s
  - This limits total simulation time to ~10 s
  - In pilot/large-scale melters, temperature profile and step changes to operation not resolved in this time frame
- Use method developed for DM1200 melter
  - Estimate a momentum source term to mimic forced convection bubbling
- To avoid having to do this for every feed type, create a response surface of bubbling rate vs. viscosity

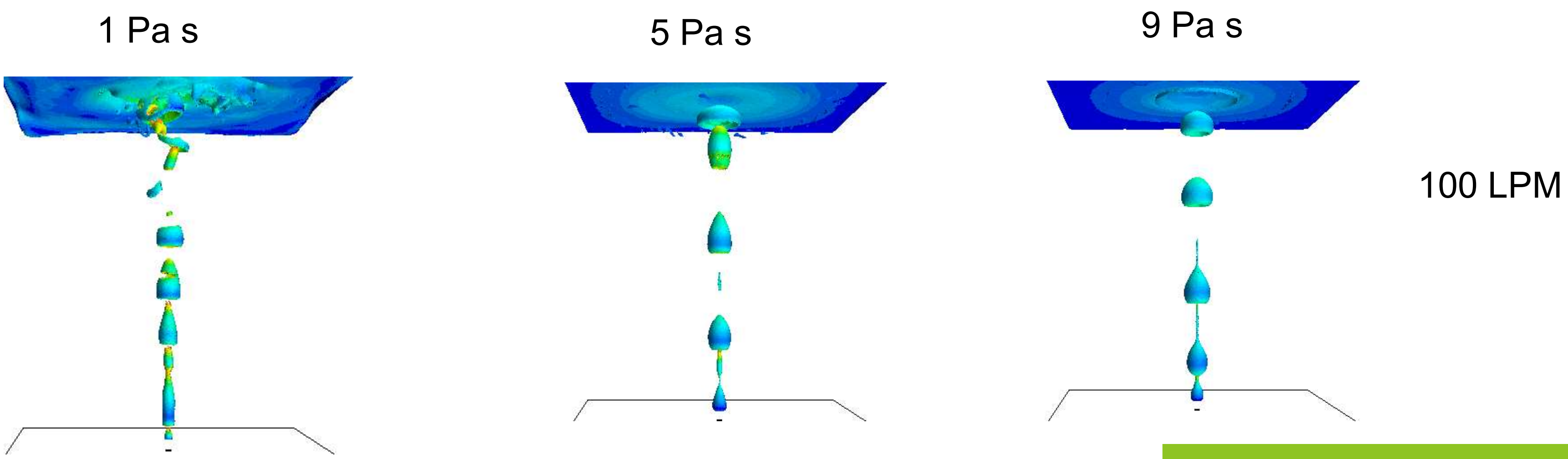




Abboud, A. W., & Guillen, D. P. (2018). A methodology to reduce the computational cost of transient multiphysics simulations for waste vitrification. *Computers & Chemical Engineering*, *115*, 64-80.

Parametric Evaluation of Bubbling Behavior

- Range of viscosity 1 to 9 Pa·s
- Range of bubbling 25-200 LPM/m^2
- Rising bubbles become larger at higher viscosities and there are less bubbles



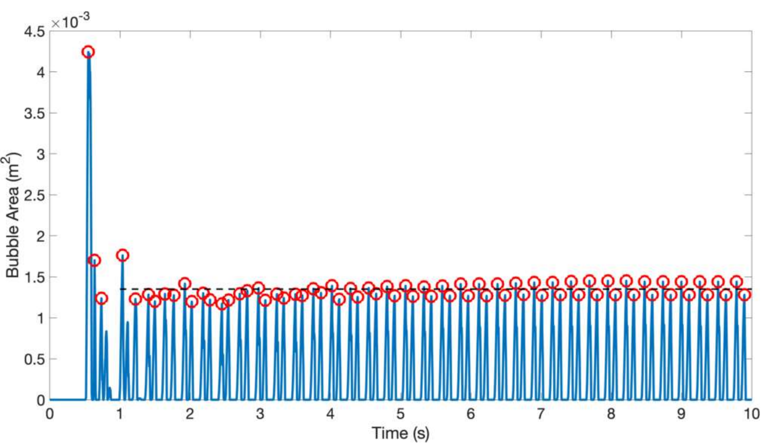
Guillen, D. P. (2016). Bubbling behavior in a waste glass melter. *WIT Trans. Eng. Sci*, *105*, 75.

Momentum Source Term Development

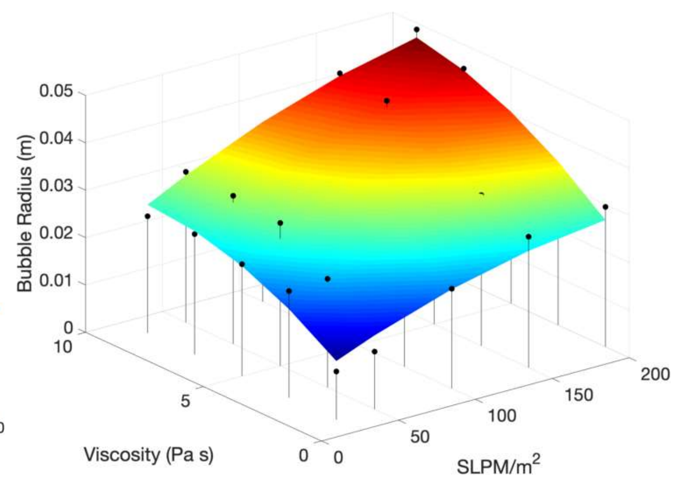
- The rising bubble surface area is monitored and used to calculate average radius at different heights
- Then matrix of simulations used to create response surface of bubble size and # of bubbles

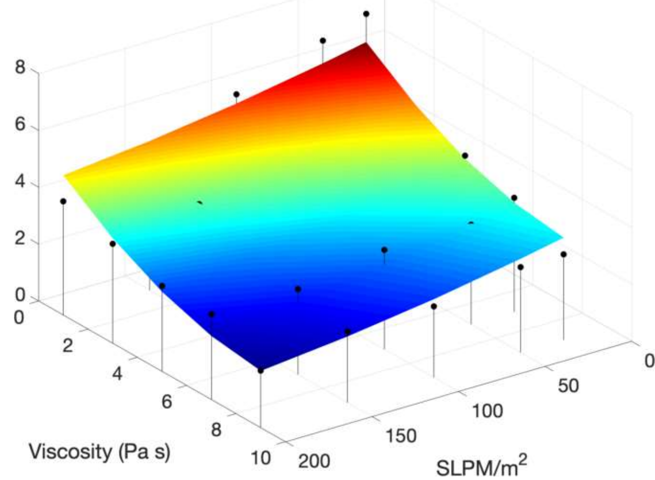
Bubble Radius response surface

Bubble Number response surface



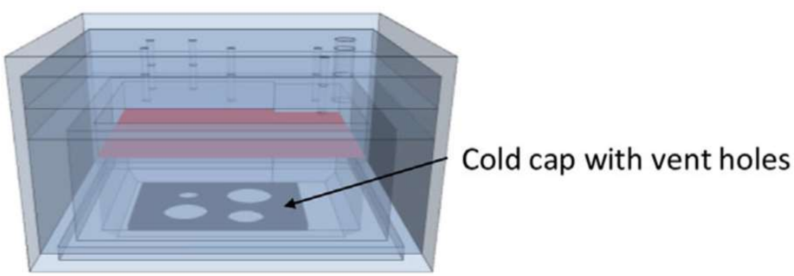
Average bubble radii (single case)

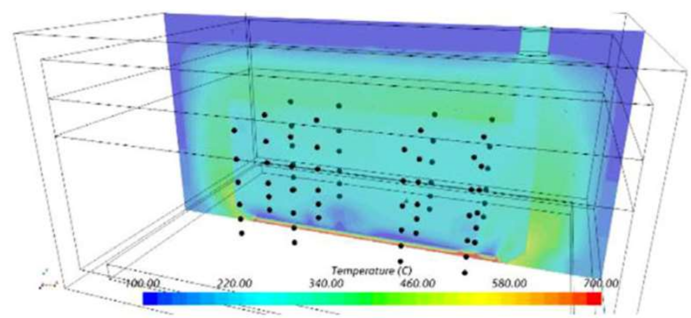




Non-Visual Feedback of Melter Temperature

- Relate cold cap coverage and topology to plenum temperature measurement
  - Inverse problem solved with the help of artificial intelligence
  - Model trained on 1000 samples → *more data is better*
  - Evaluated several algorithms: artificial neural network, support vector machine, random forest, convolutional neural network
- Potentially useful for controlling full-scale radioactive melters that don't allow for visual feedback





A.W Abboud, D.P. Guillen, B. Christensen, Prediction of Melter Cold Cap Topology from Plenum Temperatures with Computational Fluid Dynamics and Machine Learning, *International Journal of Ceramic Engineering & Science* 4, 257-269, 2022. https://doi.org/10.1002/ces2.10134.

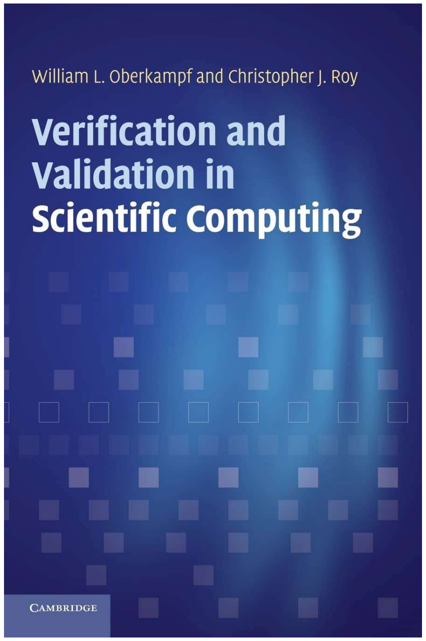
Mesh Convergence

- Run simulations on 3 meshes – coarse, medium, fine
  - Resolve mesh in regions of large gradients
  - Extract result for quantity of interest
- Use √2 scaling between meshes

$$\hat{p} = \frac{\left|\ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)\right|}{\ln(r)}$$

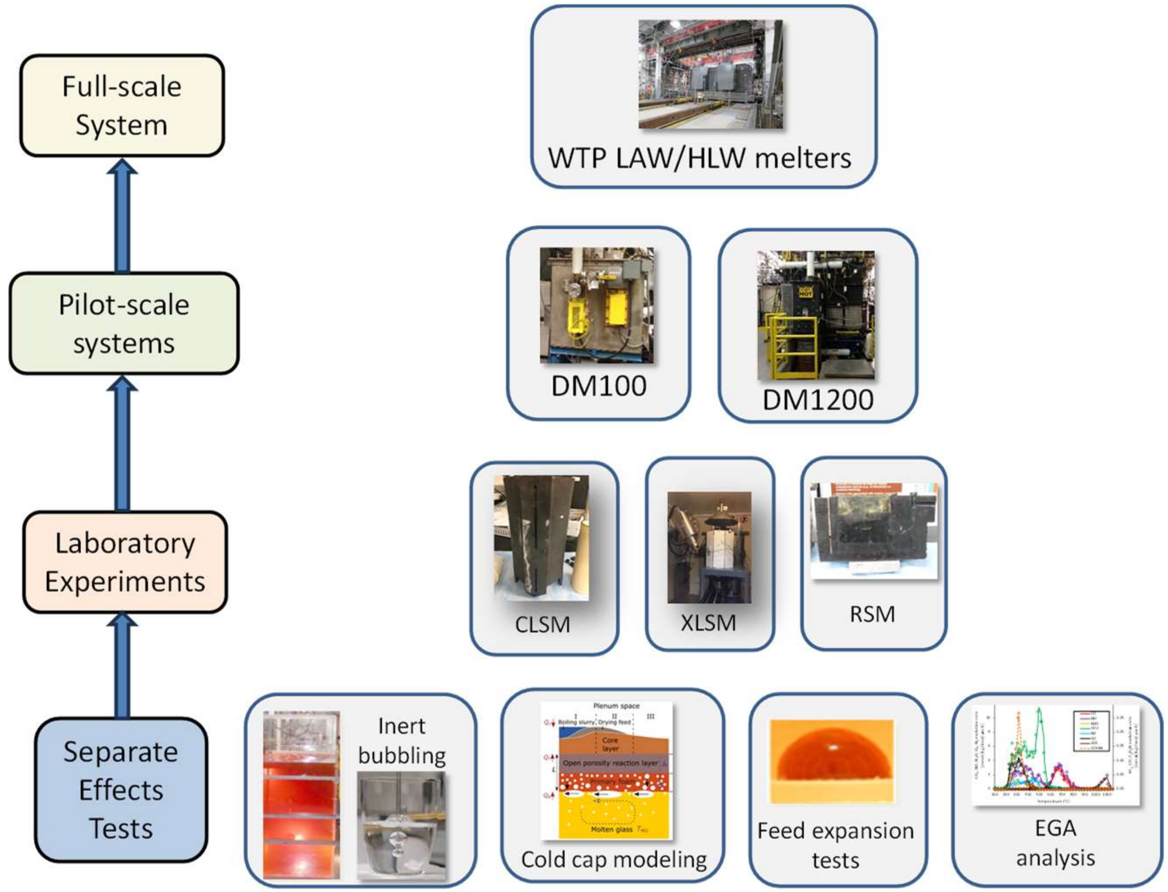
- Discretization uncertainty

$$GCI = \frac{F_s}{r^{\hat{p}} - 1}\left|\frac{f_2 - f_1}{f_1}\right|$$



Validation Hierarchy

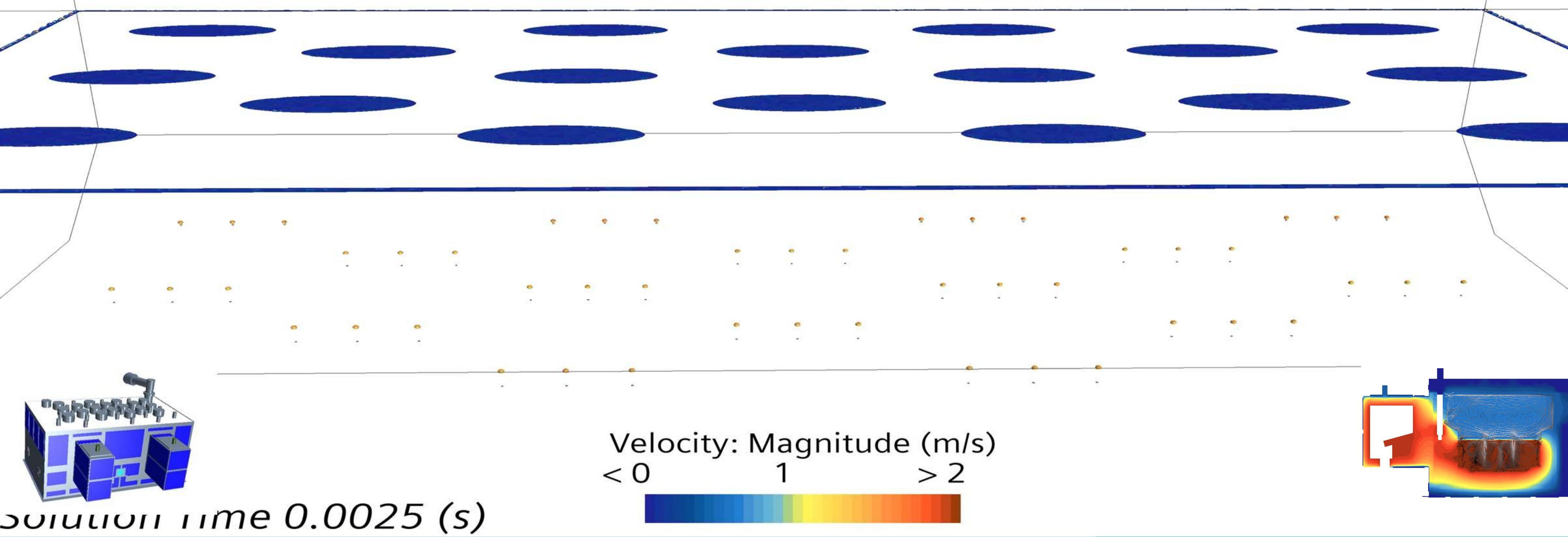
- Model increasingly levels of complexity to increase confidence in full-scale prediction
  - Simple to complex cases Oberkampf & Roy approach
- Investigate physics using separate effects tests
- Develop models using data and insight from laboratory experiments
- Validate with pilot-scale data



D. P. Guillen, A. W. Abboud, R. Pokorny, W. C. Eaton, D. Dixon, K. Fox, A. A. Kruger, Development of a Validation Approach for an Integrated Waste Glass Melter Model, *Nuclear Technology*, 203(3), 244-260, 2018. https://doi.org/10.1080/00295450.2018.1458559

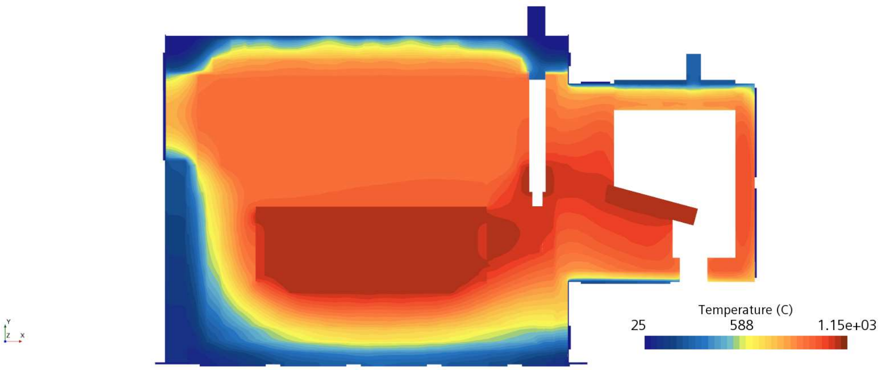
Bubbling Flow in the Low Activity Waste Treatment and Immobilization Plant

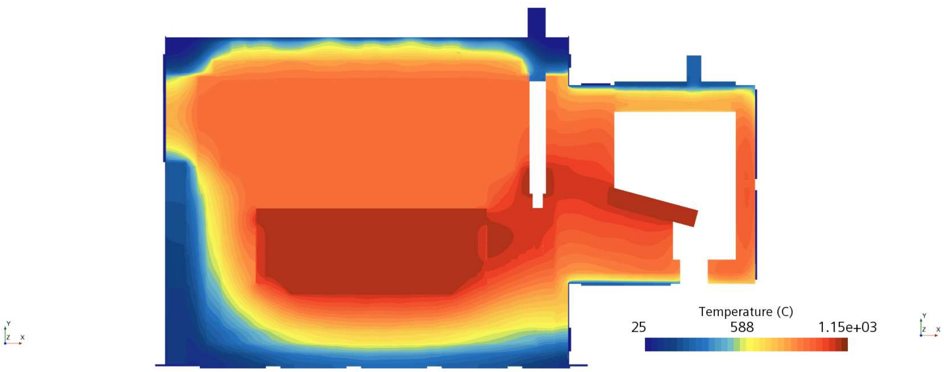
Video shows an isosurface of the bubbling in a WTP LAW melter colored by velocity. Forced convection via bubbling is used in the WTP to improve heat transfer from the molten glass to the cold cap layer where the batch-to-glass conversion kinetics occur. After discharge, this allows for long-term storage of the Hanford waste in a stable solid form.



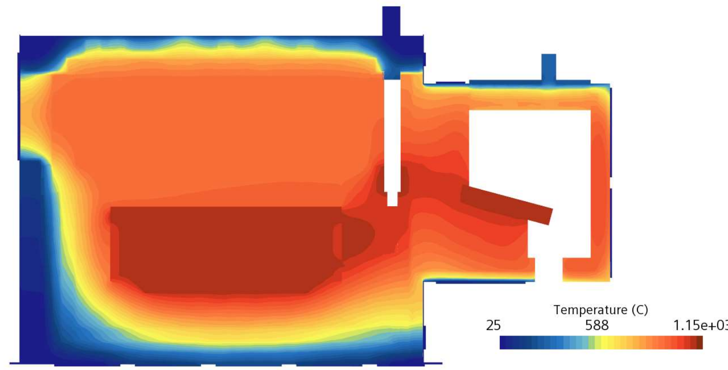
Failure Mode Assessment

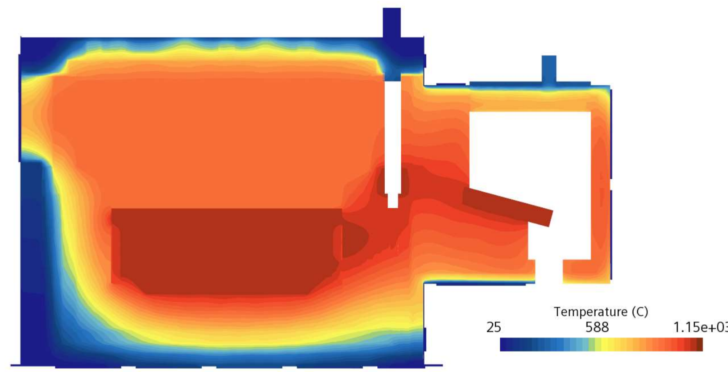
Power Failure





Electrode Failure

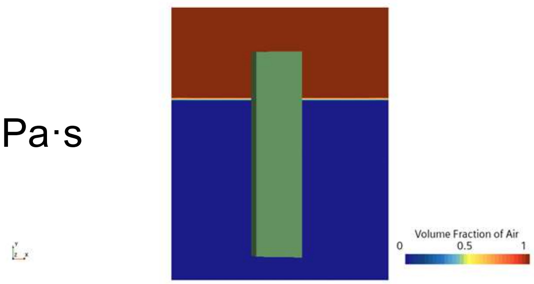


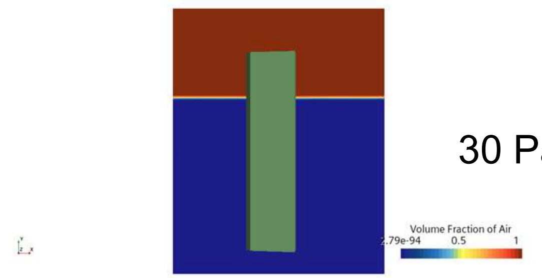


Refractory Corrosion Assessment

- Rotating finger experiments at UCT Prague; will compare with static and bubbled tests
- Refractory coupon in surrogate molten waste glass
- Determine neckline and bulk corrosion to evaluate refractory lifetime

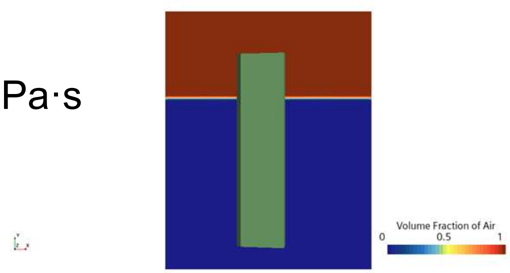
9 Pa·s

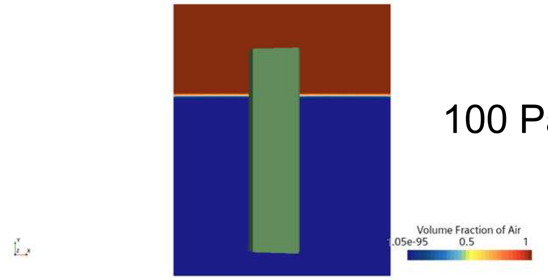




30 Pa·s

60 Pa·s





100 Pa·s

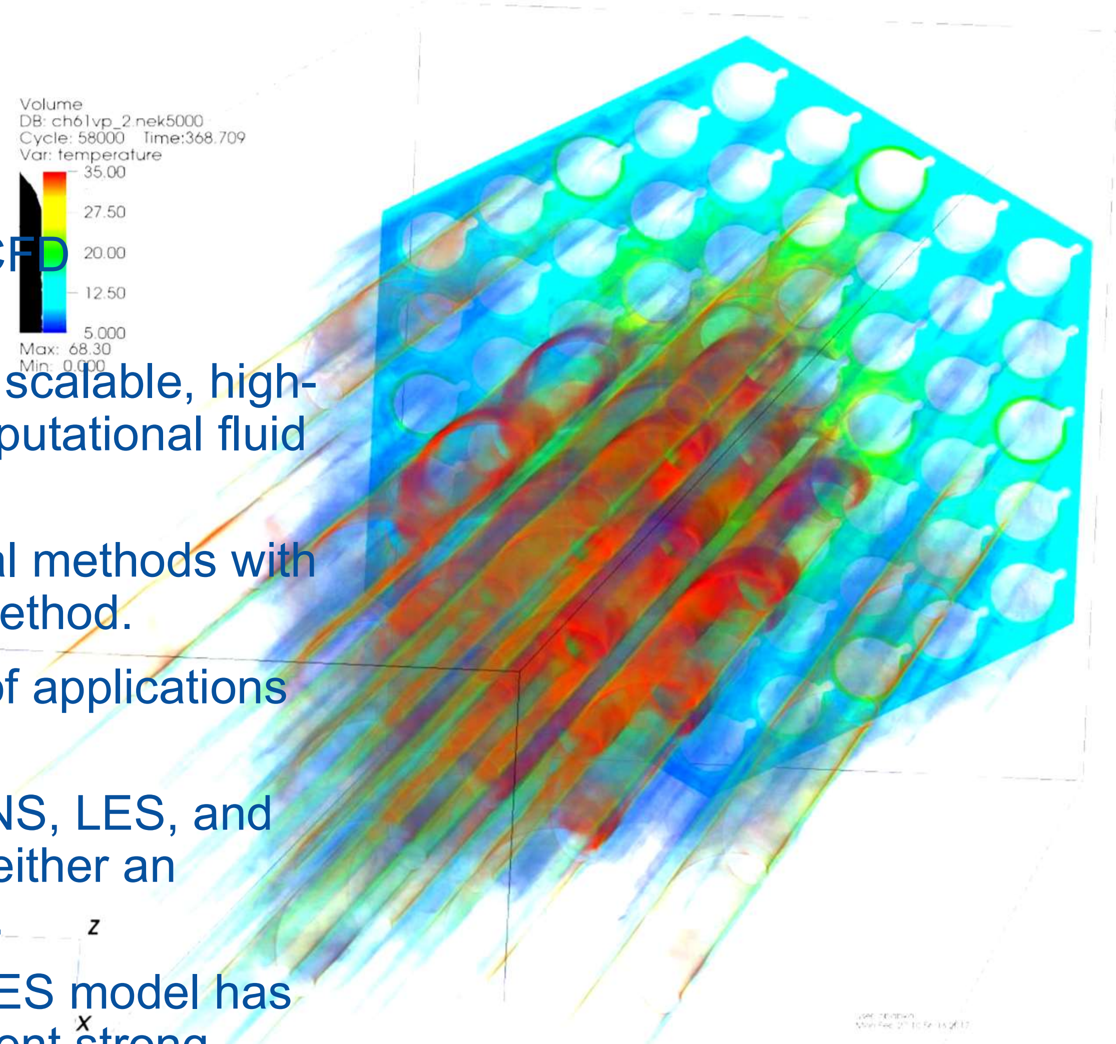
Nek5000 CFD Tool

- Incompressible and low Mach-number Navier-Stokes
- Spectral element discretization
- High-order conformal curved quadrilateral/hexahedral meshes
- Semi-implicit $2^{nd}/3^{rd}$ order adaptive timestepping
- Conjugate fluid-solid heat transfer
- LES and RANS turbulence models
- Two-phase flow capability being added

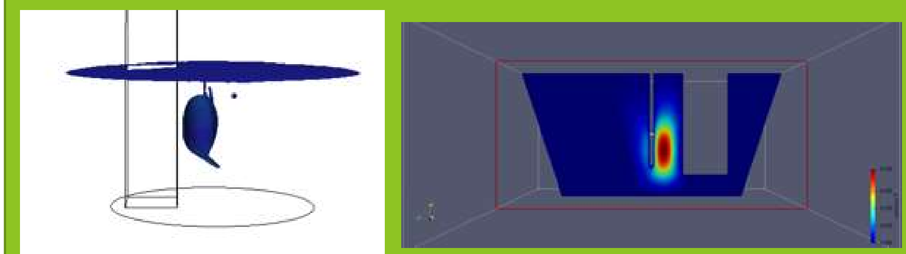
- Runs much faster than STAR-CCM+
  - GPU variant available (NekRS)
  - Lower CPU resources needed
- Computational scalability
  - Multiprocessor capability on INL's supercomputer
- Open source (free) vs. expensive license
- Amenable to machine learning studies
- High fidelity turbulence modeling (DNS & LES)

Nek5000 Description

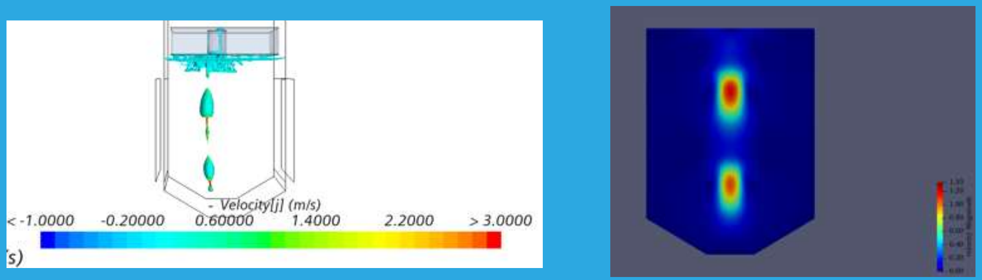
- DOE-NEAMS tool for high-fidelity CFD simulations
- Nek5000 is an open-source, highly scalable, high-order, spectral-element-based computational fluid dynamics code.
- It combines the accuracy of spectral methods with the flexibility of the finite element method.
- It has been used for a wide range of applications in nuclear energy.
- It has the capabilities to perform DNS, LES, and unsteady RANS simulations using either an incompressible or low-Mach model.
- Its high-fidelity capability with the LES model has been well documented with consistent strong performance in international benchmarks.



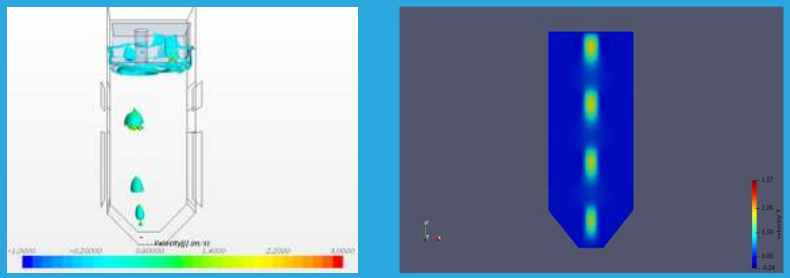
Results of Momentum Source Term Addition in Nek



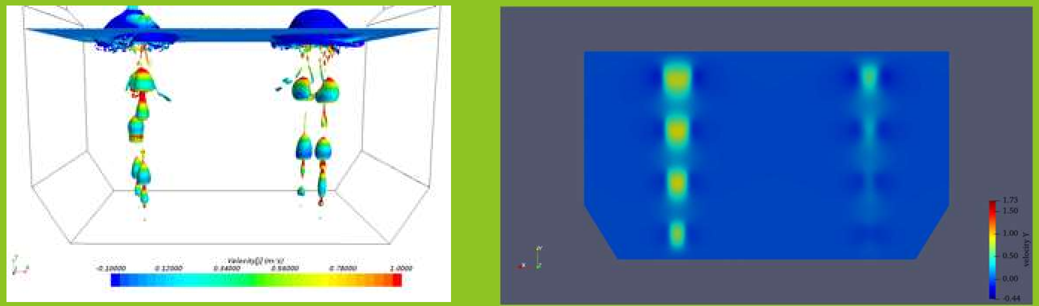
Crucible Model



DM100-WV Model



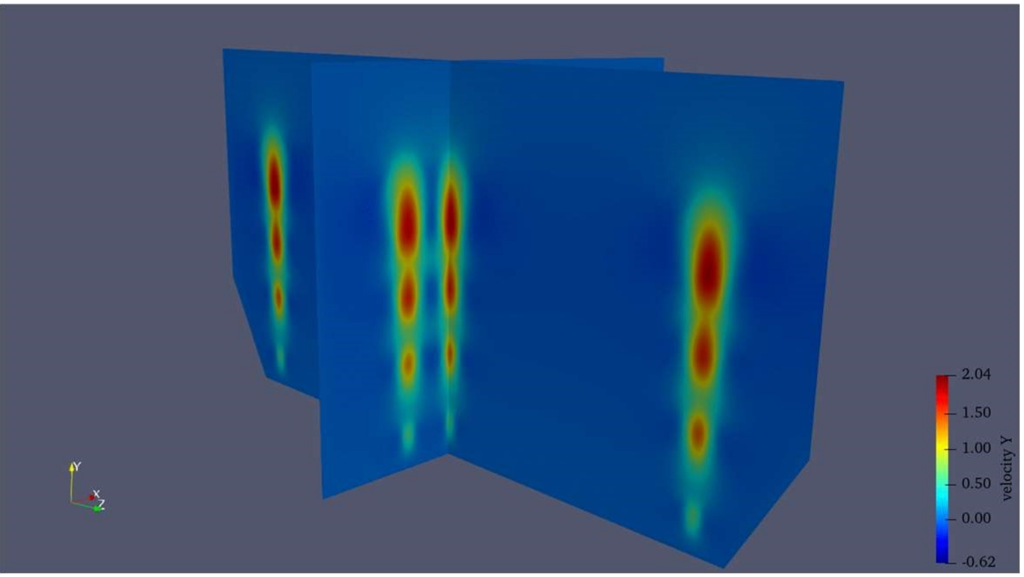
DM100-BL Model



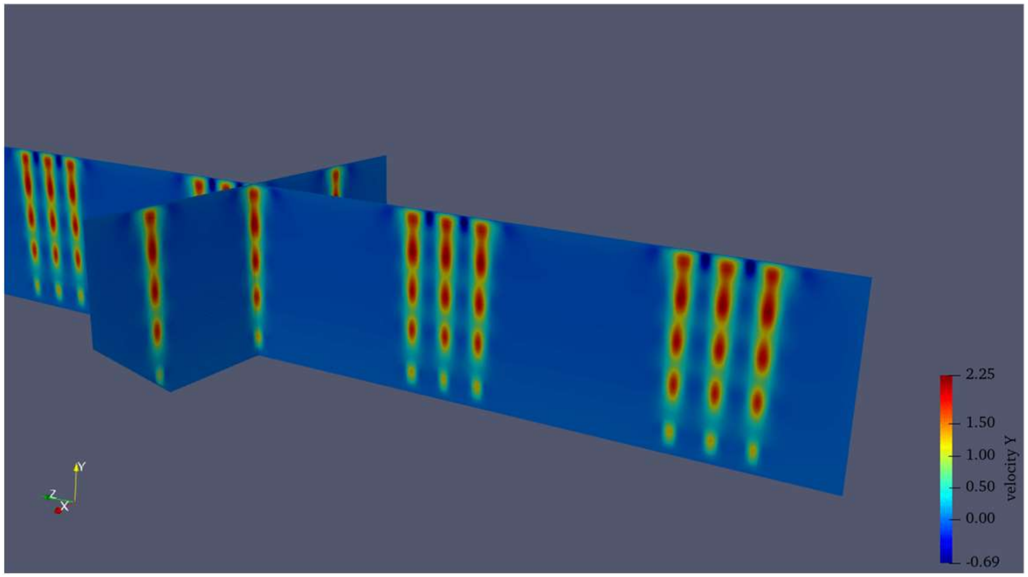
DM1200 Model

Nek Models of Bubbling in Full-Scale WTP Melters

WTP-LAW

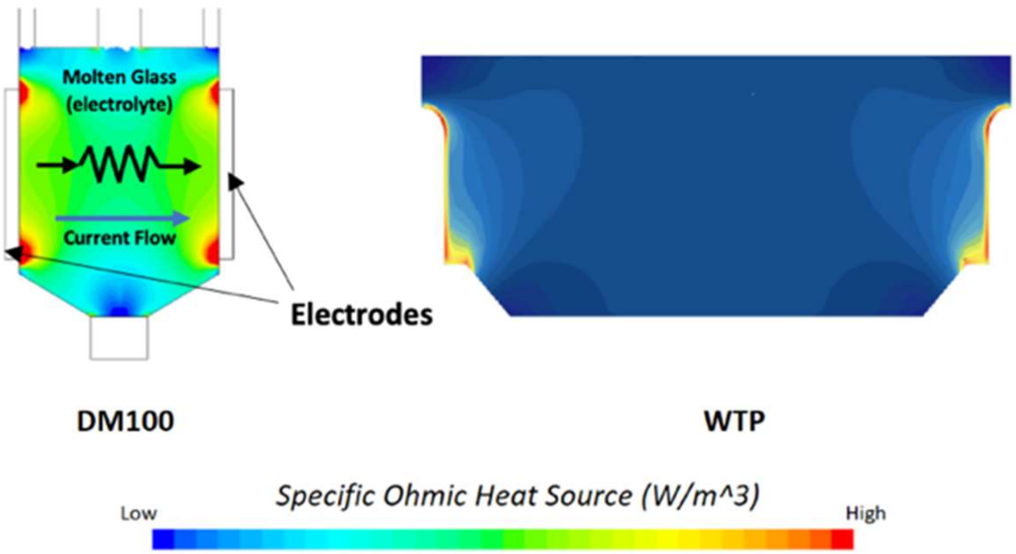


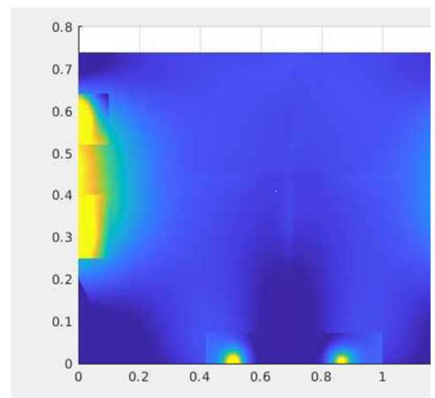
WTP-HLW

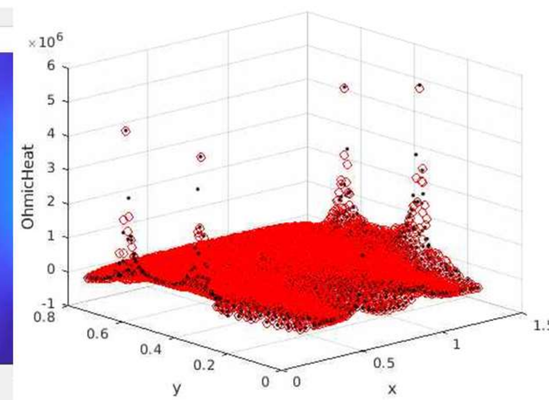


Joule Heating

- Create set of fitted polynomials to represent heating





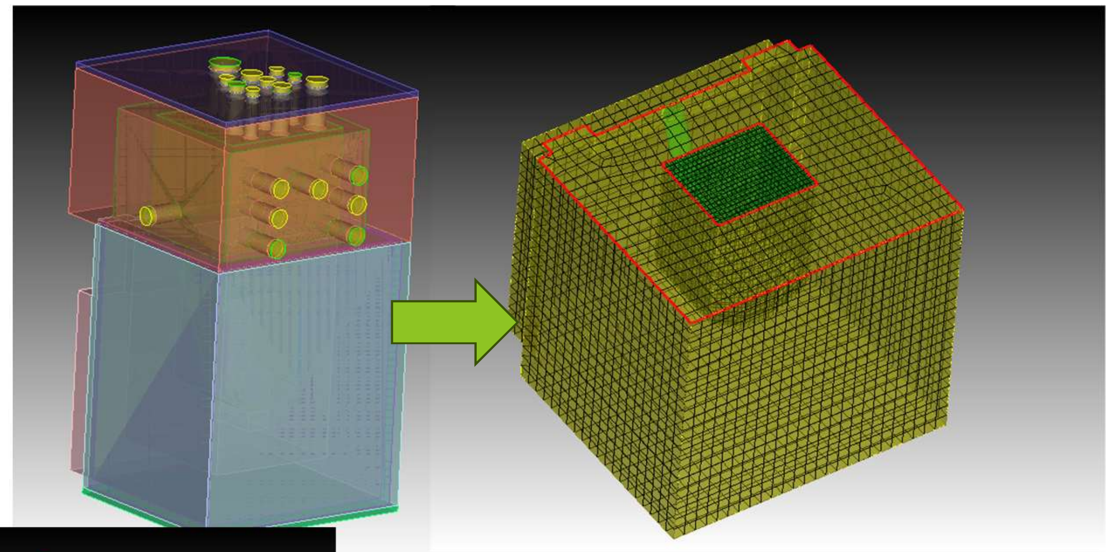


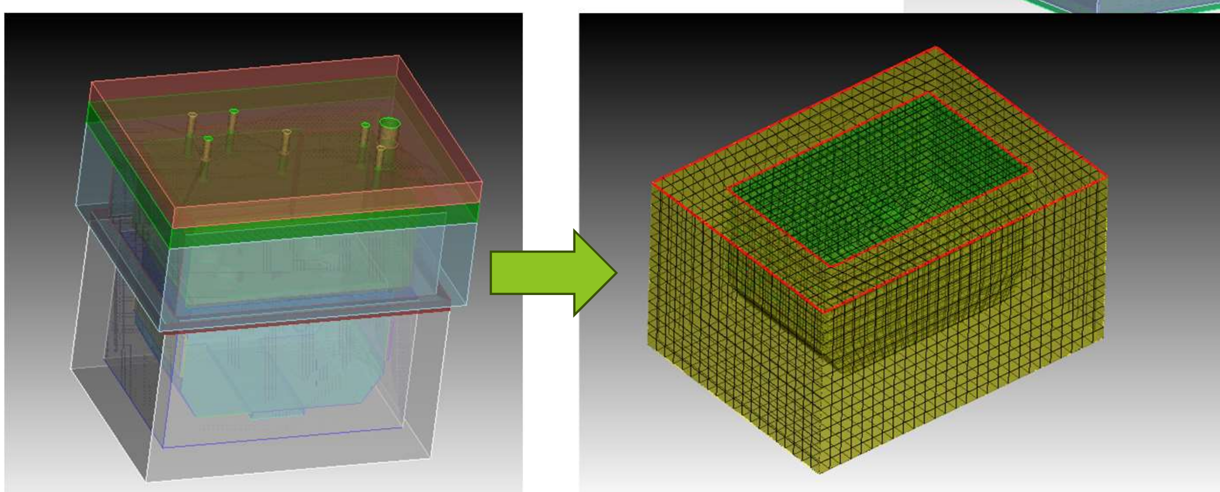
Melter	Integral of Joule Heating (W/m*)	Integral of Piecewise Fit (W/m*)	Error (%)
DM100WV	71515	70939	0.81%
DM100BL	66786	66197	0.88%
DM1200	165972	165195	0.47%
WTP	178373	177133	0.69%

*2D integral

Conjugate Heat Transfer

- Only 1 solid phase in Nek
- Create geometric representation of refractory layers for melt only
- Add plenum in when level set code complete (ANL)





Summary

- A suite of CFD models have been developed to predict both separate and integral effects in waste glass melters
- The modeling team and experimentalists work closely together
- Models incorporate data from laboratory and pilot-scale tests
  - The capability is useful for understanding the physicochemical processes occurring in waste glass melters
  - Have the potential to assist with startup, operations and troubleshooting at the plant

Acknowledgements

Funding for this work was provided by Dr. Albert Kruger of the U.S. DOE's Waste Treatment and Immobilization Plant Project of the Office of River Protection. This work was performed by Battelle Energy Alliance, LLC under the DOE Idaho Operations Contract DE-AC07-05ID14517. This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.


INL
Idaho National Laboratory