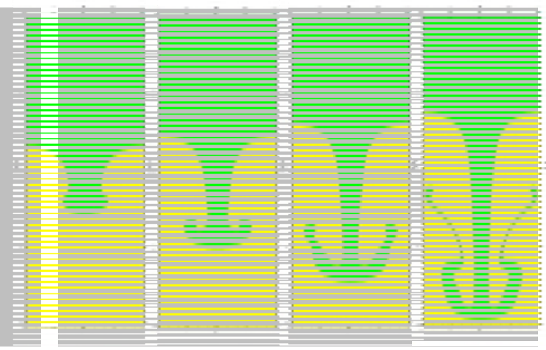
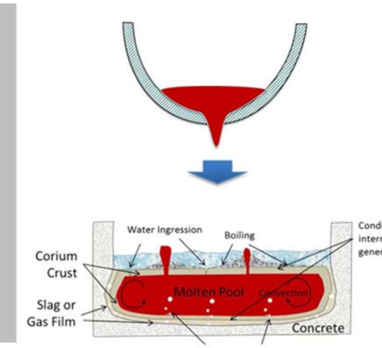
SAND2017-7268C

Exceptional service in the national interest

Sandia National Laboratories





Computational Models for Molten Corium Flow and Reaction with Concrete

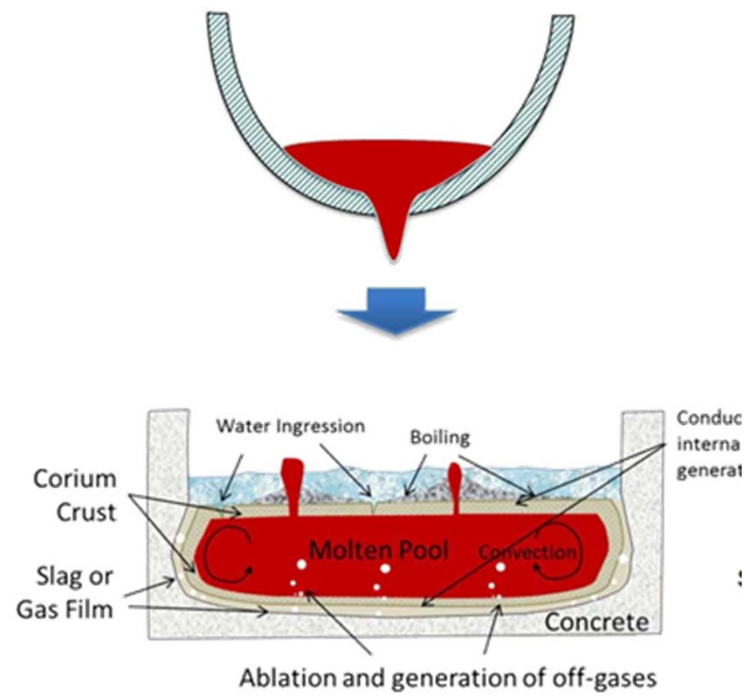
Rekha Rao, Alec Kucala, David Noble, Yifeng Wang, Jeremy Templeton, and David Louie
Sandia National Laboratories
Albuquerque, NM 87185-0836

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND NO. 2011-XXXXP

Nuclear Reactor Accidents: "Core-On-The-Floor"

- During a Nuclear Reactor Accident, one possible scenario is for the reactor to melt down and drop a hot mixture of fuel rods and cladding on the concrete below the reactor
- This is termed "Core-On-The-Floor," since the Corium, a mixture of ZrO_2 cladding and UO_2 fuel become molten, and breach the reactor
- The Corium can react with water and concrete to form hydrogen gas, which is highly combustible

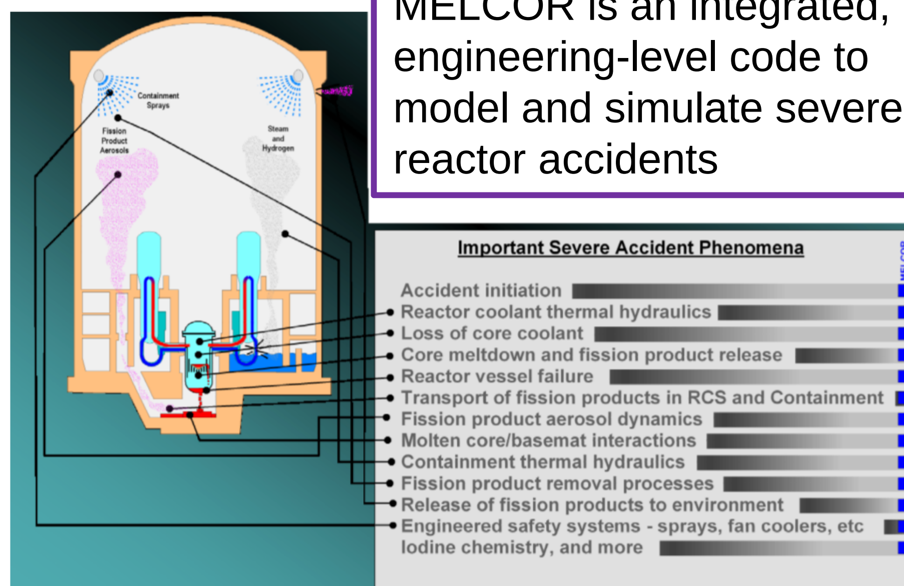


We are trying to develop predictive models of Corium spreading to incorporate into MELCOR, Sandia's Nuclear Reactor Safety Code

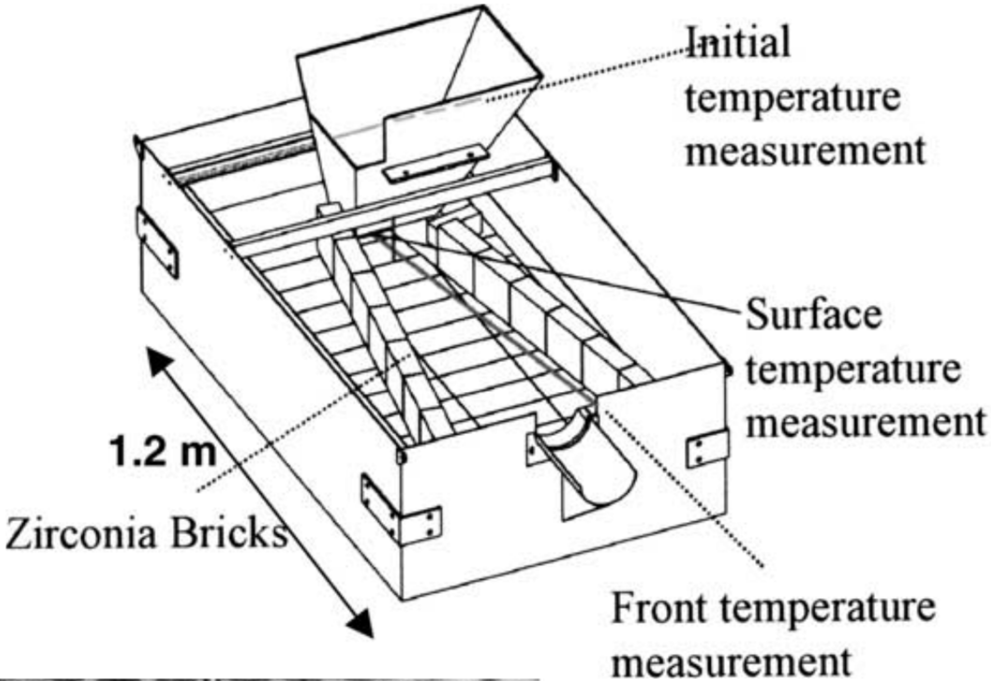
Motivation: Extend Reactor Safety Using Detailed Multiphysics Modeling

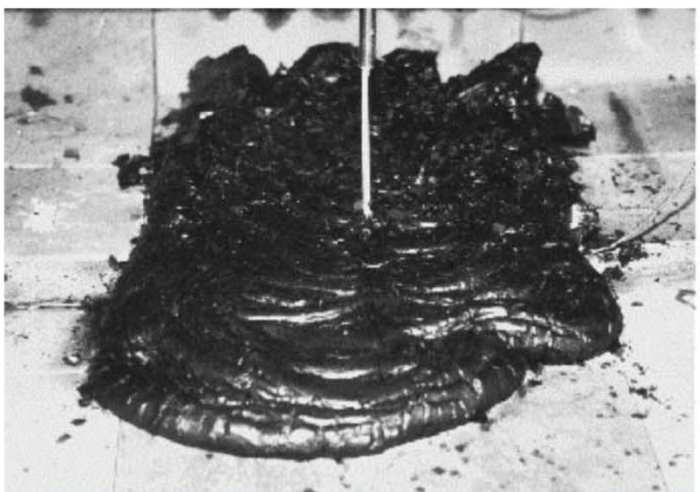
- Develop more accurate model to help understand molten reactor material transport in severe reactor accidents
  - Manage and mitigate reactor containment loads through improved designs
- Enhance ability to model Corium flow
  - Multiphase flow and heat transfer
  - Improve treatment for interfacial chemistry and dynamics
  - Follow surface topology and material breakup with advanced free surface flow algorithms

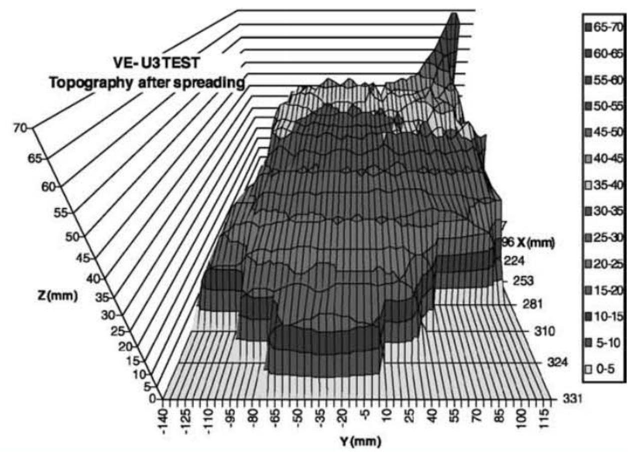
MELCOR is an integrated, engineering-level code to model and simulate severe reactor accidents



Corium Spreading Experiment







Journeau et al., Nuc. Eng. Design, 2003

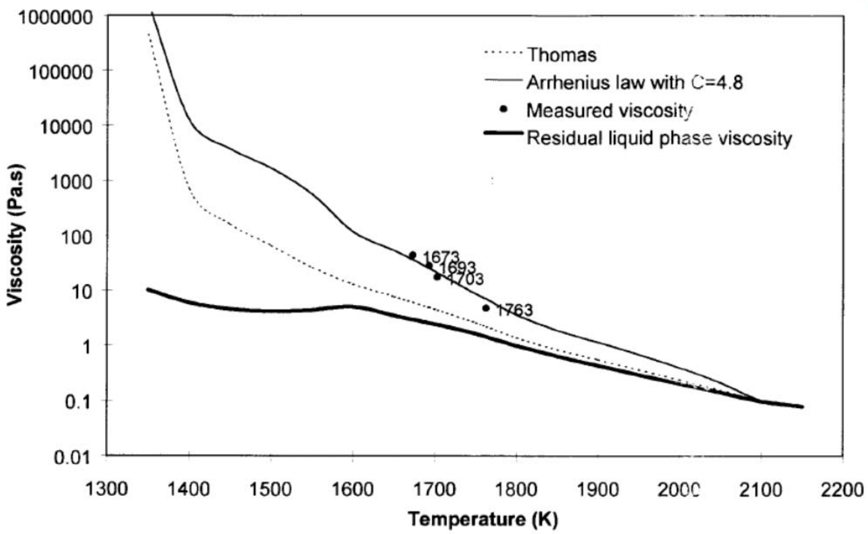
Ramacciotti Viscosity Model

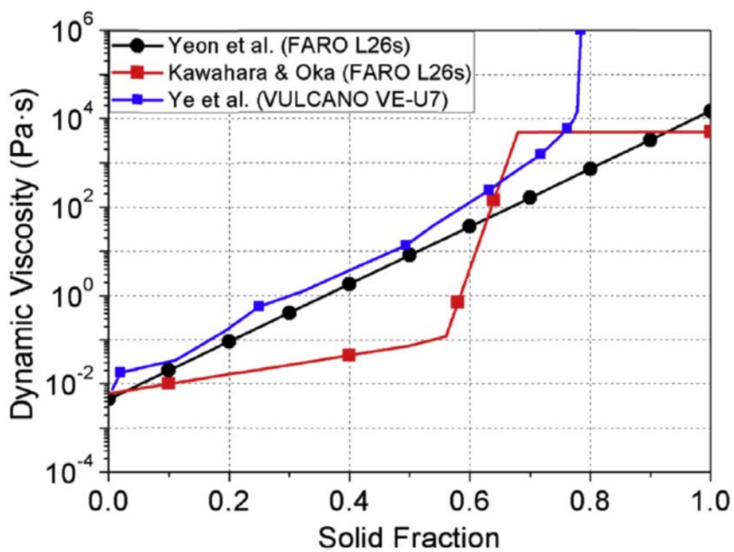
Viscosity is temperature-dependent

- It increases from water-like to solid between the liquidus and solidus temperatures
- It ranges from .0045Pa s above 2670ºC and solidifies to 147100 Pa s below 2575ºC

Table 1
Properties of molten corium.

Property	Value
Density	8000 kg/m³ [a]
Liquidus Temperature	2670 °C [b]
Solidus Temperature	2575 °C [b]
Specific Heat	565 J/kg/K [c]
Fusion Heat	362 kJ/kg [c]
Thermal Conductivity	2.88 W/m/k [c]
Liquid Dynamic Viscosity (Melt Temperature at 2670 °C)	0.0045 Pa s [c]
Surface Tension	0.45 N/m [c]



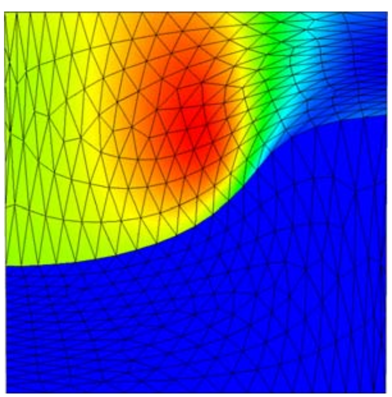
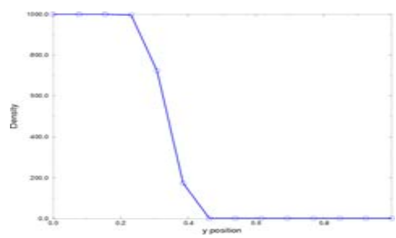
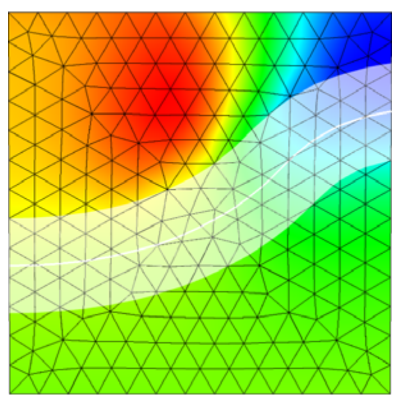
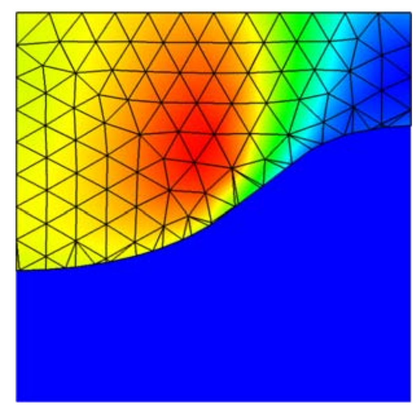


$$\mu = \mu_l \cdot \exp(2.5 \cdot C \cdot f_s)$$

$$f_s = \frac{T_l - T}{T_l - T_s}.$$

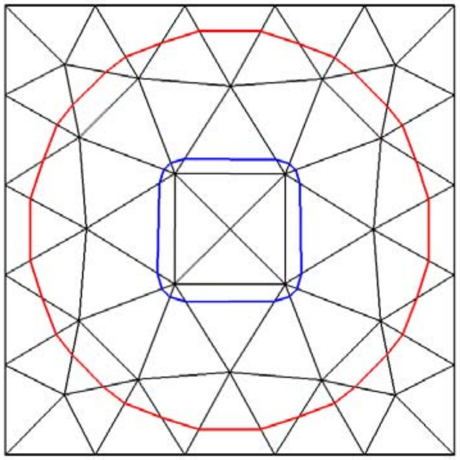
Ramacciotti et al., Nuc. Eng. Design, 2001 Na et al., Prog. Nuc. Energy, 2017

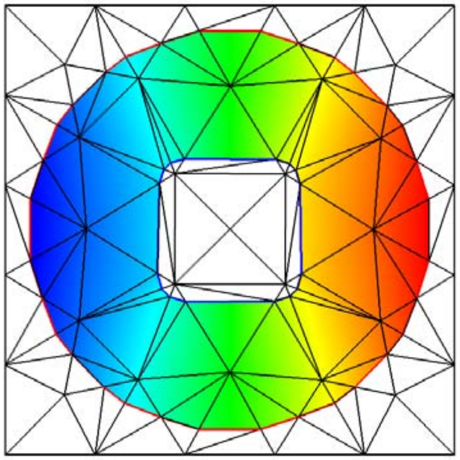
Finite Element Methods for Moving Interfaces in Fluid/Thermal Applications Tested at Sandia

		Enriched Finite Element Methods	
ALE	Diffuse LS	XFEM	CDFEM
• Separate, static blocks for gas and liquid phases • Static discretization 	• Single block with smooth transition between gas and liquid phases • Static discretization  	• Single block with sharply enriched elements (weak or strong) spanning gas and liquid phases • Interfacial elements are dynamically enriched to describe phases	• Separate, dynamic blocks for gas and liquid phases • Interfacial elements are dynamically decomposed into elements that conform to phases 

Conformal Decomposition Finite Element Method (CDFEM)

- Simple Concept (Noble, et al. 2010)
  - Use one or more level set fields to define materials or phases
  - Decompose non-conformal elements into conformal ones
  - Obtain solutions on conformal elements
- Related Work
  - Li et al. (2003) FEM on Cartesian Grid with Added Nodes
  - Ilinca and Hetu (2010) Finite Element Immersed Boundary
  - S. Soghrati and P.H. Geubelle (2012) Interface Enriched Finite Element
- Properties
  - Supports wide variety of interfacial conditions (identical to boundary fitted mesh)
  - Avoids manual generation of boundary fitted mesh
  - Supports general topological evolution (subject to mesh resolution)
- Similar to finite element adaptivity
  - Uses standard finite element assembly including data structures, interpolation, quadrature





Formulation: Capillary Hydrodynamics

Navier - Stokes

- Incompressible with a pressure for each phase

$$\nabla \cdot u = 0,\ \rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u = -\nabla P + \nabla \cdot \mu\left(\nabla u + \nabla u^t\right) + \rho g$$

- Galerkin, Backward Euler, Moving mesh term

$$\int_\Omega \rho \frac{u - u^n}{\Delta t} N_i \, d\Omega + \int_\Omega \rho\left(u - \dot{x}\right) \cdot \nabla u \, N_i \, d\Omega +$$

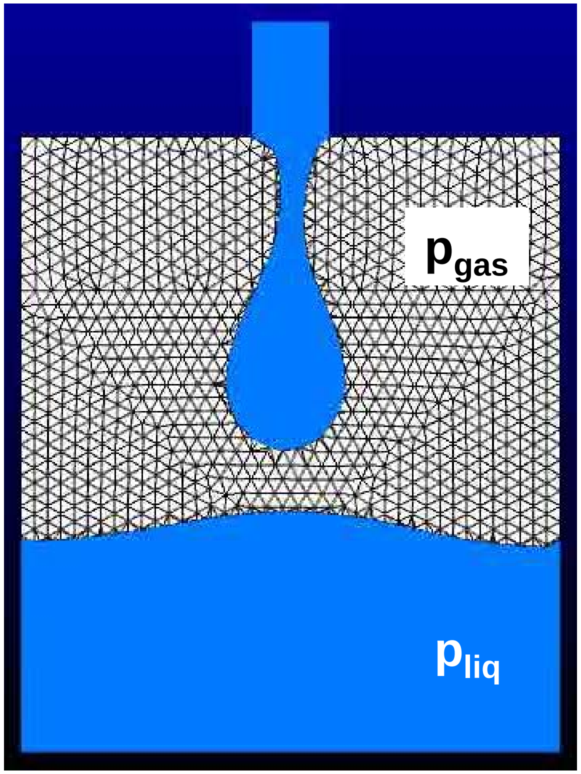
$$\int_\Omega \left[-P\,I + \mu\left(\nabla u + \nabla u^t\right)\right] \cdot \nabla N_i \, d\Omega - \int_\Omega \rho g \, N_i \, d\Omega + \int_\Gamma S \, N_i \ d\Gamma = 0$$

- PSPG stabilization

$$\int_\Omega \nabla \cdot u \, N_i \, d\Omega + \int_\Omega \tau_u \left[-\nabla P + \rho g\right] \cdot \nabla N_i \, d\Omega = 0$$

- SUPG stabilization

$$N_i \Rightarrow N_i + \tau_u \, u \cdot \nabla N_i,\ \tau_u = \left[\left(\frac{2}{\Delta t}\right)^2 + u_i g_{ij} u_j + 12\left(\frac{\mu}{\rho}\right)^2 g_{ij} g_{ij}\right]^{-\frac{1}{2}}$$



Formulation: Interface Dynamics

Level Set Equation

- Advection equation

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0$$

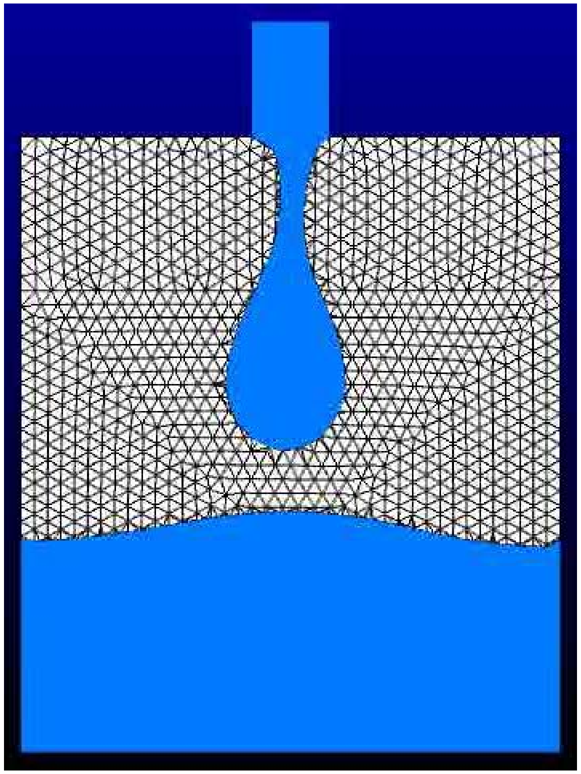
- Galerkin, Backward Euler

$$\int_{\Omega} \frac{\phi - \phi^n}{\Delta t} N_i \, d\Omega + \int_{\Omega} u \cdot \nabla \phi \, N_i \, d\Omega = 0$$

- SUPG stabilization

$$N_i \Rightarrow N_i + \tau_\phi \, u \cdot \nabla N_i , \; \tau_\phi = \left[\left(\frac{2}{\Delta t} \right)^2 + u_i g_{ij} u_j \right]^{-\frac{1}{2}}$$

- Periodic renormalization
  - Compute nearest distance to interface



Models: Liquid-Air Interface

Capillary Force

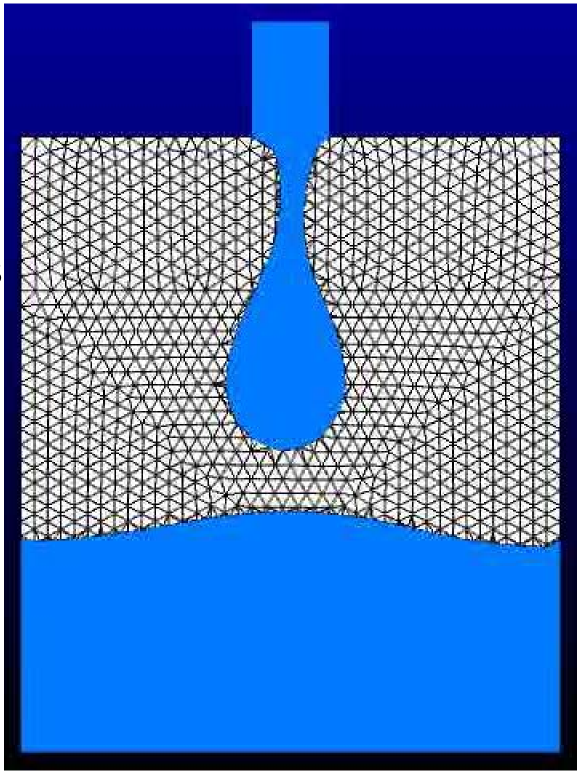
- Same model used in ALE simulations
  - Jump in stress due to interfacial tension
  - Laplace-Beltrami implementation avoids second derivatives

$$\int_{\Gamma} \left(\gamma\kappa\,\mathbf{n} + \nabla_s \gamma\right) N_i \; d\Gamma = \int_{\Gamma} \gamma \nabla_s N_i \; d\Gamma, \; \nabla_s \equiv \left(\mathbf{I} - \mathbf{nn}\right)\nabla$$

Interface Stabilization

- Surface viscosity type stabilization
  - Based on a paper by Hysing (2010)

$$\int_{\Gamma} \mu_s \nabla_s u \cdot \nabla N_i \; d\Gamma$$



Heat Transfer: Liquid Phase Only

Energy Equation

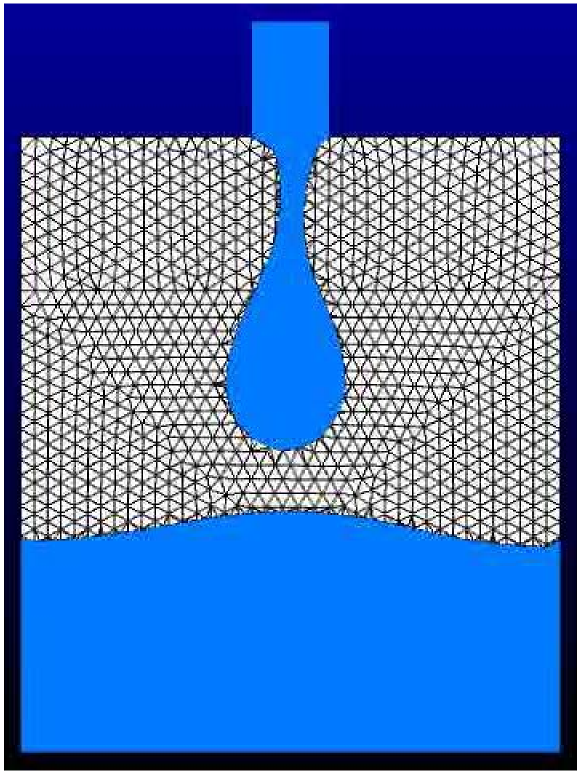
- Solve heat transfer in the liquid phase only

$$\rho C_{pf}\frac{\partial T}{\partial t} + \rho C_{pf} v \bullet \nabla T = \nabla \bullet (k \nabla T) + \rho \varphi_e \Delta H_{rxn}\frac{\partial \xi}{\partial t}$$

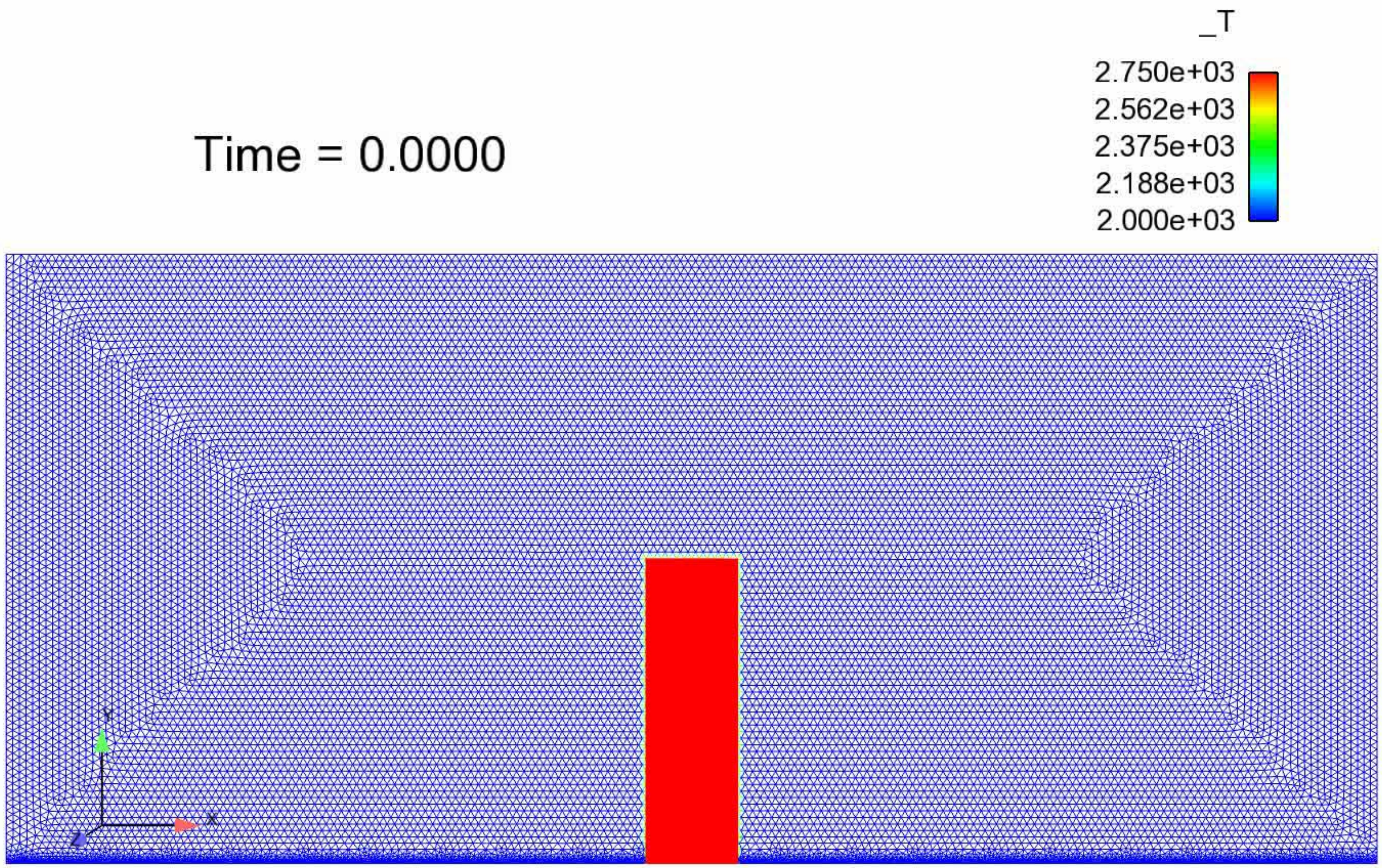
Heat transfer coefficients used for turbulent heat transfer in air

- Radiation and convection in air phase

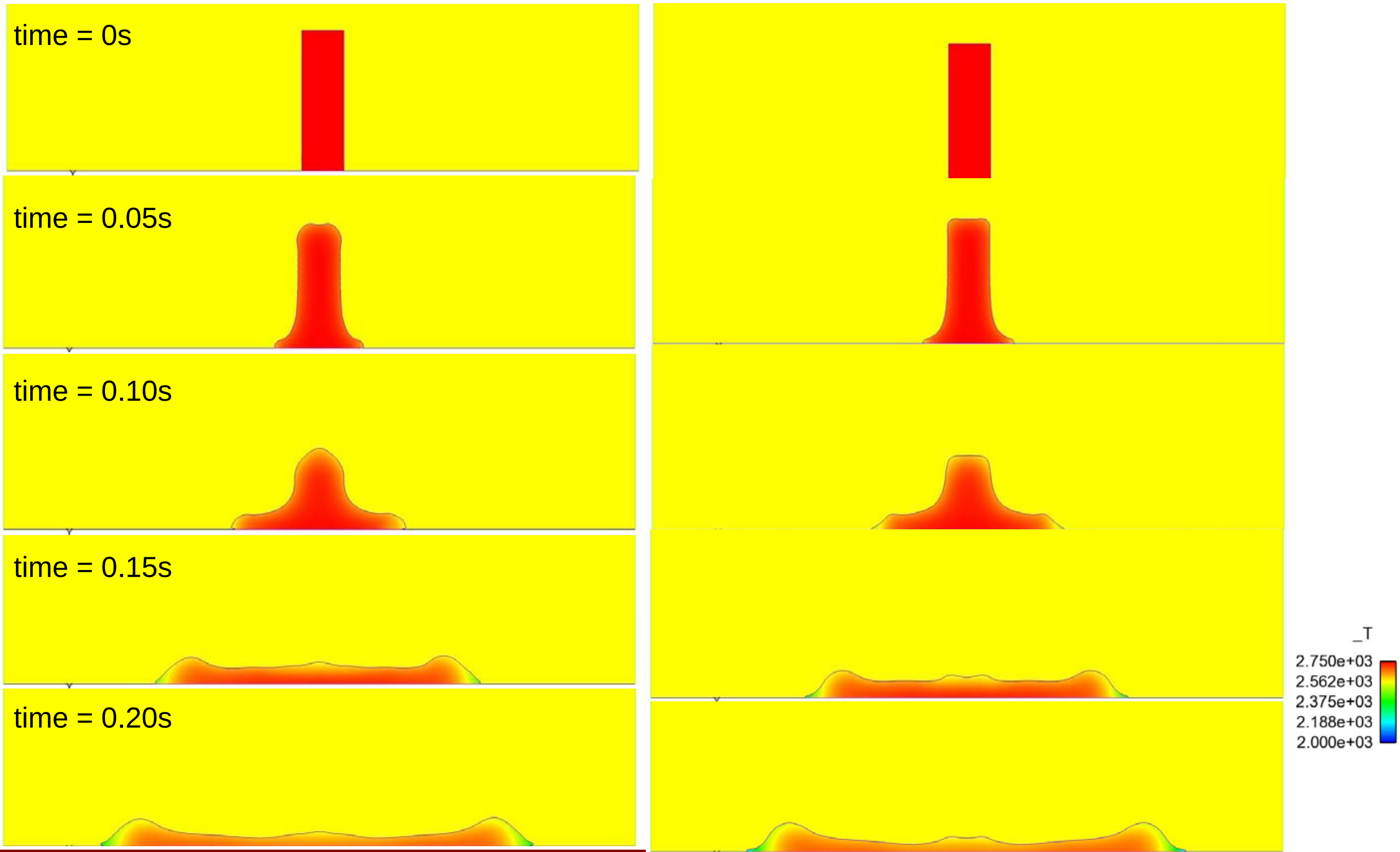
$$q_{surf} = \int_{\Gamma} h_{conv}(T - T_{ref}) + h_{rad}(T^4 - T_{ref}^4)\, d\Gamma$$



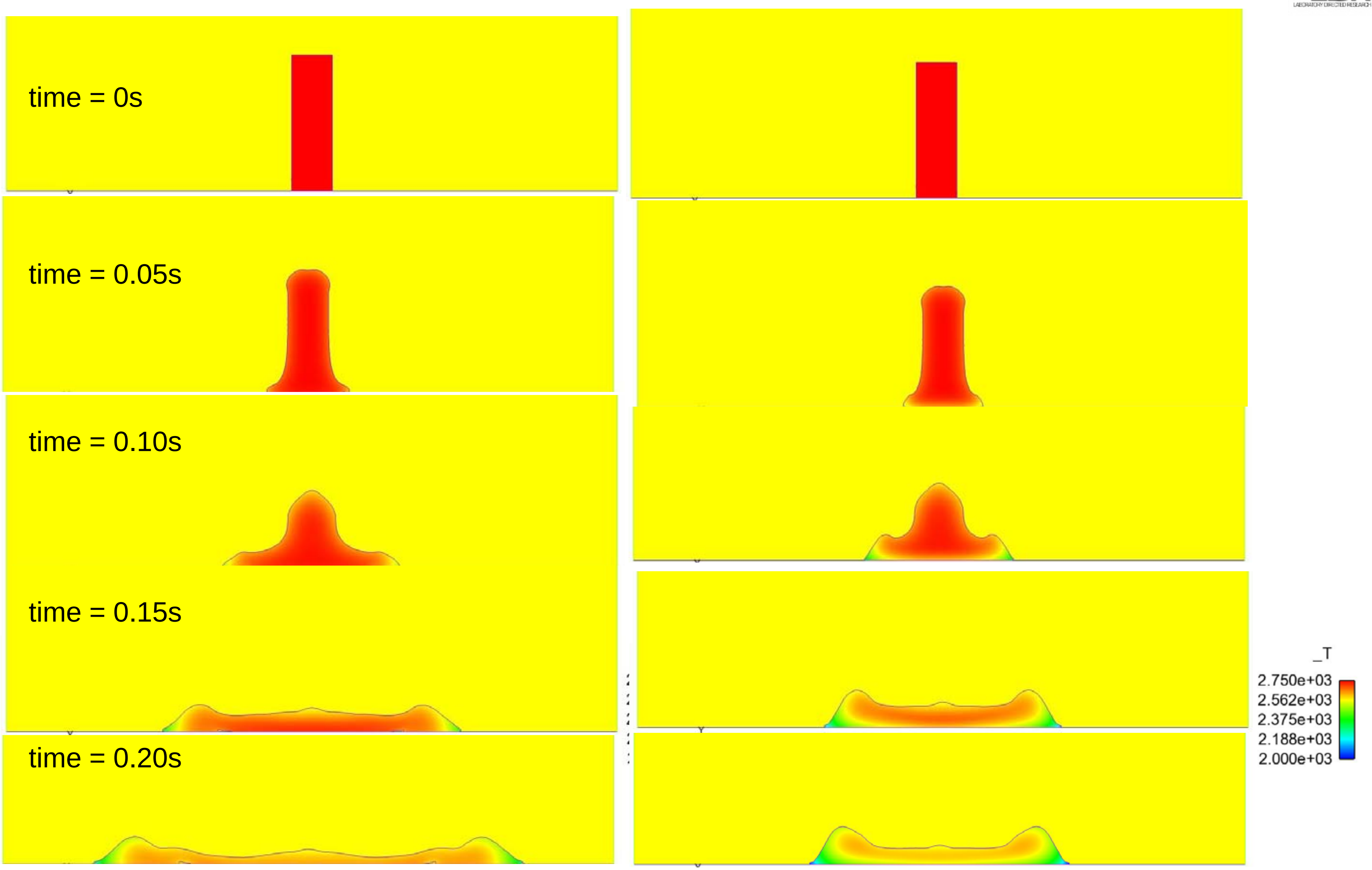
2D Corium Spreading



Corium Spreading: Variable Surface Tension vs. No Surface Tension



Cooling on the Bottom: Small vs. Large Heat Flux

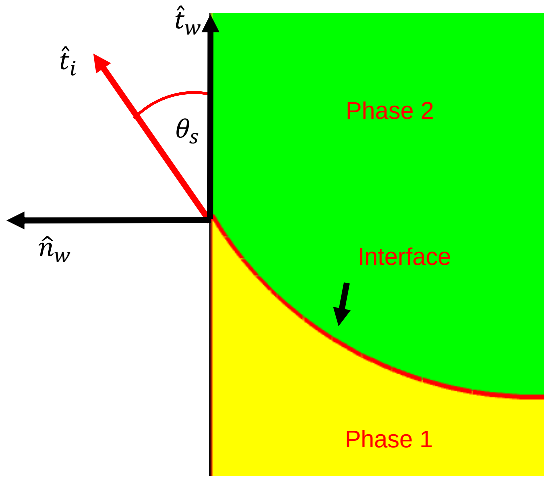


Moving contact line model

Wetting Line Force

$$\vec{f} = \gamma \hat{\tau}_i$$

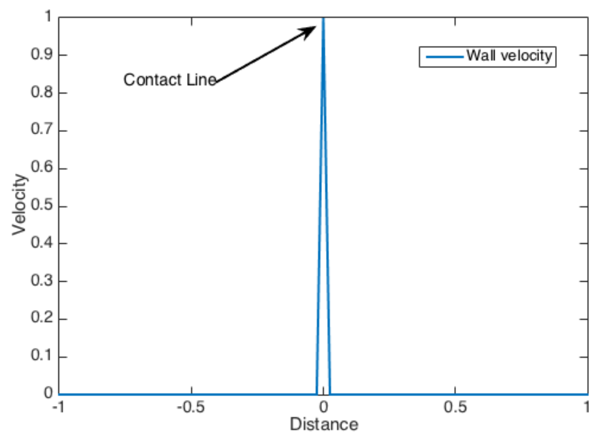
$$\hat{\tau}_i = \hat{\tau}_w \cos\theta_s + \hat{n}_w \sin\theta_s$$



Navier-Slip Condition

$$\vec{f} = \frac{\mu}{\beta}(\vec{v}_w - \vec{v}_{CL})$$

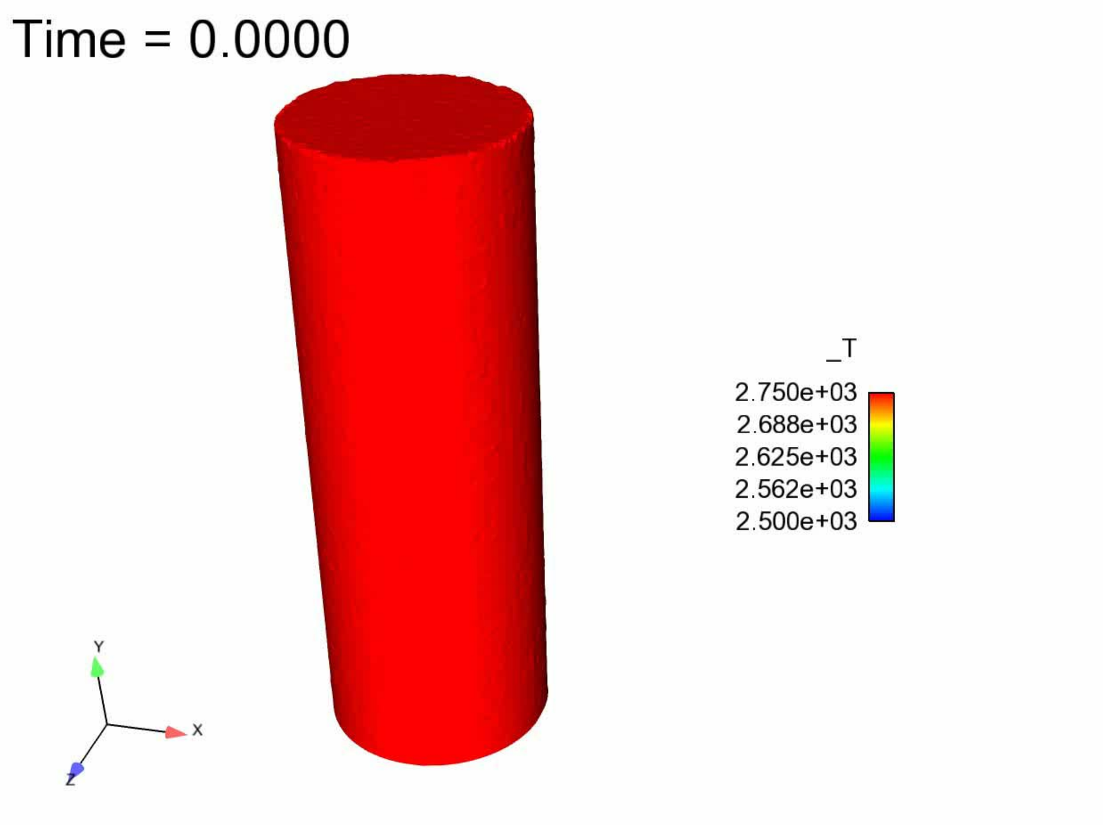
$$Flux = \int \vec{n} \cdot \vec{f} \phi^i \mathrm{d}S$$



- Assume microscopic (static) contact angle is a constant (θ_s) (hydrodynamic type method)
- For a given fluid pair, specify kinematic and physical properties, surface tension force (γ), and static contact angle (θ_s)
- Pull contact line with surface tension force at Young's equilibrium contact angle
- Select the Navier-Slip length (β) to fit to experimental data

3D Spreading Model (CDFEM)

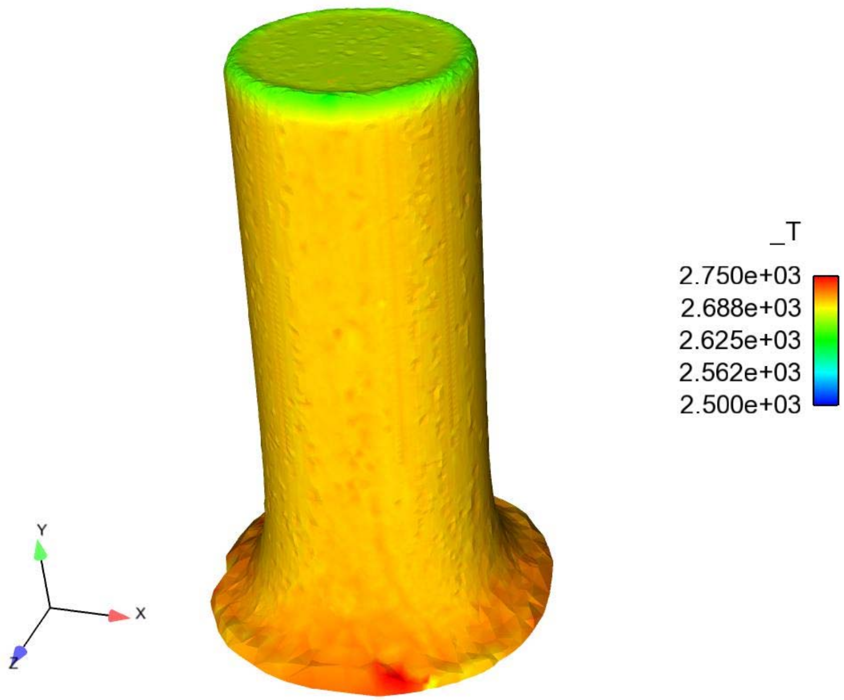
- Column slumping similar to 2D examples
- Wetting line entrains air and has difficulty maintaining mesh integrity

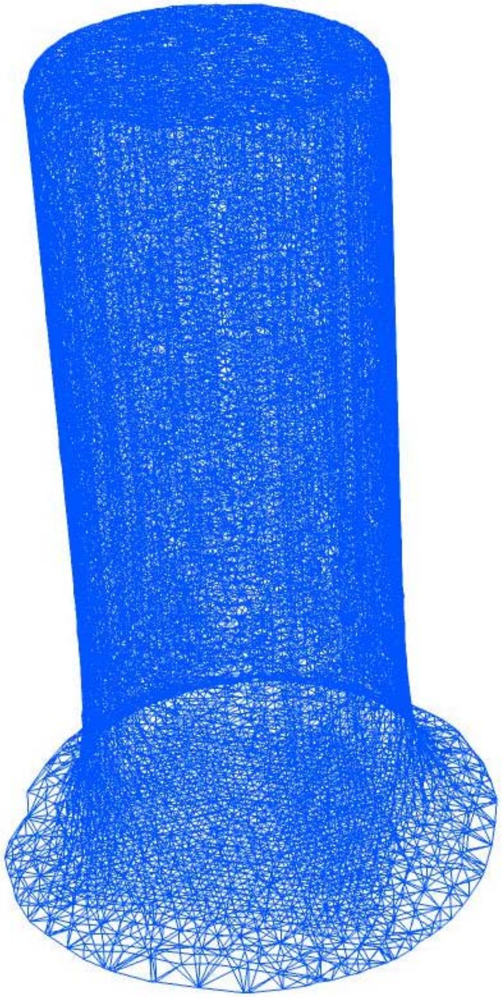


3D Spreading Model (CDFEM)

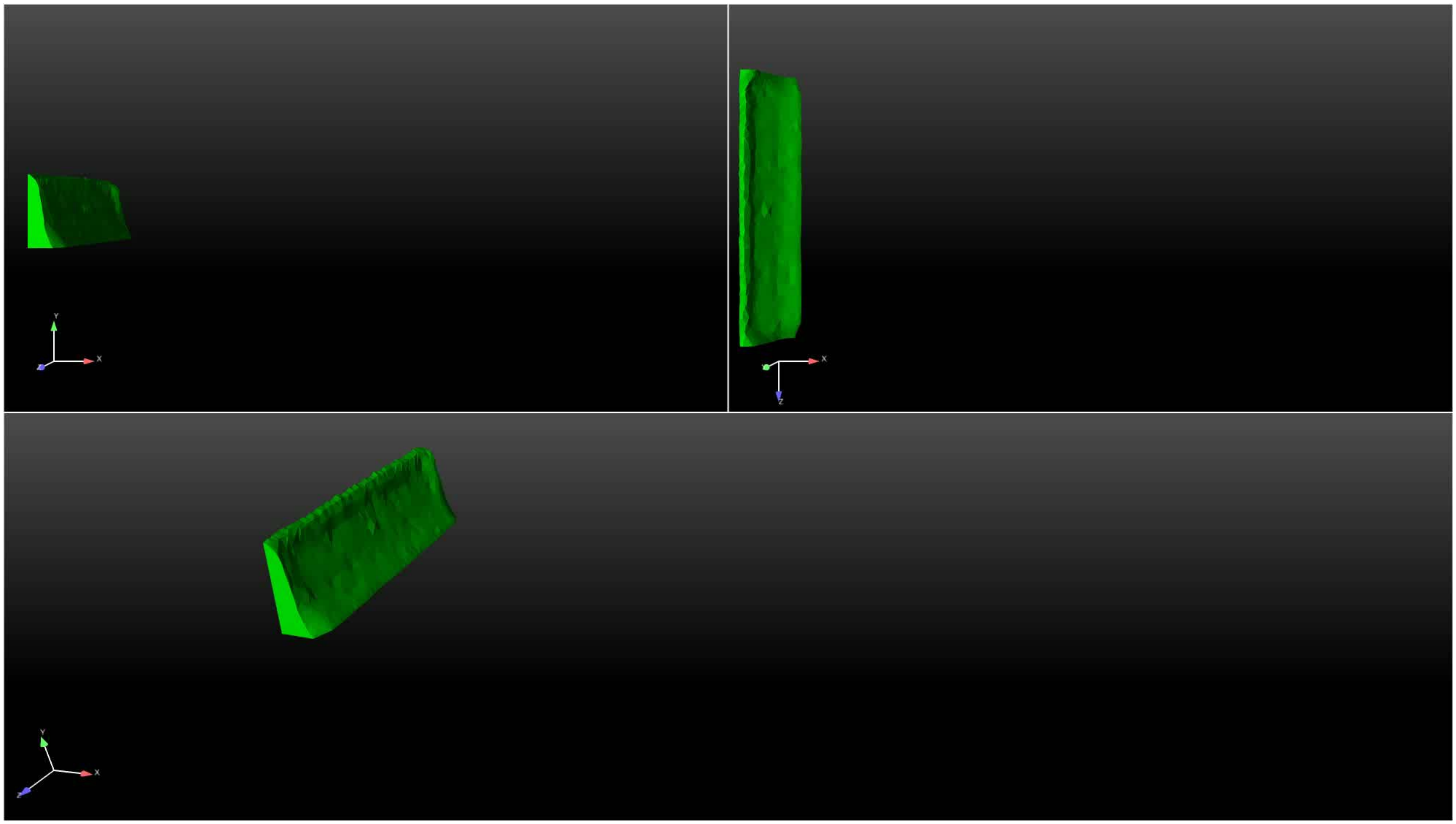
- Column slumping similar to 2D examples
- Wetting line entrains air and has difficulty maintaining mesh integrity

Time = 0.1261

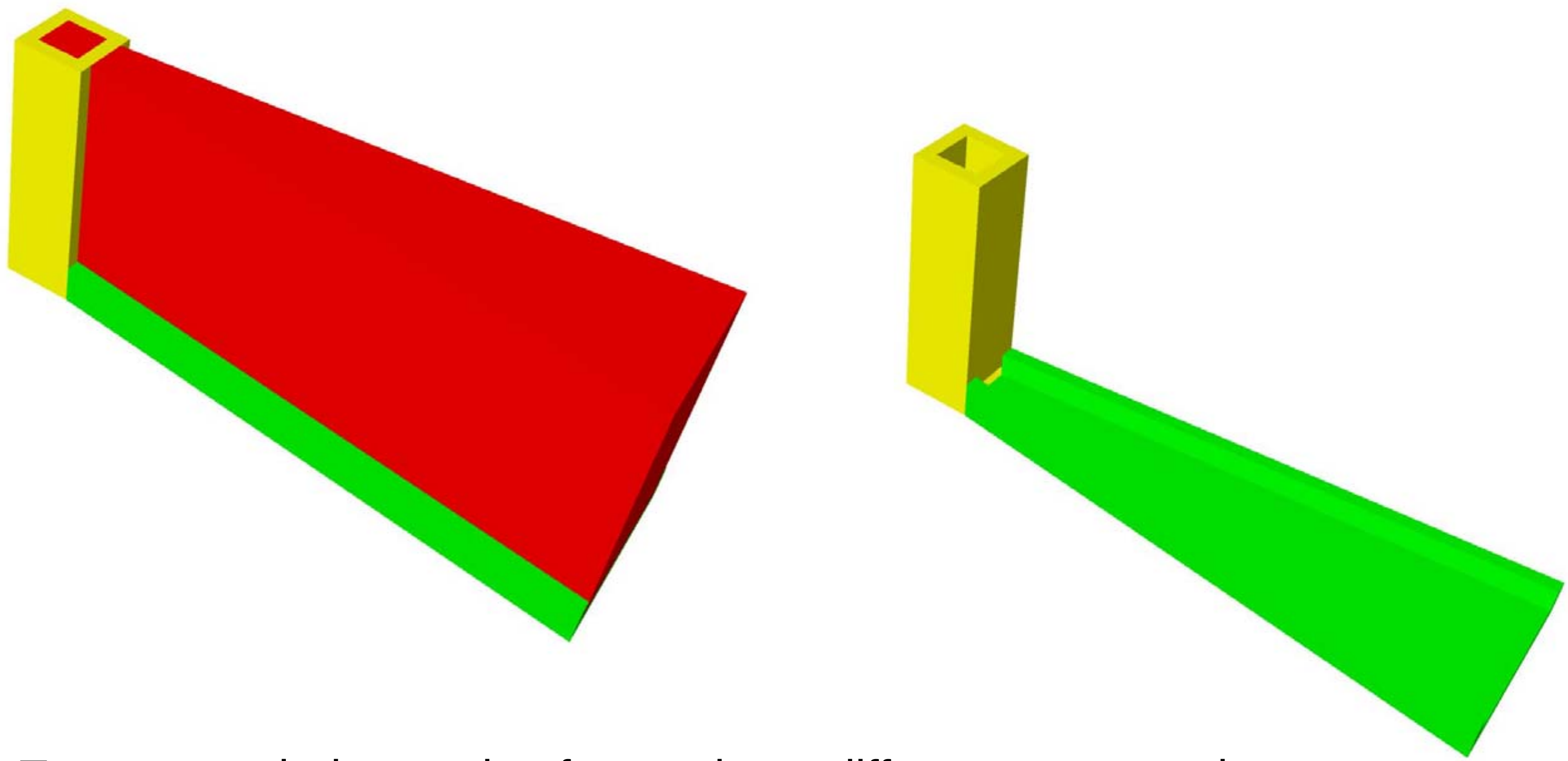




3D Spreading Model (CDFEM)

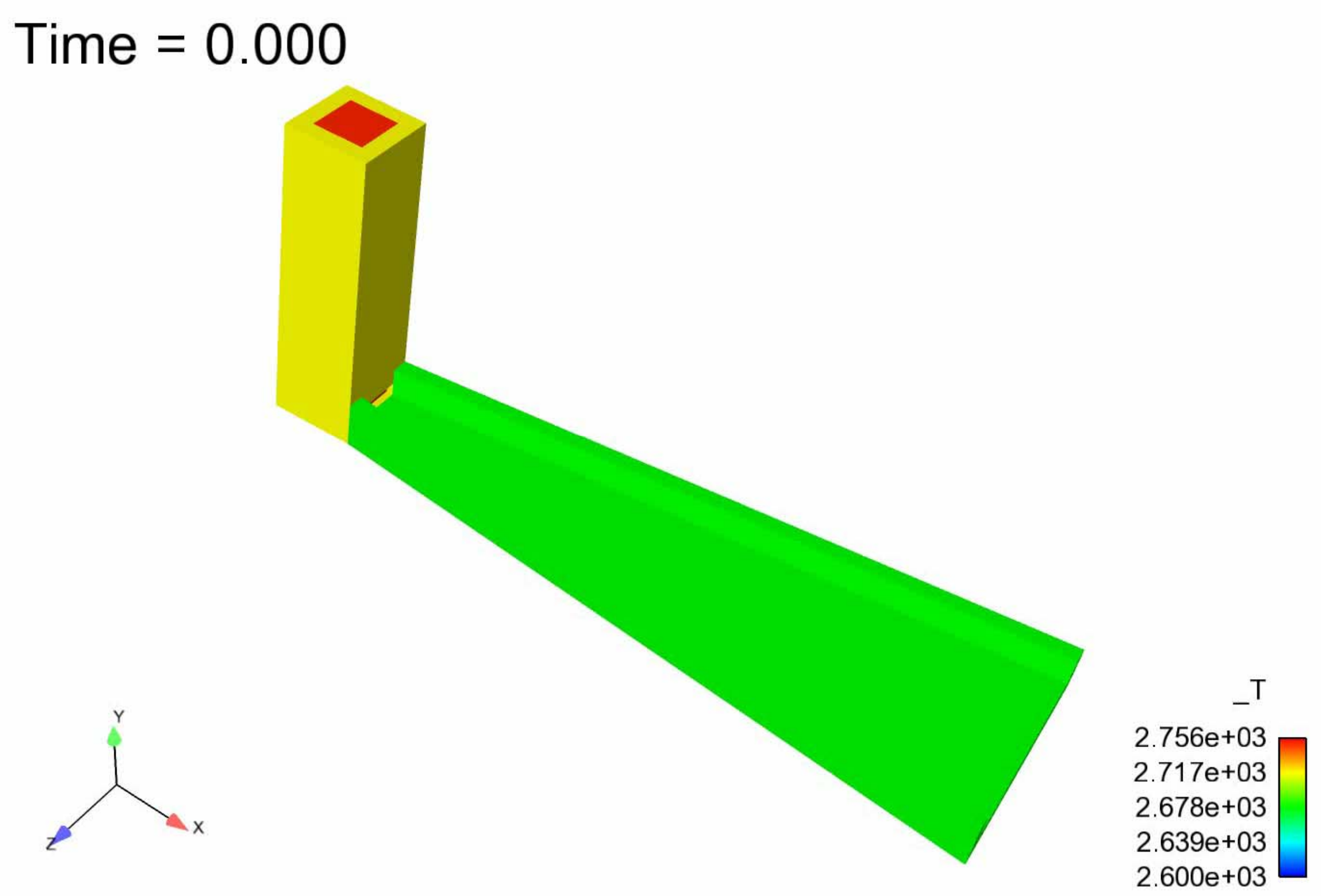


3D Corium Spreading in Trough: Level Set Method: Diffuse Interface



- Try to smooth the wetting front using a diffuse representation
- Level set method: Red phase has corium and air
- Corium fills the chute at time 0 and flows with gravity into the trough
- Yellow and green parts are steel

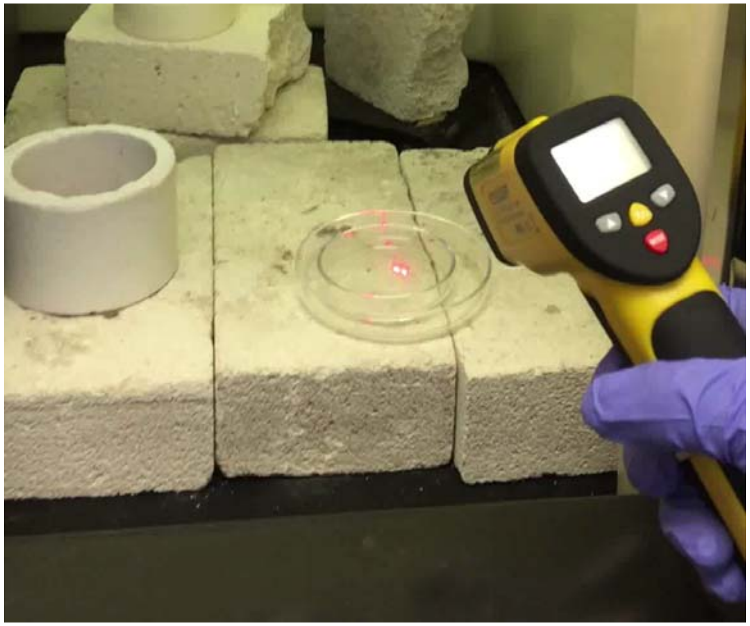
3D Corium Spreading in Trough



- For level set, there is currently no way to apply boundary condition on the free surface for radiative heat loss
- Cooling is applied through the steel trough

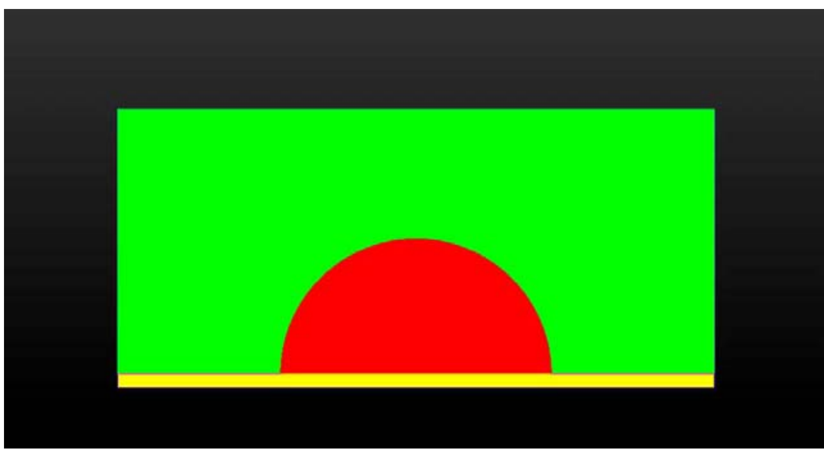
Experiments for Flow and Solidification

- Benchtop experiments were carried out on model system
  - Developed experimental procedures for testing the proposed concept using PbO as a surrogate for Corium.
  - Tested molten PbO at 975^{o}C onto silica dish.
  - Surface temperatures were monitored during the pour experiments

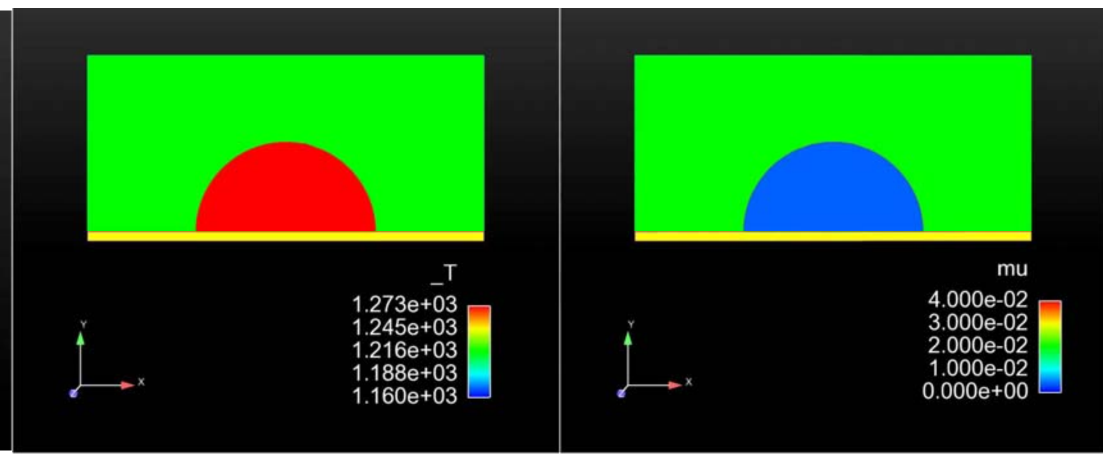


Experimental Modeling – Lead Oxide Spread

- Spread of melt modeled using Aria
  - Finite-element code using level set method to discretize the melt
  - Spread rate influenced by surface tension and gravity forces
- Effect of heat transfer on spread rate has been modeled
  - Viscosity – temperature relationship influences spread rate
  - Spread is halted when external heat transfer is applied at lead boundary
- Demonstrate Aria's capability for modeling molten spreading and solidification

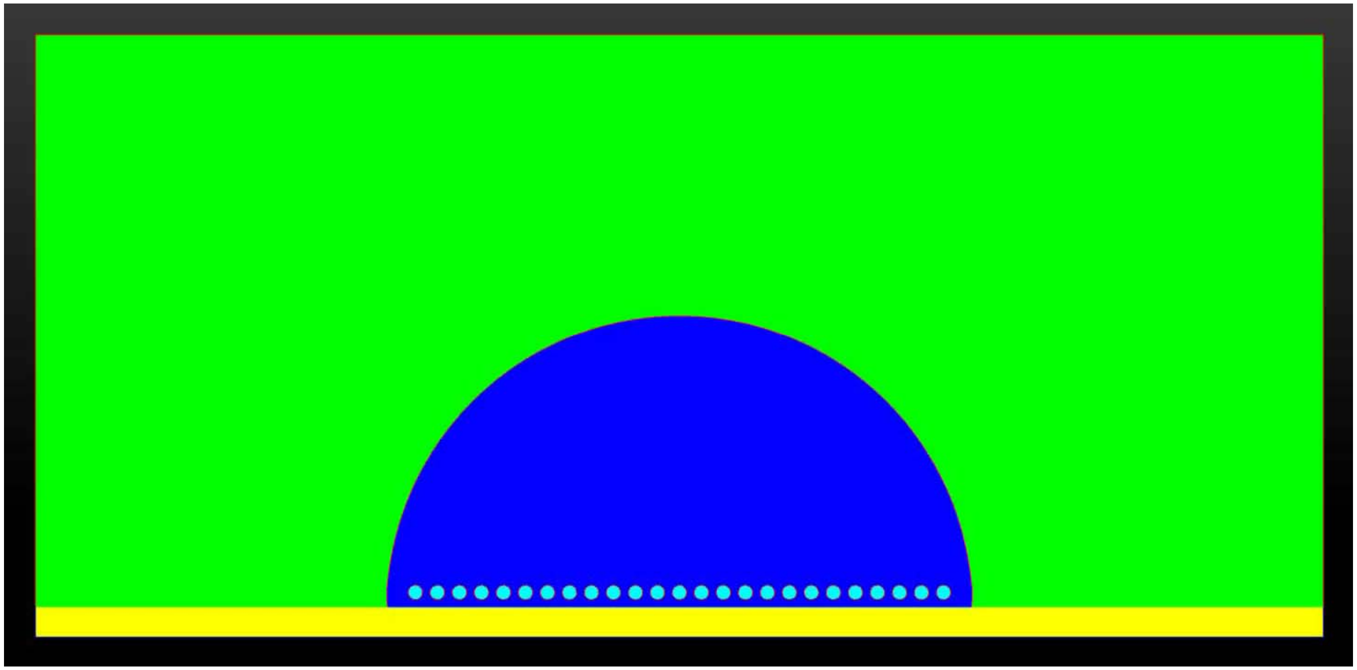


Spread of lead oxide with no heat heat flux



Spread of lead oxide as a function of viscosity & temperature due to heat flux

Experimental Modeling – CO_2 bubbles



- CO_2 bubble rise can be modeled
  - Initial array of CO_2 bubbles emanate from $CaCO_3$-PbO boundary
  - Heat flux boundary conditions change local viscosity
  - Bubbles rise via buoyant forcing and local convection inside spreading melt
  - Coalescence of bubbles
- Better heat transfer model under development
  - $CaCO_3$ endothermic reaction

Conclusions

- We are working on modeling Corium flow after a nuclear accident to support MELCOR, a reactor safety code
- CDFEM is used to solve the spreading of the molten Corium material
  - Problem is difficult:
    - High temperatures involved with high Peclet number
    - Low viscosity of melt, temperature-dependence and solidification
    - Low capillary number and wetting of free surface
- Next steps:
  - Low-order turbulence model
  - Smoothing of the wetting line to improve mesh quality and reduce numerical air entrainment