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A Control Volume Finite Element Approach for Modeling Molten Corium Spreading and Solidification

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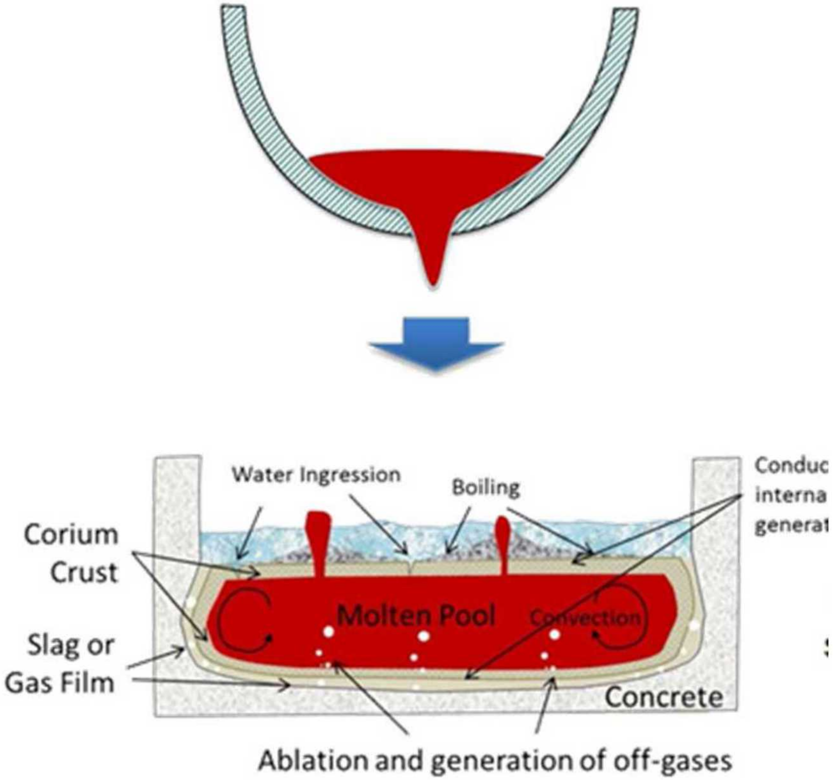
Nuclear Reactor Accidents

- When the nuclear facilities cooling system fails during a nuclear reactor accident, one possible scenario is a core breach
- A core breach occurs when a viscous molten mixture of nuclear fuel (UO_2), cladding, and structural supports, deemed "corium" breaches the containment vessel in a nuclear reactor
  - Temperature of this material can exceed 3000 º Celsius
- The molten corium can escape containment forming a melt pool, flowing along the reactor cavity ablating the concrete structure
- The corium can react with water and concrete to form hydrogen gas, which is highly combustible

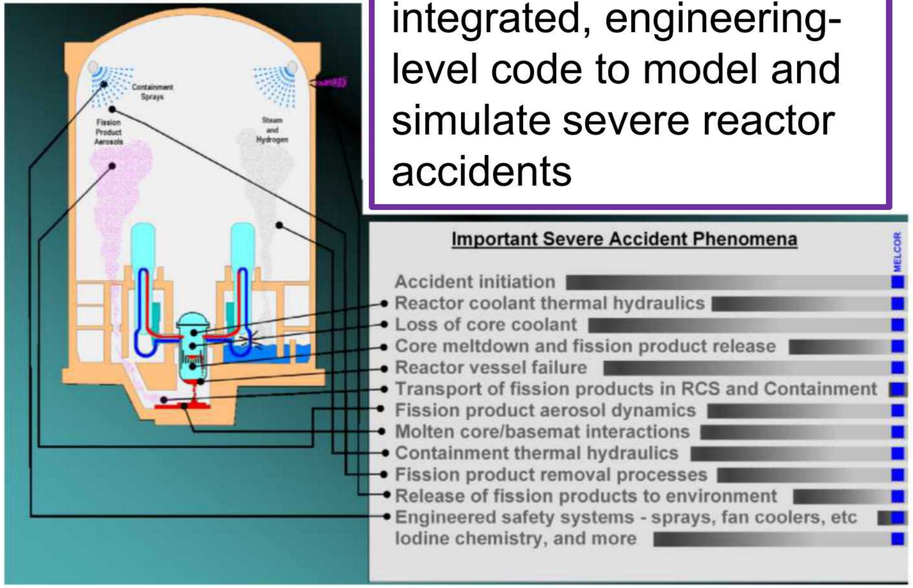


We are developing predictive models of corium spreading to incorporate into MELCOR, Sandia's Nuclear Reactor Safety Code

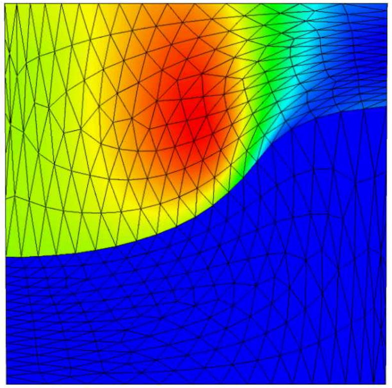
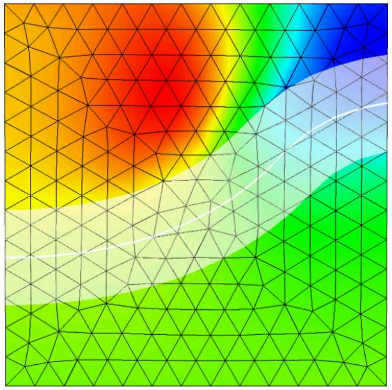
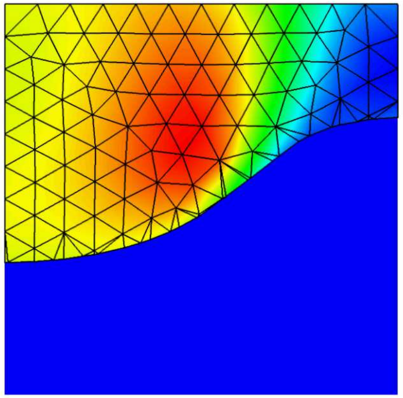
Corium Spreading

- Corium flow is characterized by an undulating flow where the corium transitions between solid/liquid phase change
- Corium flow is difficult to model using conventional methods
  - High temperatures involved with high Peclet number
  - Low viscosity of melt, temperature-dependence and solidification
- Use a CVFEM-CDFEM methodology to model corium flow
  - Multiphase flow and heat transfer
  - Follow surface topology and material breakup with advanced free surface flow algorithms
- Modeling effort motivated to aid in the development of more accurate low-order spreading models for MELCOR and to engineering new design methods to prevent containment breach in a nuclear accident scenario

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

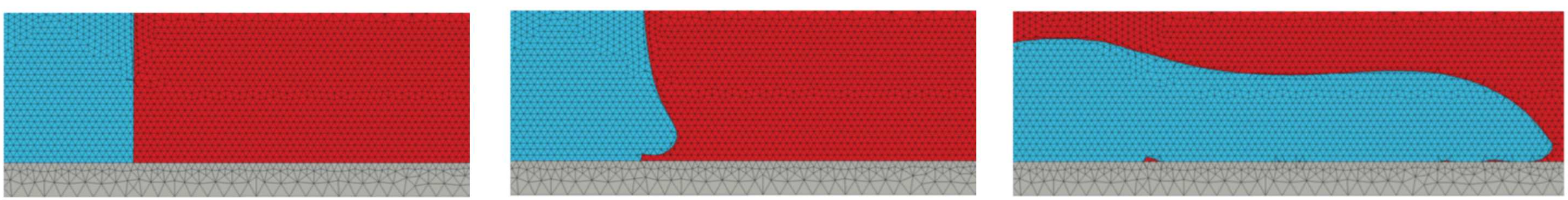


Finite Element Methods for Moving Interfaces in Fluid/Thermal Applications Tested at Sandia

		Enriched Finite Element Methods	
ALE	Diffuse LS	XFEM	CDFEM
• Separate, static blocks for gas and liquid phases • Static discretization • Mesh quality can be become a problem, leading to re-meshing of geometry 	• Single block with smooth transition between gas and liquid phases • Static discretization • Interface "smearing" 	• 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)

- 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
- Modeling the molten flowing corium poses challenges for numerical models due to presence of large Peclet numbers and Reynolds numbers
  - GFEM technique is sometimes inadequate for suppressing spurious oscillations
  - CVFEM discretization for advection dominated flow and heat transport
  - CDFEM tracks the corium/air interface on an existing background mesh
- CVFEM-CDFEM approach
  - Spreading of molten corium in 2D and 3D
  - CVFEM formulation suppress spurious oscillations associated with high Pe and Re flow regimes



Governing Equations

Conservation Equations

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u}\right) = -\nabla p + \nabla \cdot \left(\mu\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right)\right)$$

$$\rho C_{\mathrm{P}}\left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) - \nabla \cdot (k \nabla T) = \dot{q}$$

Level Set Equation

$$\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\,\phi = 0$$

Interface Boundary Conditions

$$[\mathbf{u}]_{\Delta} = 0, \qquad \mathbf{x} \in \Gamma_{\mathrm{F}}$$

$$[-p\mathbf{I} + \mu(\mathbf{x})\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right)]_{\Delta} \cdot \hat{\mathbf{n}} = -\gamma \kappa \hat{\mathbf{n}}, \qquad \mathbf{x} \in \Gamma_{\mathrm{F}}$$

Time-discretization scheme (2nd Order)

Momentum Prediction

$$\int_{\Omega^n} (\nabla\cdot\tilde{\mathbf{u}})\, w_i \mathrm{d}\Omega = 0,$$

$$\int_{\Omega^n} \rho \left(\frac{\frac{3}{2}\tilde{\mathbf{u}} - 2\mathbf{u}^n + \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} + (\tilde{\mathbf{u}}\cdot\nabla)\,\tilde{\mathbf{u}} \right)\cdot \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Omega^n} -P\mathbf{I} + \mu\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^t\right)\cdot\nabla\mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Gamma_f^n} \sigma\left((\mathbf{I}-\mathbf{nn}) + \Delta t \underline{\nabla}\tilde{\mathbf{u}}\right)\cdot\nabla\mathbf{w}_i \mathrm{d}\Gamma = 0,$$

Levelset Advection

Momentum Correction

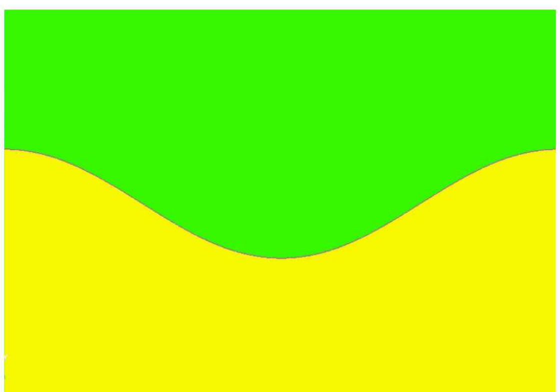
$$\int_{\Omega^{n+1}} \left(\nabla\cdot\mathbf{u}^{n+1}\right) w_i \mathrm{d}\Omega = 0.$$

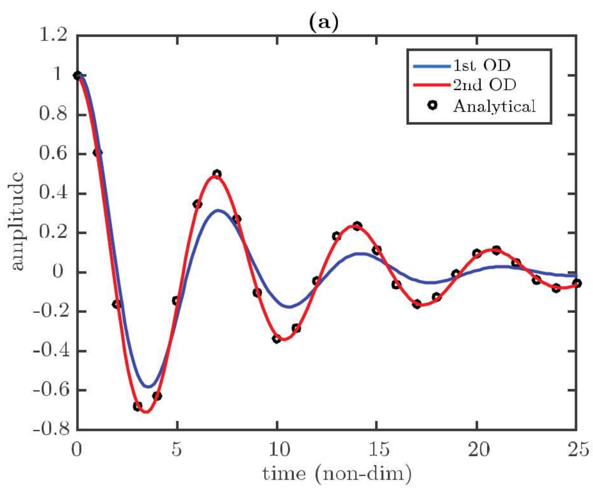
$$\int_{\Omega^{n+1}} \rho \left(\frac{\frac{3}{2}\mathbf{u}^{n+1} - 2\mathbf{u}^n + \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} + \left(\left(\mathbf{u}^{n+1} - \dot{\mathbf{x}}\right)\cdot\nabla\right)\mathbf{u}^{n+1} \right)\cdot \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Omega^{n+1}} -P\mathbf{I} + \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^t\right)^{n+1}\cdot\nabla\mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Gamma_f^{n+1}} \sigma\left((\mathbf{I}-\mathbf{nn}) + \Delta t \underline{\nabla}\left(\mathbf{u}^{n+1} - \tilde{\mathbf{u}}\right)\right)\cdot\nabla\mathbf{w}_i \mathrm{d}\Gamma = 0,$$

Verification and validation (capillary wave decay)

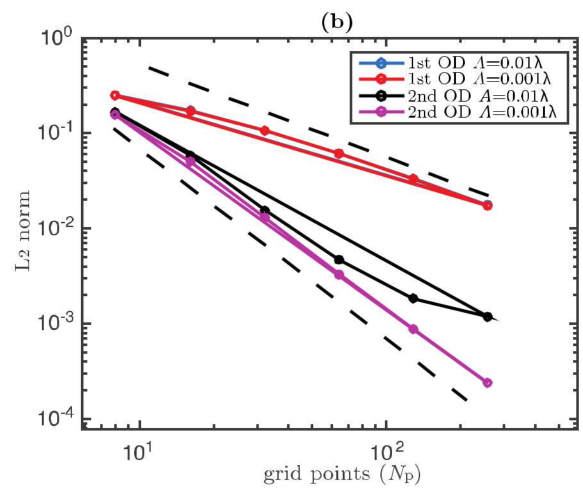
- Perturb two-phase interface with sinusoidal disturbance
- Interface shape should decay with specific frequency and rate (Prosperetti, 1981) at small amplitudes
- Accurate prediction of capillary wave frequency and amplitude decay
- CDFEM discretization of interface accurately captures surface tension dynamics
- 2nd order mesh convergence observed

Interface Dynamics





Convergence



Viscosity model

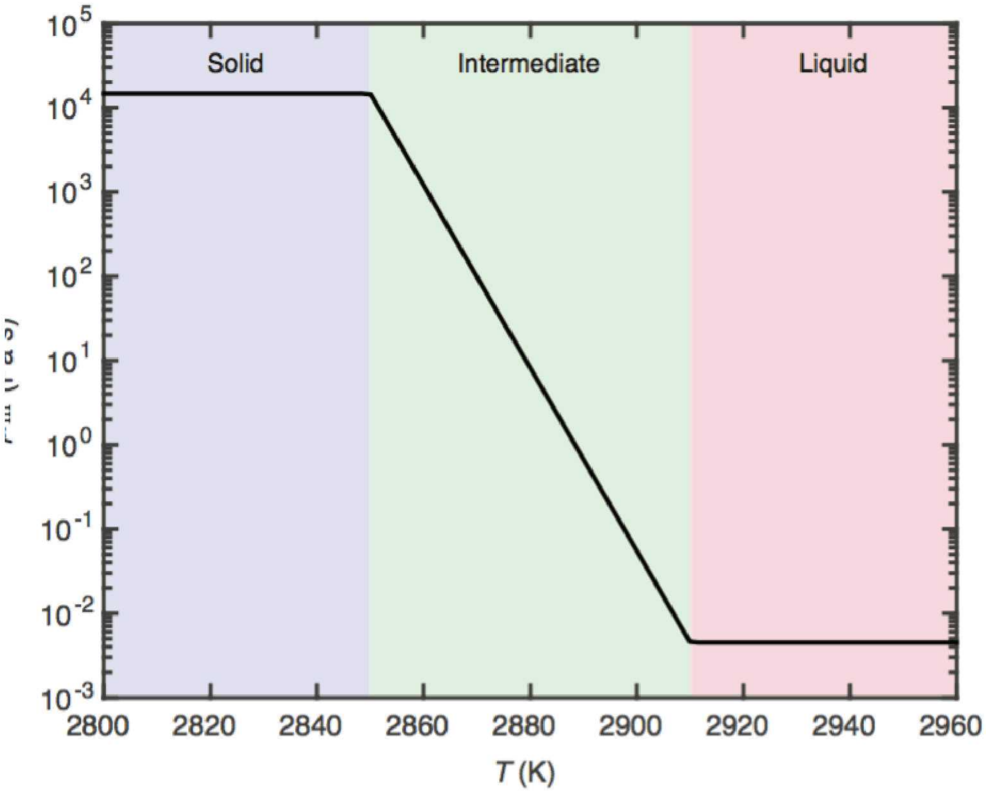
- Ramacciotti (2001) temperature-dependent viscosity model used for psuedo-solidification.

Table 1: Some static properties for the corium melt

Property	**Value (Units)**
Density (ρ_m)	8000 ($kg \cdot m^{-3}$)
Specific Heat (C_P)	565 ($J \cdot kg^{-1} \cdot K^{-1}$)
Thermal Conductivity (k_m)	(2.88 $W \cdot m^{-1} \cdot K^{-1}$)
Surface Tension (γ)	0.45 ($N \cdot m^{-1}$)
Liquidus Temperature (T_L)	2910 (K)
Solidus Temperature (T_S)	2860 (K)
Emmisivity (ϵ)	0.80

$$f = \frac{T_L - T}{T_L - T_S}$$

$$\mu_m = \mu_L e^{2.5 \cdot C \cdot f}$$



Viscosity as a function of temperature (Ramacciotti, 2001)

Interface Modeling

Navier-Slip Condition

$$\int_{\Gamma_S^{n+1}} \left(\left(-p\mathbf{I} + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}} \right)^{n+1} \right) \cdot \hat{\mathbf{n}} \right) w_i \mathrm{d}\Gamma_S = \int_{\Gamma_S^{n+1}} \frac{\mu_m}{\beta} \left(\mathbf{u}_w - \mathbf{u}^{n+1} \right) \cdot \mathbf{w}_i \mathrm{d}\Gamma_S,$$

Corium/Steel Heat Transfer

$$T_s - T_m = 0 \quad \text{on } \Gamma_S$$

$$(k_s \nabla T_s - k_m \nabla T_m) \cdot \hat{\mathbf{n}} = \frac{k_s}{h} (T_s - T_m) \quad \text{on } \Gamma_S$$

Corium Radiactive Heat Decay (Na et. al; 2017)

$$\dot{q}_d = 0.095 \dot{q}_0 t^{-0.26}$$

Corium/Air Radiative Heat Transfer

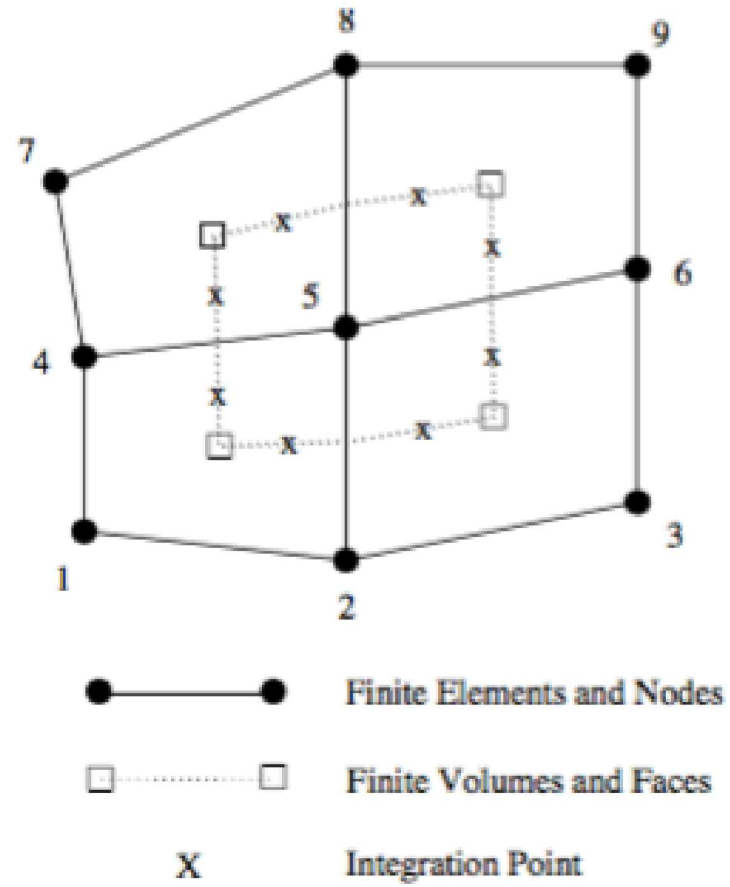
$$q = c_{rad} \left(T^4 - T_{ref}^4 \right)$$

Corium/Air Convective Heat Transfer

$$q = h (T - T_{ref})$$

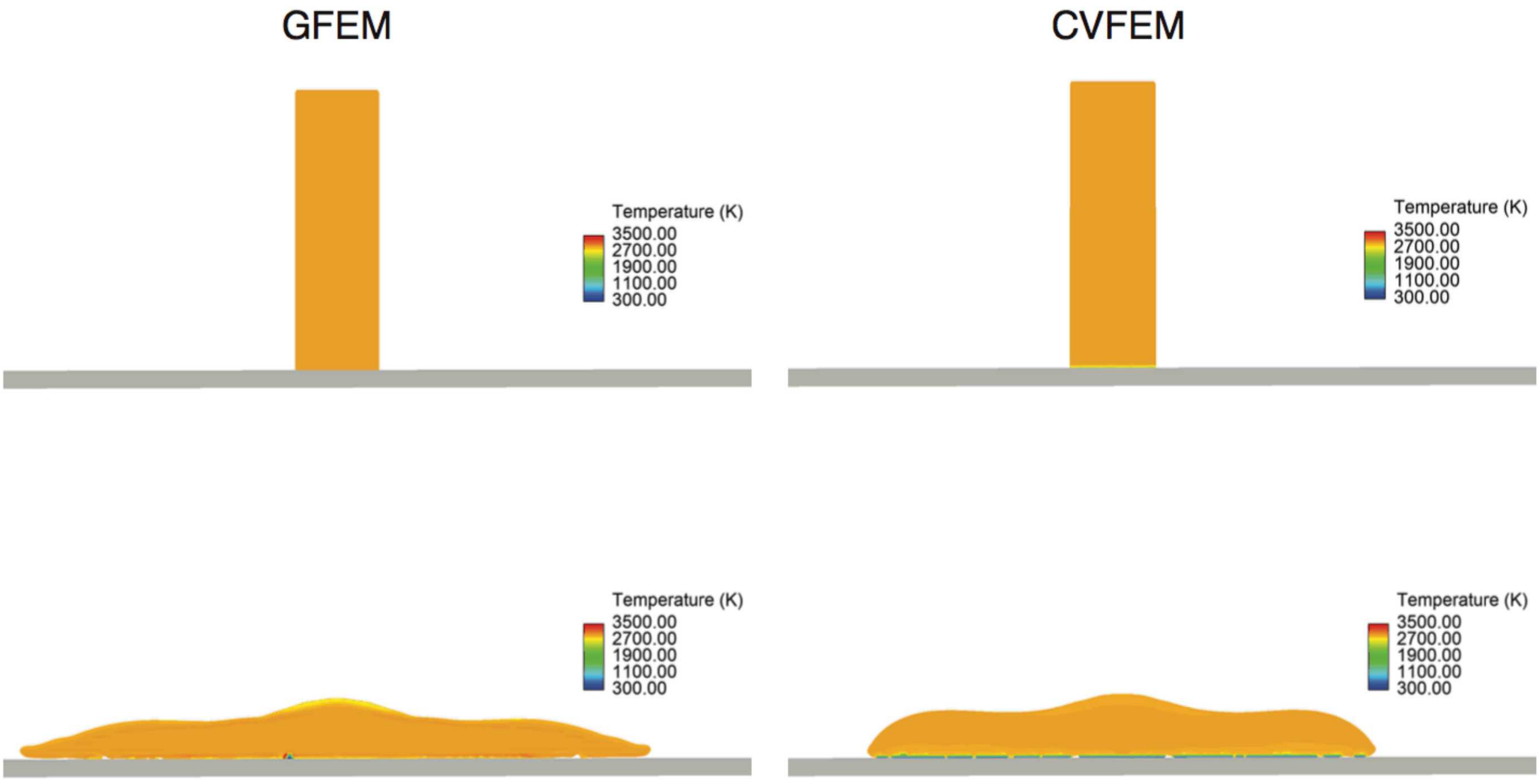
CVFEM - CDFEM

- Large temperature gradients, low thermal diffusivity of corium, and relatively large scale makes this a highly unstable two-phase flow problem
- Control volume finite-element methods (CVFEM) allow for a finite-volume discretization to be used in an existing finite-element framework
- Suitable for high-Peclet number flows where advection can be treated with an upwinding technique
- CVFEM used in conjunction with CDFEM can be used to simulate high Peclet number, two-phase flows

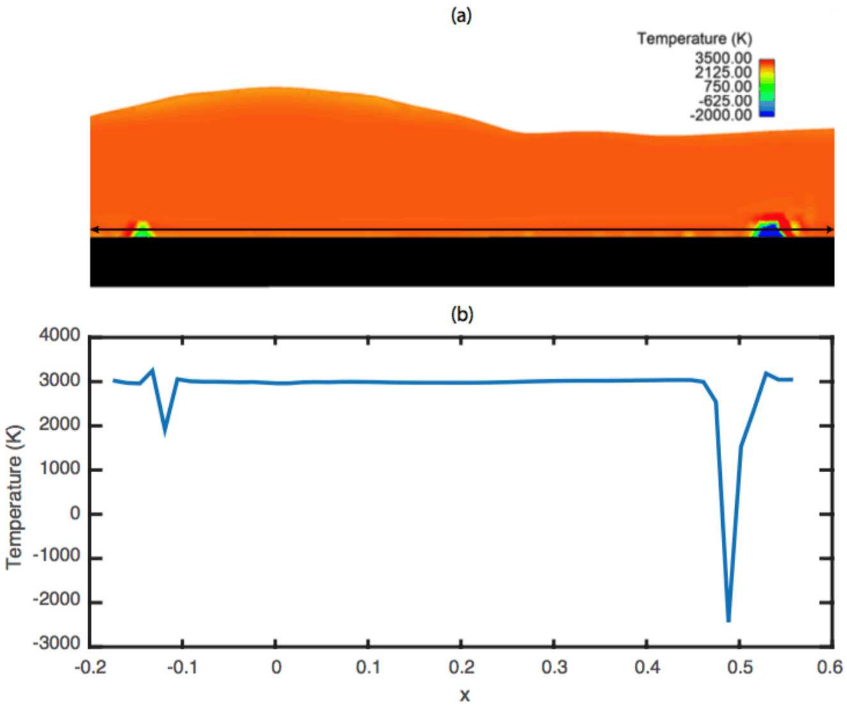


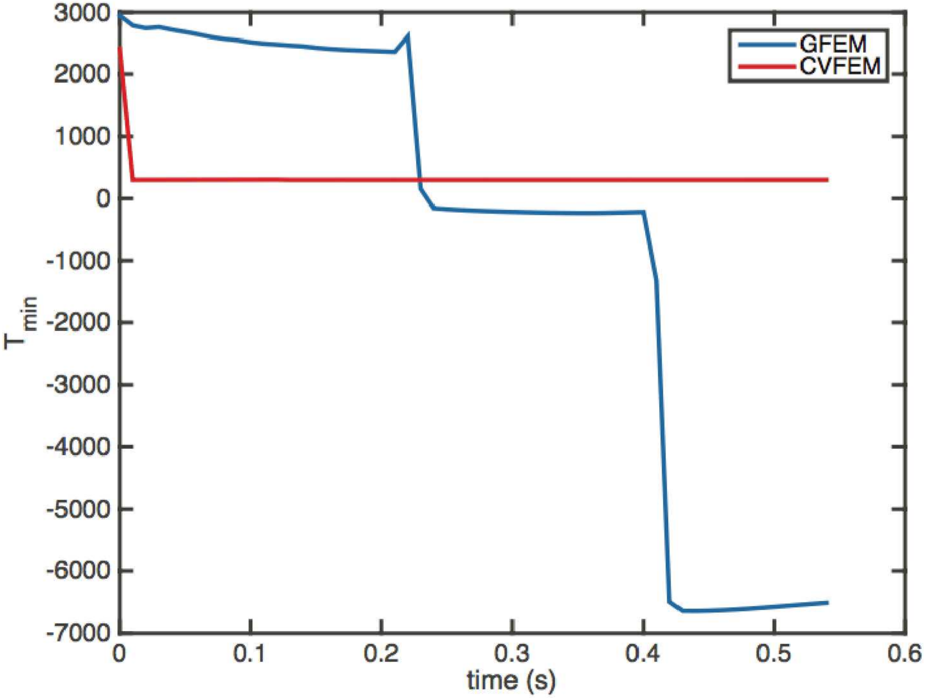
$$\int_{l}^{r} \rho \bar{u} \varphi \mathrm{d}\bar{x} \approx \frac{1}{2}(\dot{m} + |\dot{m}|)\varphi_l + \frac{1}{2}(\dot{m} - |\dot{m}|)\varphi_r$$

GFEM-SUPG vs CVFEM



GFEM-SUPG

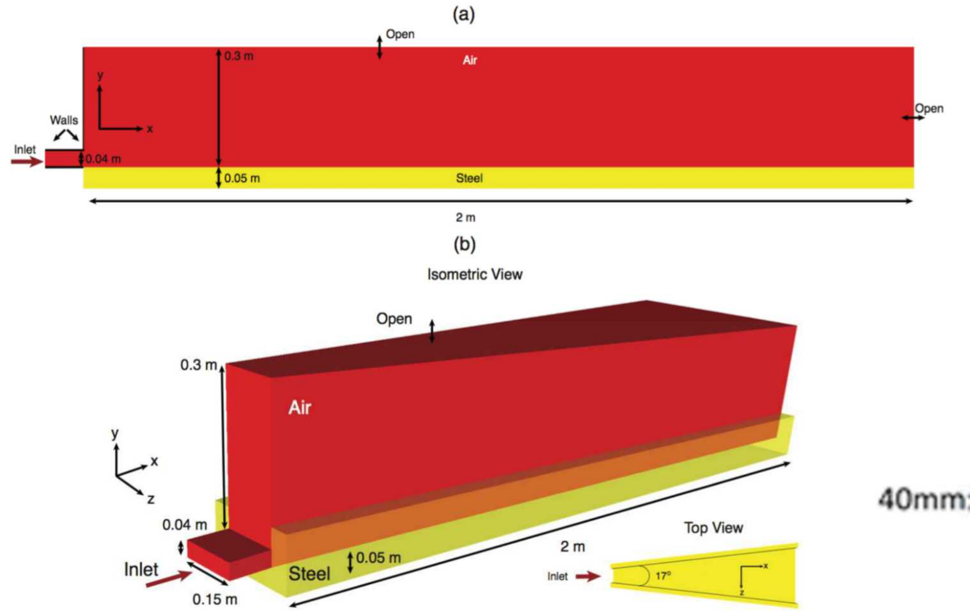




- Spurious oscillations in temperature observed using a GFEM-SUPG approach
- Spurious oscillations not present in CVFEM approach
- Upwinding seems to be effective in stabilizing temperature

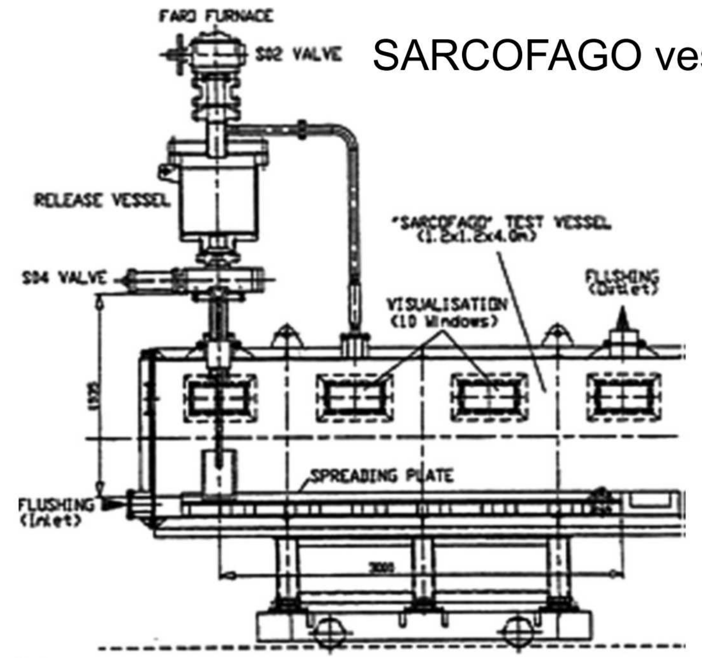
FARO L26 Corium Spreading Exp.

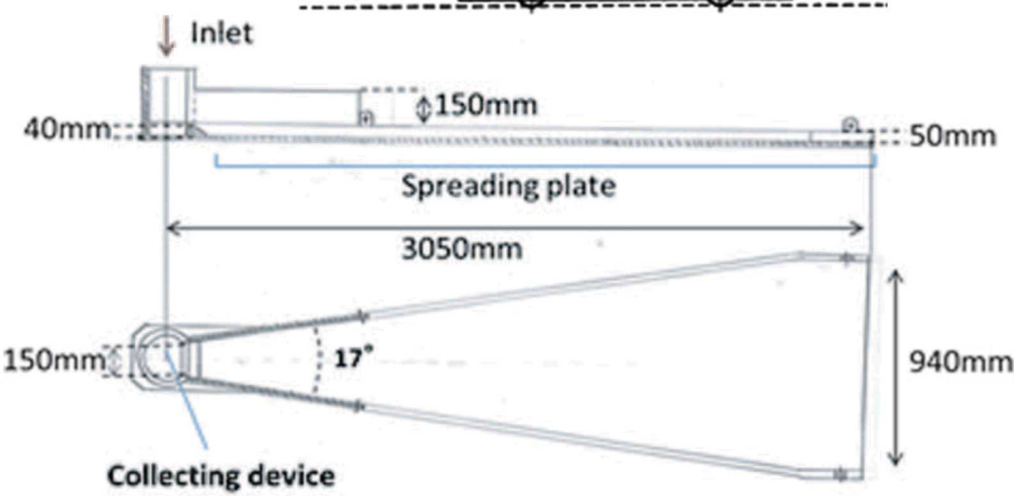
- Approximately 160 kg - 80% UO_2, 20% ZrO_2
- Spreading plate – stainless steel
- Pressure constant



Geometry for simulations of corium spreading in the FARO L26s experiment (a) 2D geometry (b) 3D geometry

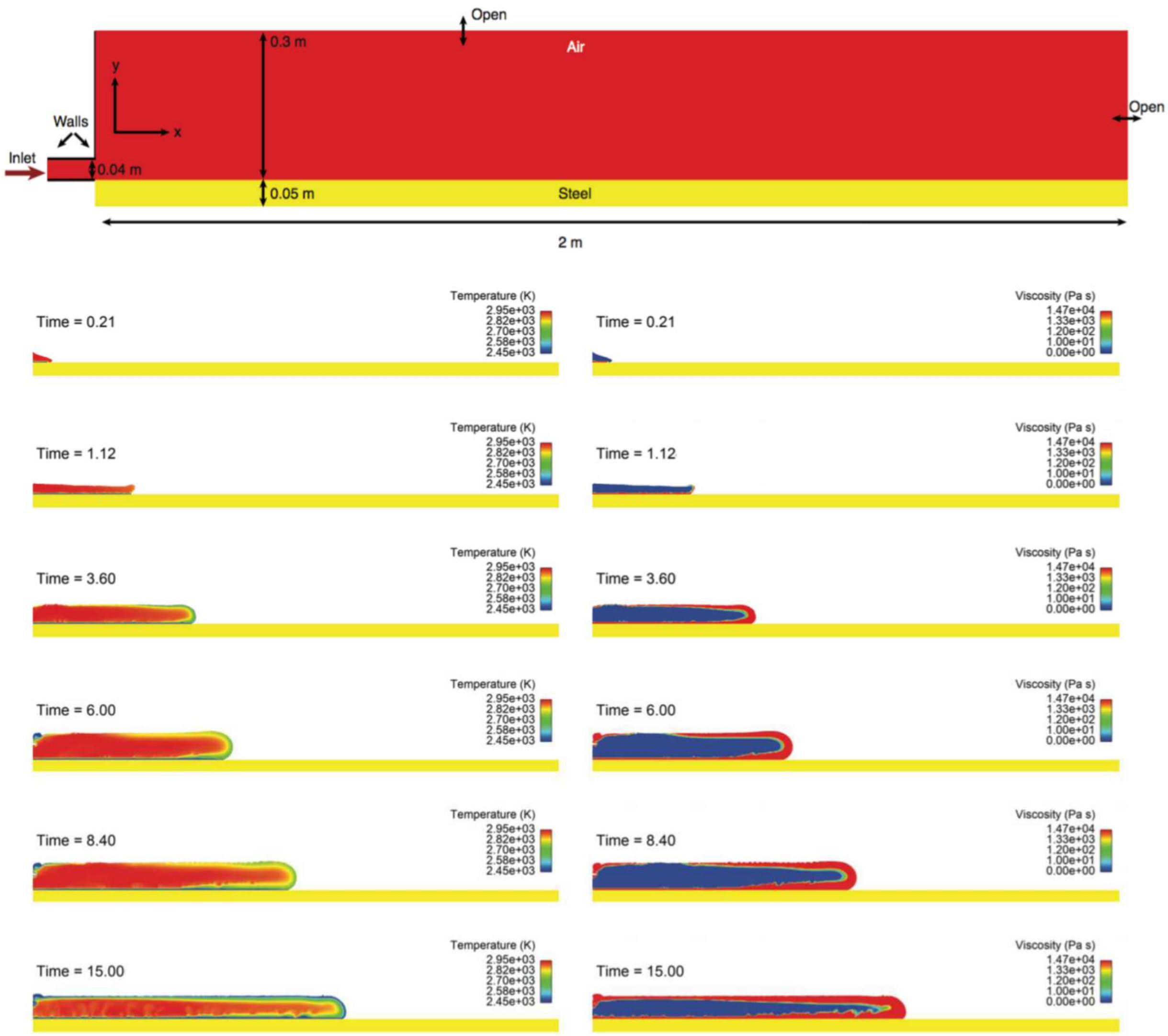
SARCOFAGO vessel



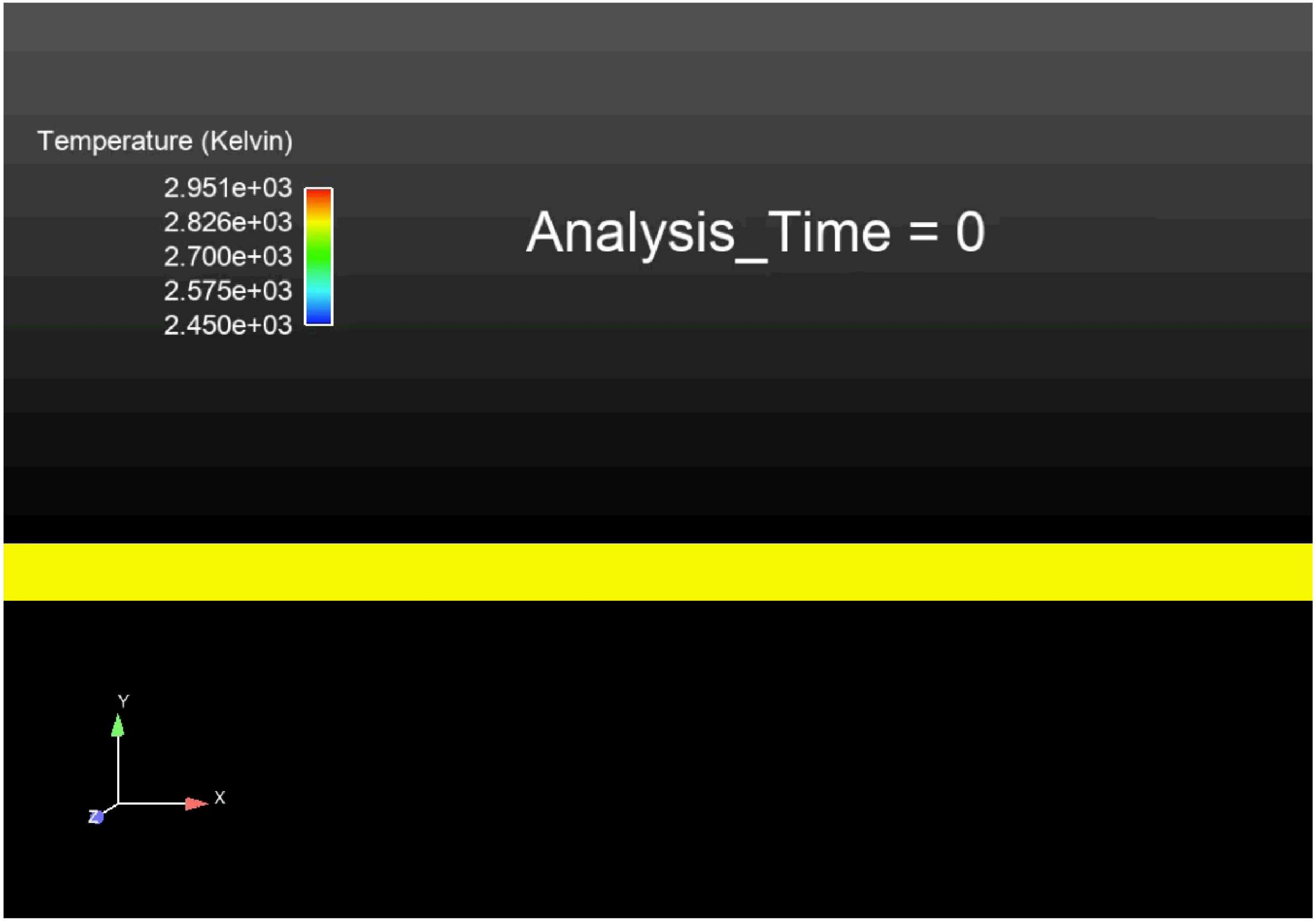


Kawahara, et al., JNST, 49:12, 1156-1164

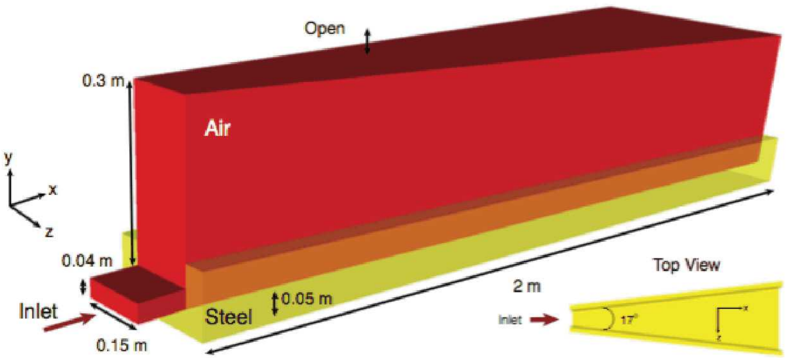
2D Corium Spread Modeling



2D Corium Spread Modeling (cont.)



3D Corium Spread Modeling



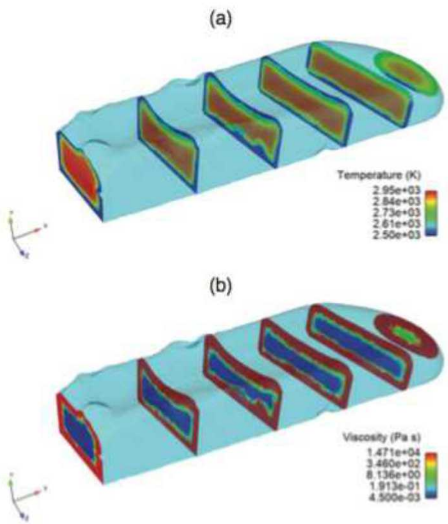


Figure 12: Contours of (a) temperature and (b) viscosity taken at a time snapshot $t = 10$ s at various (y-z) planes showing the three-dimensional effects of the melt solidification process.

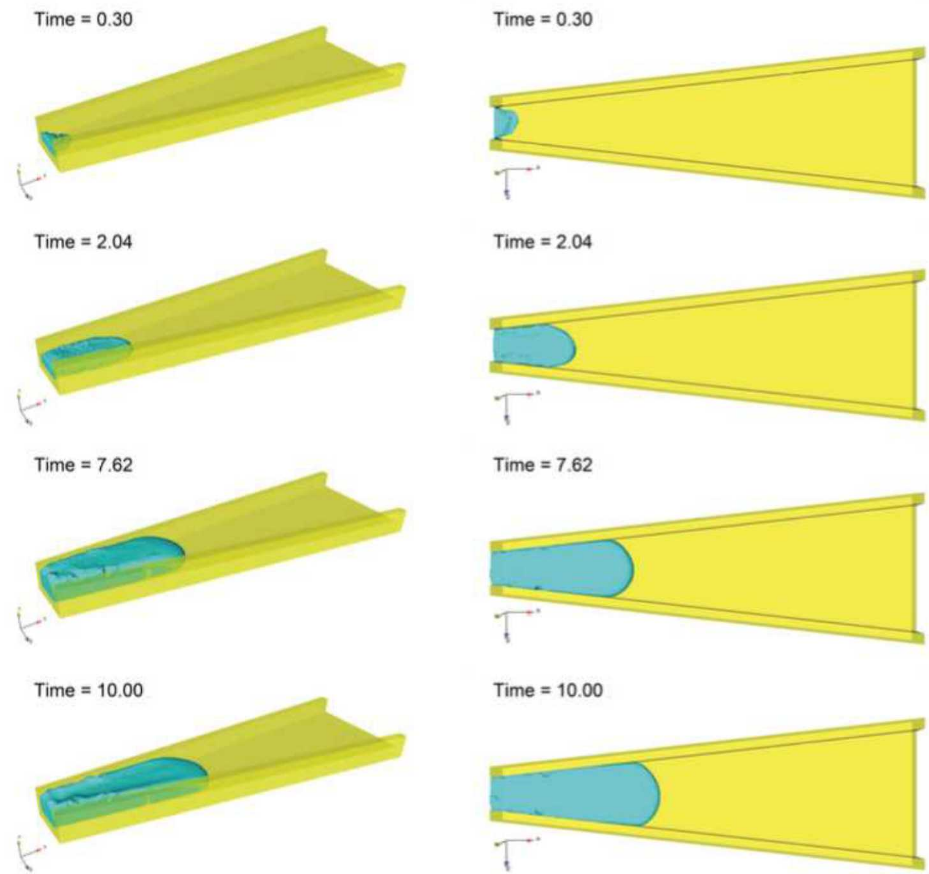
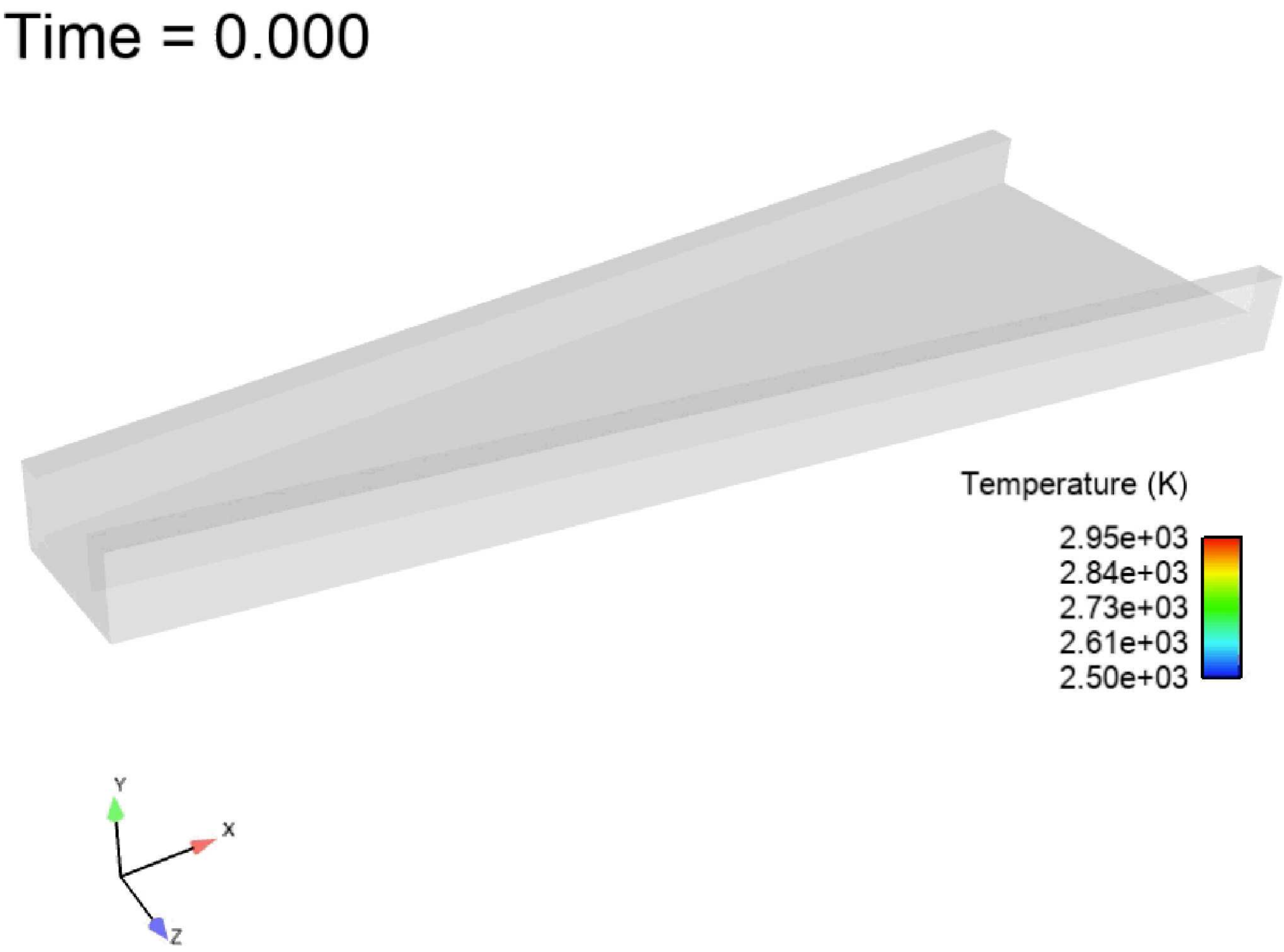


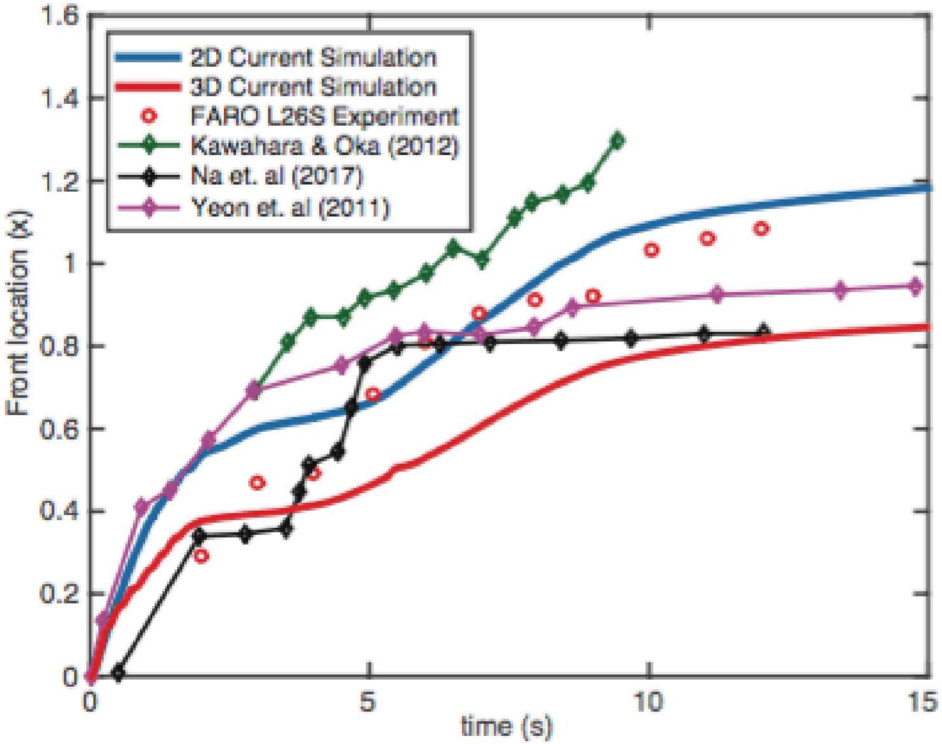
Figure 11: Material phase blocks of the melt (blue), and steel (yellow) as a function of time as the melt spreads and solidifies for the 3D simulation in an isometric view (left) and top-down view (right). First evidence of solidification occurs at $t = 2.04$ s.

3D Corium Spread Modeling (cont.)



Corium Spreading Simulations

- FARO-L26s Experiment simulated – 80% UO_2, 20% ZrO_2
- 2D/3D simulations completed
- Heat loss through the melt boundary modeled
- Psuedo-solidification modeled using Ramacciotti viscosity model.
- Good agreement with experiments



Simulation results compared to experiment and other computations

Conclusions and Future Work

- Excellent agreement with 2D simulations
- 3D simulations under-predicted corium spreading front although same physics captured
  - More surface area exposed to trough side-walls
  - Higher solidification effect
- Slip lengths remain model dependent
- Scale problem up to the reactor scale (metric tons)
- Include concrete ablation model
- Develop a reduced-order model for MELCOR

Questions & Acknowledgements

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- Questions?