Modeling Effort on Chamber Clearing for IFE Liquid Chambers at UCLA

Presented by:

P. Calderoni

Town Meeting on IFE Liquid Wall Chamber Dynamics

Livermore, CA

May 5-6, 2003

Outline

This presentation will address two components of our modeling efforts on chamber clearing:

- **Vapor Condensation**
- **Droplet clearing in a pressure decay field**

Vapor Condensation Modeling - Approach

Couple UCB model for condensation at a liquid / vapor interface (based on Schrage kinetic theory) with Tsunami calculations in 2-D volume

Apply "enhanced" Tsunami to simulate flibe vapor condensation experiments, maintaining all assumptions implicit in Tsunami and condensation model

Compare with experiments
Evaluate effect of measured interface conditions:
traces of non condensable gases
vapor density dropping into transitions regime
accumulation of less volatile BeF2

Generalize liquid / vapor interface model:
add diffusional layer at the interface for non condensable gases
add velocity and temperature slip at the interface
add diffusional layer at the interface for BeF_2

Gas dynamics modeling in IFE liquid chambers

Gas dynamics regime characterized by Knudsen number:

$$Kn = \frac{\lambda}{L}$$ ⇨ **mean free path:** $$\lambda = \frac{1}{\sqrt{2}\,\pi\, d^2 n}$$

⇨ **characteristic length**

Upper limit of mean free path in HYLIFE: 4.7 cm

Considering: Hard-sphere model diameter d = 4 A Lowest density in HYLIFE chamber = $3X10^{13}$ #/cm^3

Kn < 0.01 Continuum Regime

Mean free path small compared to system - molecular collision dominate - gas approximated as continuos medium

0.01 < Kn < 0.1 Slip regime

Gas approximated as continuos several mean free paths away from adjoining medium - Kinetic theory near interfaces to account for both molecular collisions and collision with system boundaries

0.1 < Kn < 3 Transition regime

Molecular collisions and collision with system boundaries are equally important

Kn > 3 Free Molecules Regime

Molecular collisions infrequent - rarefied gas kinetic theory applies

Condensation model assumptions

2-D gas dynamics calculation assumptions:

- **Two dimensional geometry**
- **Gas phase is a continuum**
- **Gas state changes are isoentropic everywhere except at shock waves, which are treated as discontinuities**
- **Liquid structures are rigid - liquid inertia in the time scales of interest prevents structures from moving or deforming - no work is transferred from gas to liquid**
- **Gas viscosity is negligible - viscous time scale L^2/ν >> dynamic time scale L/c**
- **Inside the volume gas is adiabatic - conduction time scale L^2/α >> dynamic time scale L/c - radiative losses assumed to be negligible**
- **Flibe is an ideal gas law with constant γ - fitted EOS corrected for dissociation and ionization not effective in the considered range**

Condensation model assumptions

1-D liquid / vapor interface assumptions:

- Vapor condenses only on liquid surfaces present as initial condition - no droplet nucleation in the volume
- Liquid layers are semi-infinite slabs - thermal diffusion length ($\alpha\ \Delta t)^{1/2}$ << surface curvature - initial layer T is uniform - liquid T away from the interface remains constant - droplet spray cooling not considered
- Heat and mass transfer at the interface only in the normal direction - interface velocity due to mass addition is neglected because of mass continuity
- Heat transfer in the liquid layer by conduction in the normal direction - a convection term due to condensing flux introduced in the energy eq
- Liquid surface is always in thermodynamic equilibrium with the vapor - high mass transfer rates during initial transient neglected - continuum assumption
- Recombination and chemical diffusion effects for flibe are fast - vapor chemical composition is fixed by initial conditions
- Vapor composition is uniform in the volume and at the interface
- Interface kinetic theory accommodation coefficients (sticking and evaporation) are assumed to be = 1

Interface condensation: Schrage theory

The effect of condensation on the molecular motion is to impose a net flux in the direction normal to the interface:

$$\frac{dN_{u,v,w}}{N} = \left(\frac{m}{2\pi\, k_b T}\right)^{3/2} \exp\left[-\left(\frac{m}{2k_b T}\right)\left[(u-u_0)^2 + v^2 + w^2\right]\right] du\, dv\, dw$$

Integrating over v, w and positive (toward) u:

$$\phi_N^+ = n_0\left(\frac{k_b T}{2\pi\, m}\right)^{1/2}\left\{\exp\left[-u_0^2\left(\frac{m}{2k_b T}\right)\right] + u_0\sqrt{\pi}\left(\frac{m}{2k_b T}\right)^{1/2}\left[1 + erf\left(u_0\left(\frac{m}{2k_b T}\right)^{1/2}\right)\right]\right\}$$

Re-writing:

$$G^+ = p\left(\frac{\mu}{2\pi\, R_0 T}\right)^{1/2}\left\{e^{-s^2} + s\sqrt{\pi}\left[1 + erf(s)\right]\right\} \quad \textbf{where} \quad s = u_0\left(\frac{\mu}{2R_0 T}\right)^{1/2} = \frac{u_0}{(\gamma RT)^{1/2}}\left(\frac{\gamma}{2}\right)^{1/2} = M\left(\frac{\gamma}{2}\right)^{1/2}$$

$$p = \rho RT$$

Finally, the net flux across the interface:

$$G_k = f_c\, p_{vs}\, \Gamma\left(\frac{1}{2\pi\, RT_{vs}}\right)^{1/2} - f_e\, p_{ls}\left(\frac{1}{2\pi\, RT_{ls}}\right)^{1/2}$$

Modeling the interface and liquid layer

Two equations to couple liquid and vapor properties at the interface:

mass balance $$G\Big|_{x=0^-} = \rho_{vs}\, u_{vs} = \rho_{ls}\, u_{ls} = G\Big|_{x=0^+} \qquad t \geq 0$$

energy balance $$G\, h_{vs}^0 = -k_l \frac{\partial T(x,t)}{\partial x}\bigg|_{x=0} \qquad t \geq 0$$

conduction in the vapor neglected for short diffusion length - neglect radiation

Vapor stagnation enthalpy: $$h_{vs}^0 = c_{pg}\left[T_{vs} - T_{sat}(p_{vs})\right] + h_{fg}\left[T_{sat}(p_{vs})\right] + \frac{u_{vs}^2}{2}$$

Where for flibe

$$h_{fg}(T_{sat}(p_v)) = h_{fg}(T_{ref}) + (c_{pg} - c_{pl})\left[T_{sat}(p_v) - T_{ref}\right] \qquad p_{sat} = \frac{101300}{760} \times 10^{\left(9.407 - \frac{10054}{T}\right)}$$

In the liquid layer:

Energy equation $$\frac{\partial T(x,t)}{\partial t} + u_{ls}\frac{\partial T(x,t)}{\partial x} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2} \qquad 0 \leq x \leq \infty$$

with bc $$q''_{\text{int}} = -k_l \frac{\partial T(x,t)}{\partial x}\bigg|_0 \qquad t \geq 0$$

$$T(\infty,t) = T_{l\infty} \qquad t \geq 0$$

Convection term added to account for condensing mass across the interface - u_{ls} evaluated from G

Initial non-equilibrium conditions

In early stages of condensation the contact of highly superheated vapor with the cold surface causes high mass transfer rates at the interface - the effect (suction) is to increase the vapor velocity that is evaluated by Tsunami

Schrage theory fails to account for high mass transfer rates because of the surface equilibrium assumption - velocity associated with mass flux predicted by the Schrage eq can be higher than physical limitations associated with super sonic choking effect

Gas dynamics limiting flux:

$$G_{v\max} = \rho c\left(M + \frac{2}{\gamma - 1}\right)\left[\frac{\gamma - 1}{\gamma + 1}\left(M + \frac{2}{\gamma - 1}\right)\right]^{\frac{2}{\gamma - 1}} - \frac{2\rho c}{\gamma - 1}\left[\frac{\gamma - 1}{\gamma + 1}\left(M + \frac{2}{\gamma - 1}\right)\right]^{\frac{\gamma + 1}{\gamma - 1}} \qquad u_v < c$$

$$G_{v\max} = \rho u_v \qquad u_v > c$$

Correction: $G = \min\left(G_k, G_{v\max}\right)$

Numerical iteration scheme

Vapor (p, T) at the interface are given by Tsunami (as well as the gas dynamic limiting flux)

Equilibrium assumption reduces unknown liquid properties to one, surface temperature:

$$T_{ls} = \frac{G_k\left(h_{vs}^0 + c_{pl}T_{l\infty}\right) + \dfrac{k_l}{\Delta x}T_l}{G_k c_{pl} + \dfrac{k_l}{\Delta x}}$$

Condensation gives the second eq to solve for T and G:

$$G_k = f_c\, p_{vs}\,\Gamma\left(\frac{1}{2\pi RT_{vs}}\right)^{1/2} - f_e\, p_{ls}\left(\frac{1}{2\pi RT_{ls}}\right)^{1/2}$$

Iteration step: $G^n = G(T_{ls}^{n-1}) \Rightarrow T_{ls}^n = T_{ls}(G^n) \Rightarrow \dfrac{\left|T_{ls}^n - T_{ls}^{n-1}\right|}{T_{ls}^{n-1}} \le \varepsilon$

Newton-Raphson averaging method:

$$T_{ls-low}^n = T_l^{n-1}$$
$$T_{ls-high}^n = T_{ls}(G(T_{ls-low}^n)) \Rightarrow$$

$$T_{ls-high}^{n-new} = T_{ls}^n$$
$$T_{ls}^{n-new} = \frac{(T_{ls}^n + T_{ls-low}^n)}{2}$$

or

$$T_{ls-low}^{n-new} = T_{ls}^n$$
$$T_{ls}^{n-new} = \frac{(T_{ls}^n - T_{ls-high}^n)}{2}$$

In the liquid layer, using an upwind scheme for the condensation case:

$$T_i^n = T_i^{n-1} + \frac{\alpha\,\Delta t}{(\Delta x)^2}\left[T_{i+1}^{n-1} - 2T_i^{n-1} + T_{i-1}^{n-1}\right] - \frac{G^n\,\Delta t}{\rho_l\,\Delta x}\left[T_i^{n-1} - T_{i-1}^{n-1}\right]$$

$$\Delta t < \left[\frac{2\alpha}{(\Delta x)^2} + \frac{G^n}{\rho_l\,\Delta x}\right]^{-1}$$

Introducing condensation effect in Tsunami

The condensation module evaluates G at each step - the mass flux condition must now be used at Tsunami boundary cells interface instead of the usual adiabatic condition adopted at cells interfaces in the volume

Tsunami numerical scheme requires computation of mass (continuity), momentum (Riemann solver across the discontinuity) and energy (adiabatic assumption) fluxes at the edge of each cell

Mass flux is G

Energy flux from same interface balance - written in Tsunami terms:

$$Energy\ flux = G\left[\frac{\gamma\, p_{vs}}{(\gamma-1)\rho_{vs}} + \frac{u_{vs}^2}{2}\right]$$

Momentum flux determined by mirror node, introducing suction velocity:

$$U_L = \left(\rho_{vs}, u_{vs}, p_{vs}\right)^T$$
$$U_R = \left(\rho_{vs}, -u_{vs} + u_s, p_{vs}\right)^T$$

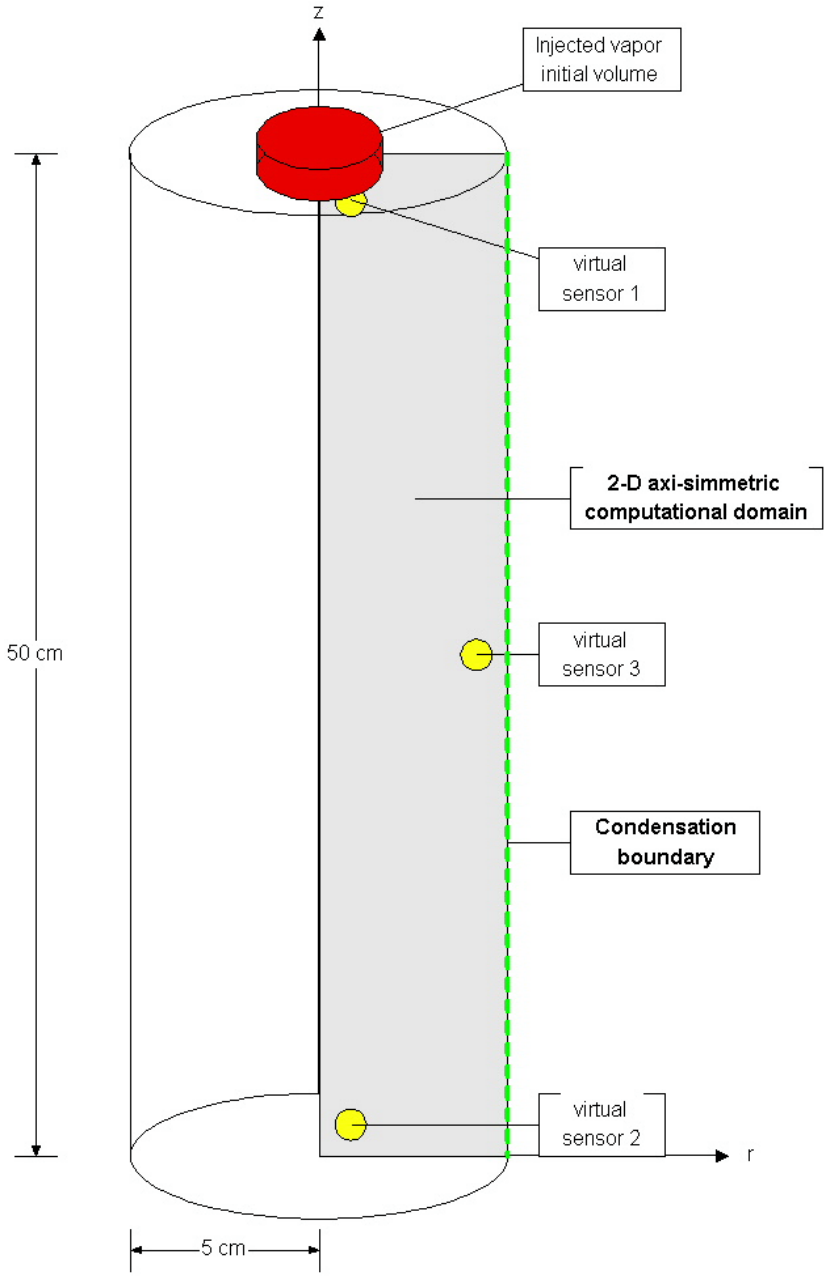
$$U^* = \left(\rho^*, u^*, p^*\right)^T \qquad G = \rho^* u^* \qquad \Delta G_{norm} = \frac{\rho^* u^* - G}{G_{v\max}} < \varepsilon$$

Iteration scheme:

$$u_s^0 = 2\frac{G}{\rho_{vs}}$$

$$u_s^k = u_s^{k-1}\left(1 - \Delta G_{norm}^{k-1}\right) \qquad if\ G > 0$$
$$u_s^k = u_s^{k-1}\left(1 + \Delta G_{norm}^{k-1}\right) \qquad if\ G < 0$$

Numerical domain geometry



Background gas is flibe, considered as an ideal gas with:

$$m = 0.0331 \frac{kg}{mol}$$

$$\gamma = \frac{C_p}{C_v} = 1.4$$

Initial background conditions specified as:

$$\rho_0 = \frac{p_0 \cdot W}{R \cdot T_0} \qquad e_0 = \frac{R \cdot T_0}{\gamma - 1}$$

Uniform grid: 10 x 100 cells - 0.5 x 0.5 cm each

Injected gas considered by Tsunami as DEBRIS, initially available in a 3 x 3 cell volume V_0

Initial superheated vapor conditions specified as total injected mass [kg] and total initial energy [J]

Code runs - parameters case study

Tsunami BC recovered:

Boundary conditions:

$u_s = 0$ → **Open interface**

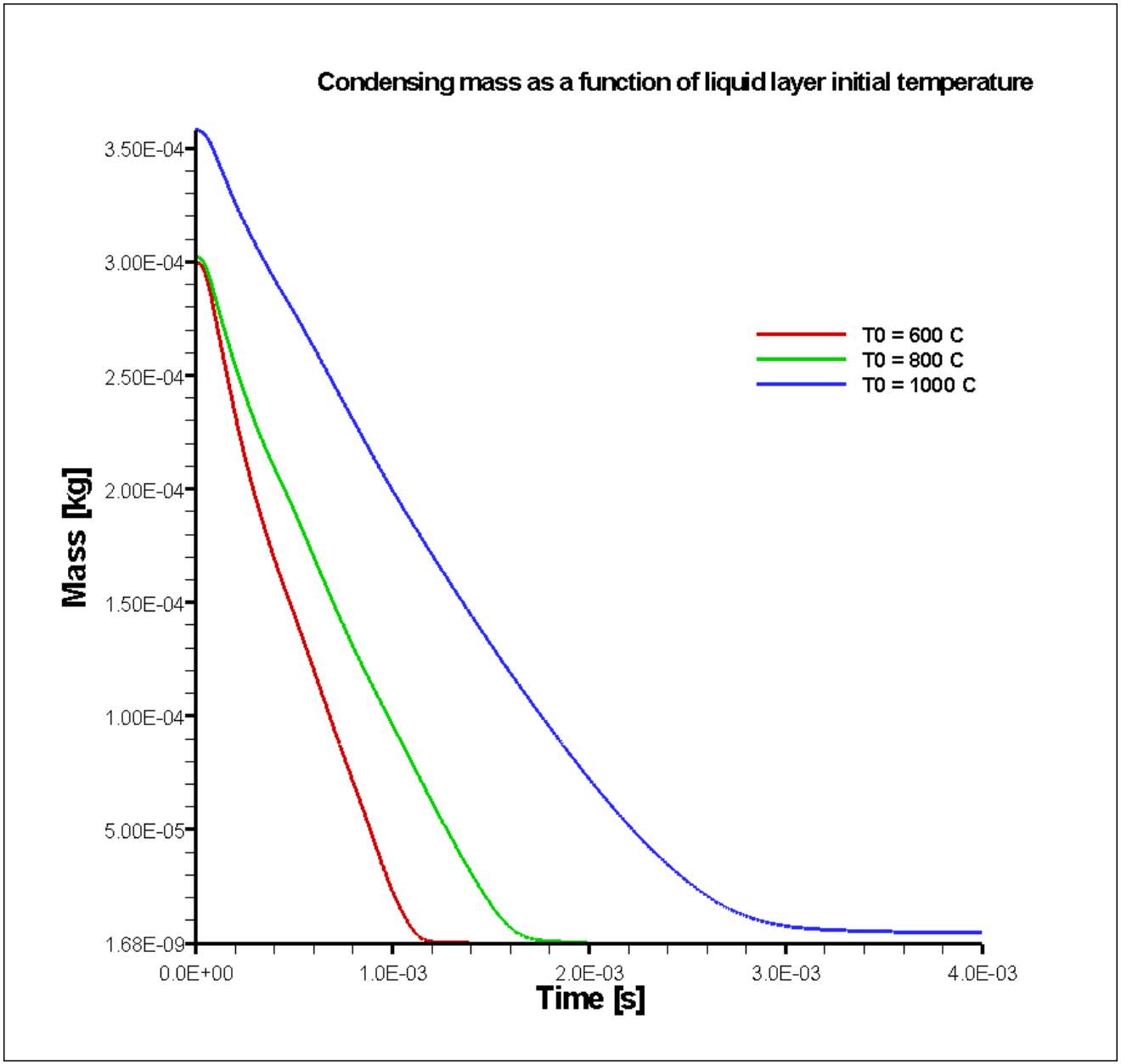
$u_s = 2\ u_{vs}$ → **Impermeable surface**

Condensation

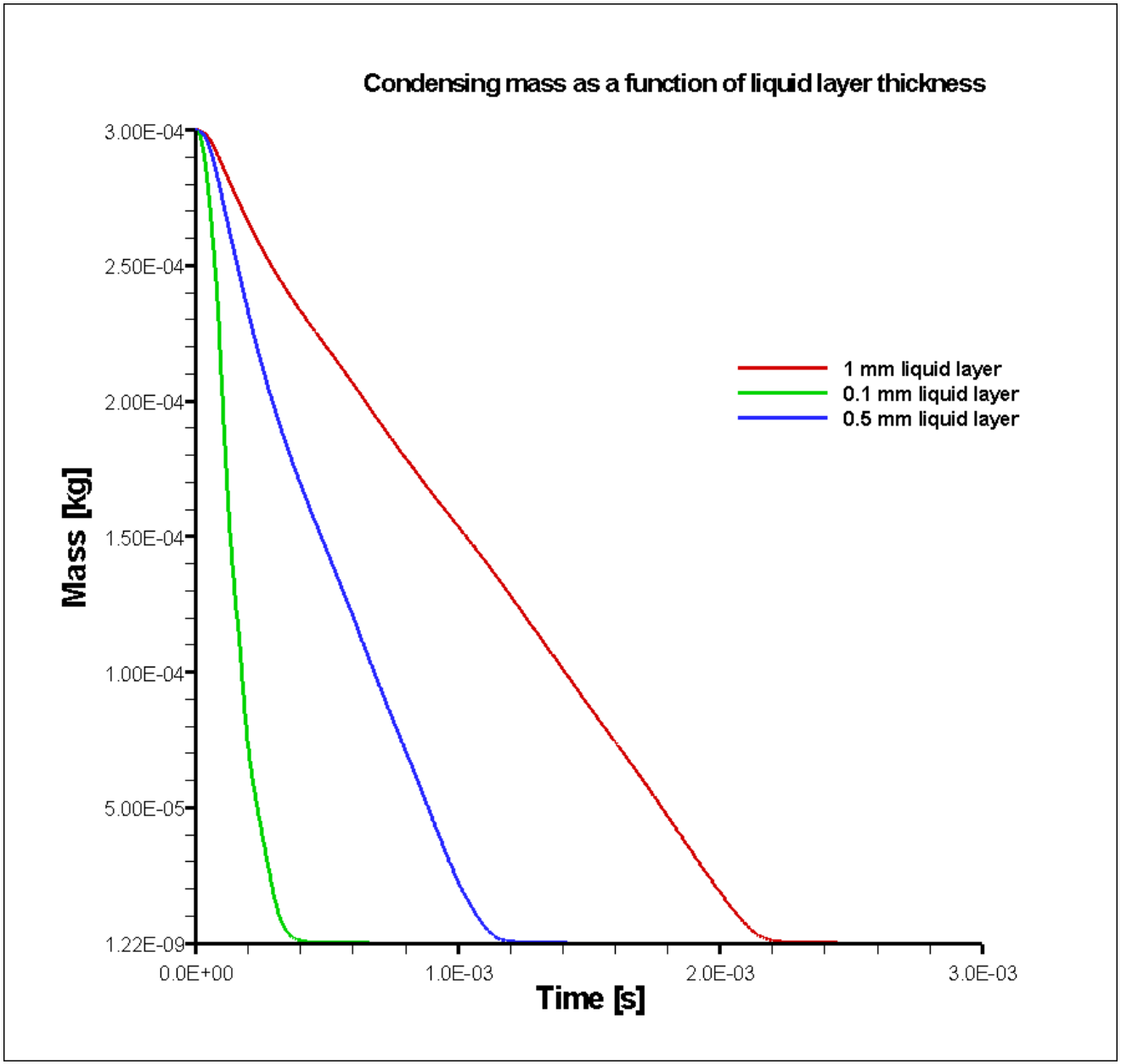
Top and bottom boundary are impermeable

Parametric study for:	**Reference case:**
Initial liquid temperature (constant at solid wall interface)	**600 C**
Liquid layer thickness	**0.5 mm**
Sticking coefficient at the interface	**fc = 1**

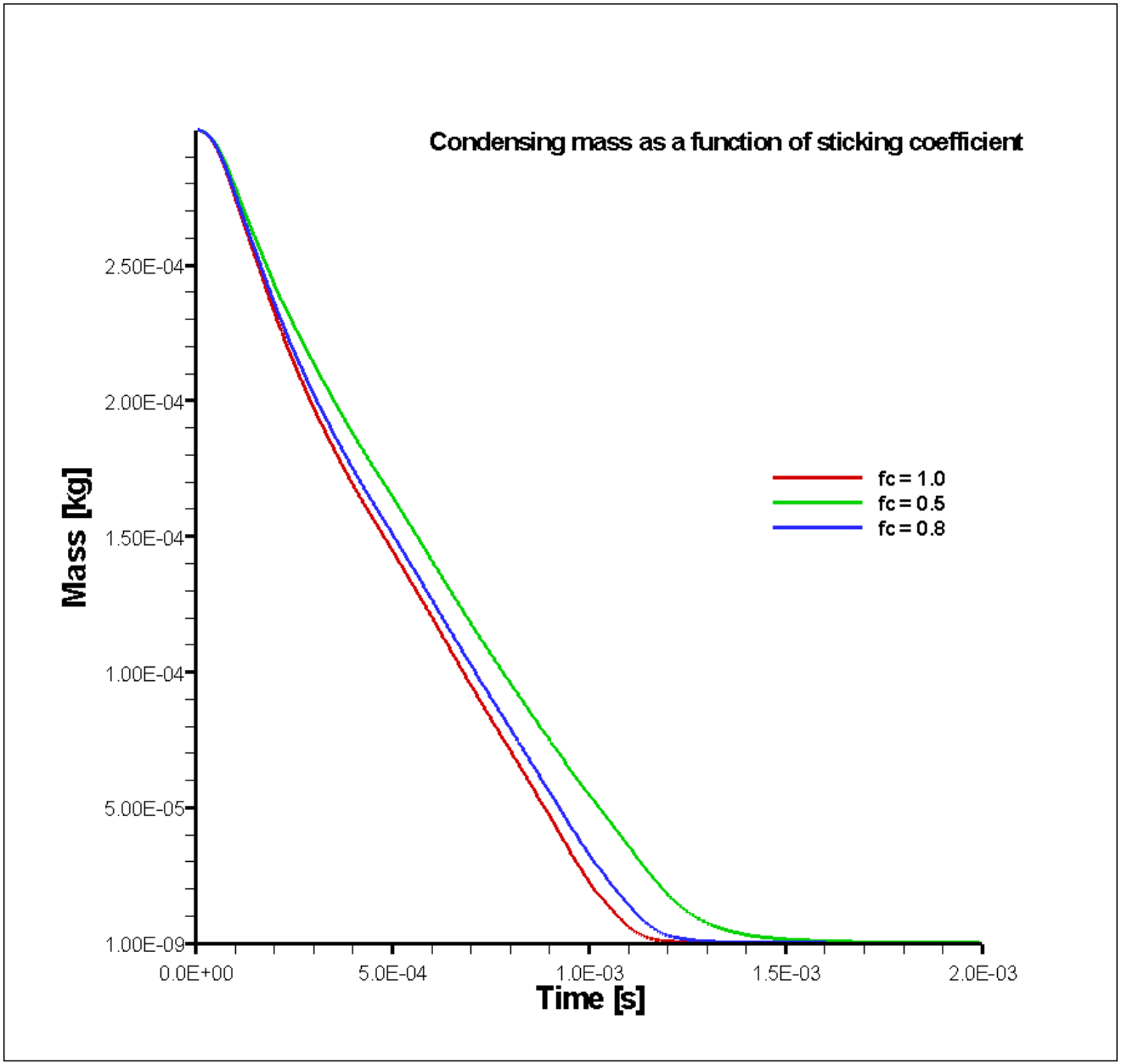
Liquid initial temperature



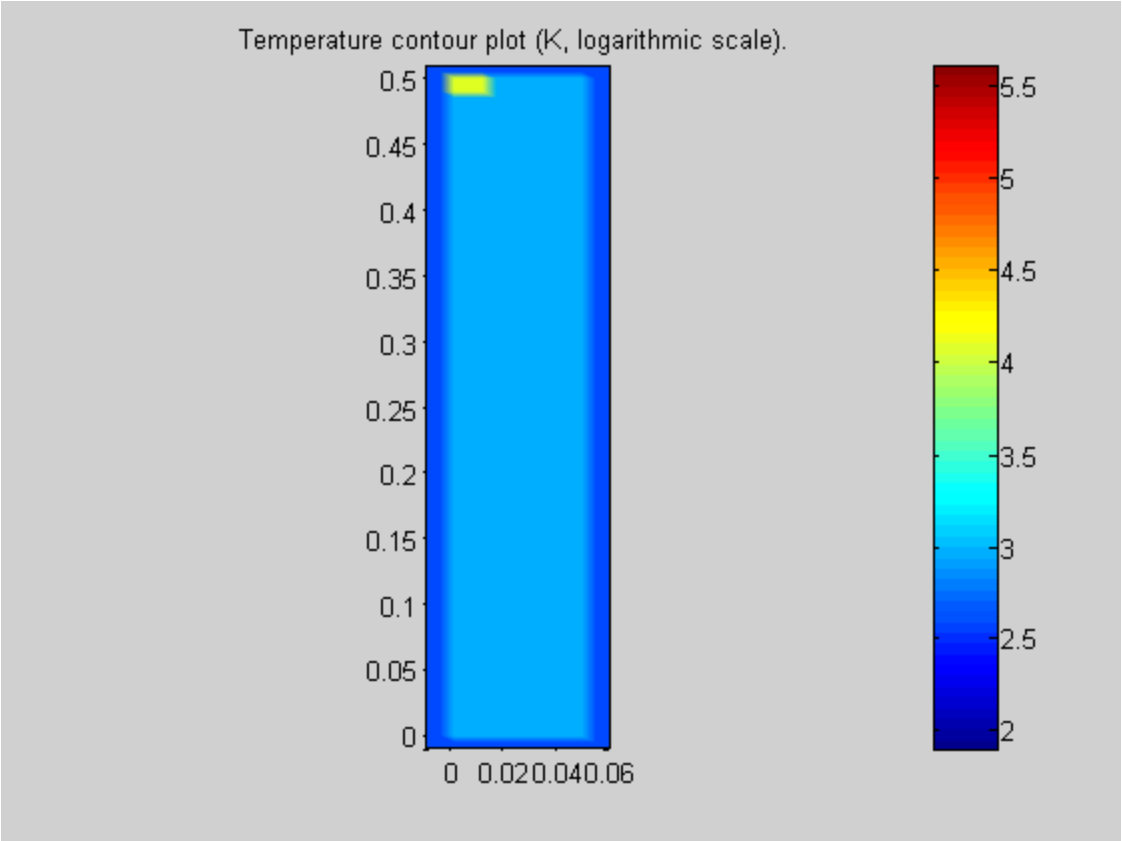
Liquid layer thickness



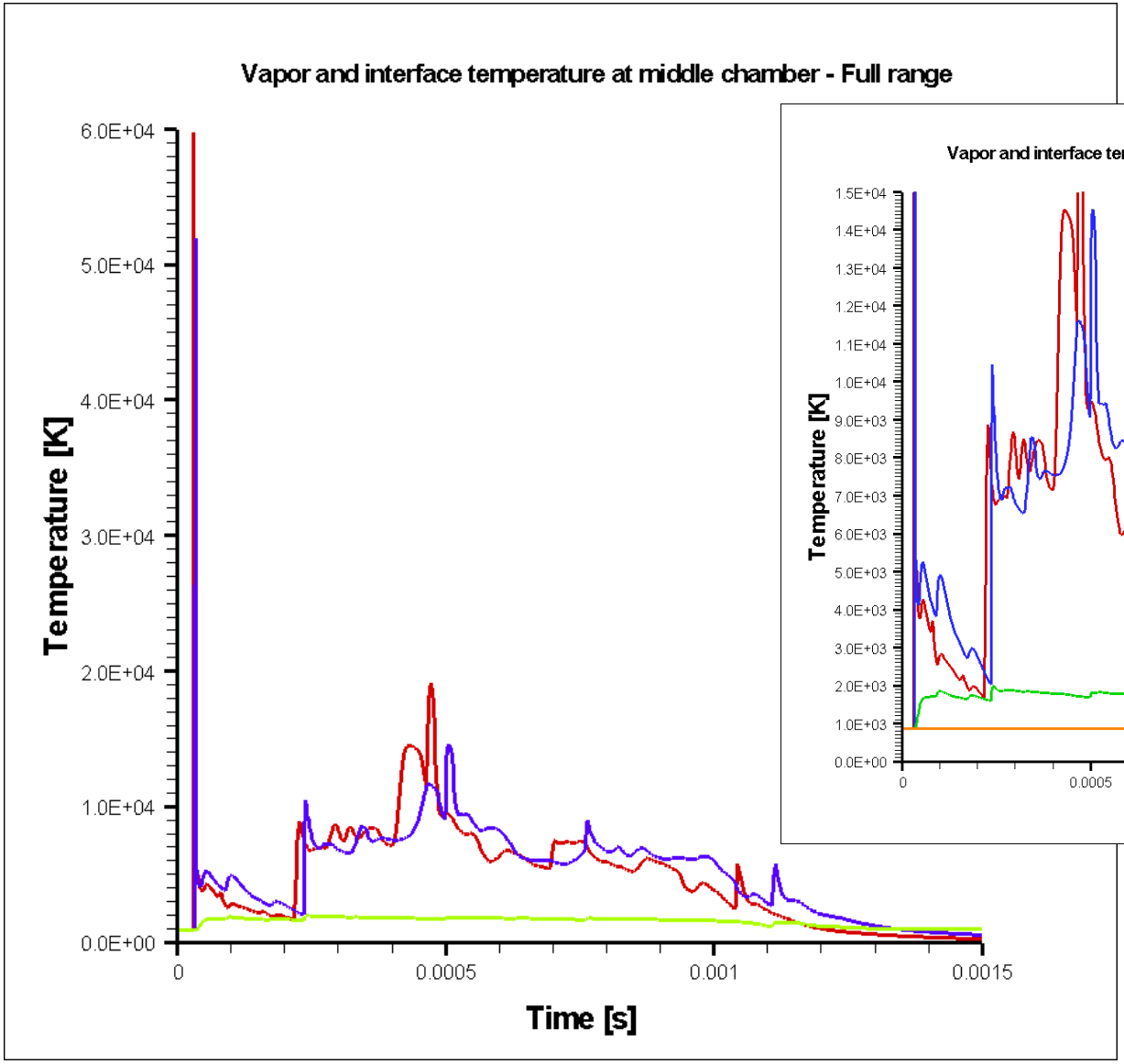
Liquid initial temperature

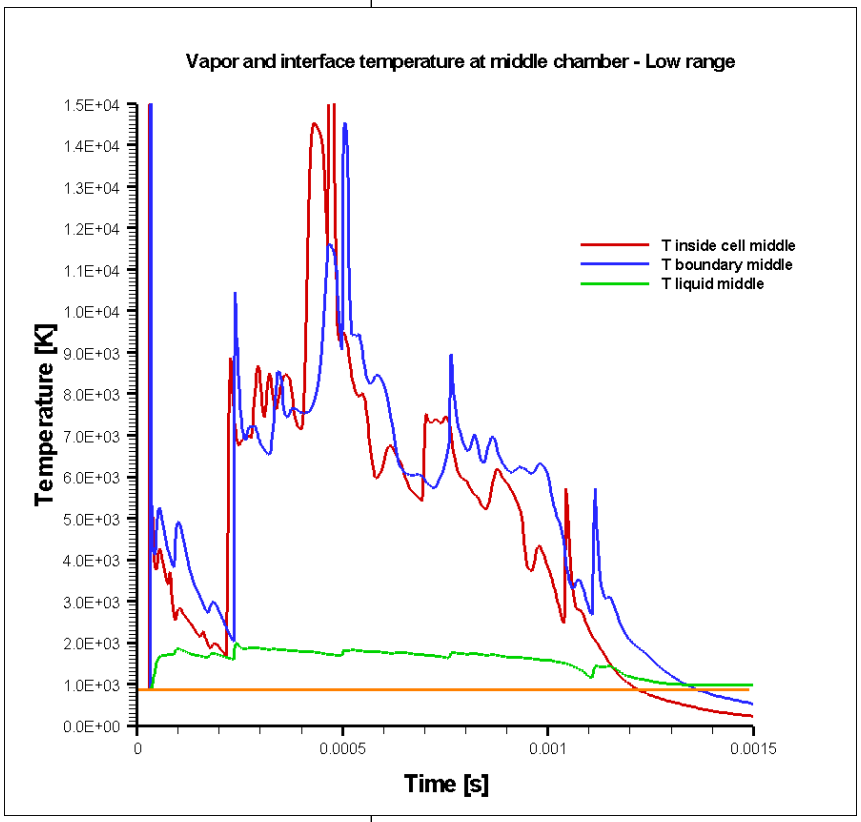


Temperature distribution in the 2-D axi-symmetrical numerical domain as a function of time for the reference case



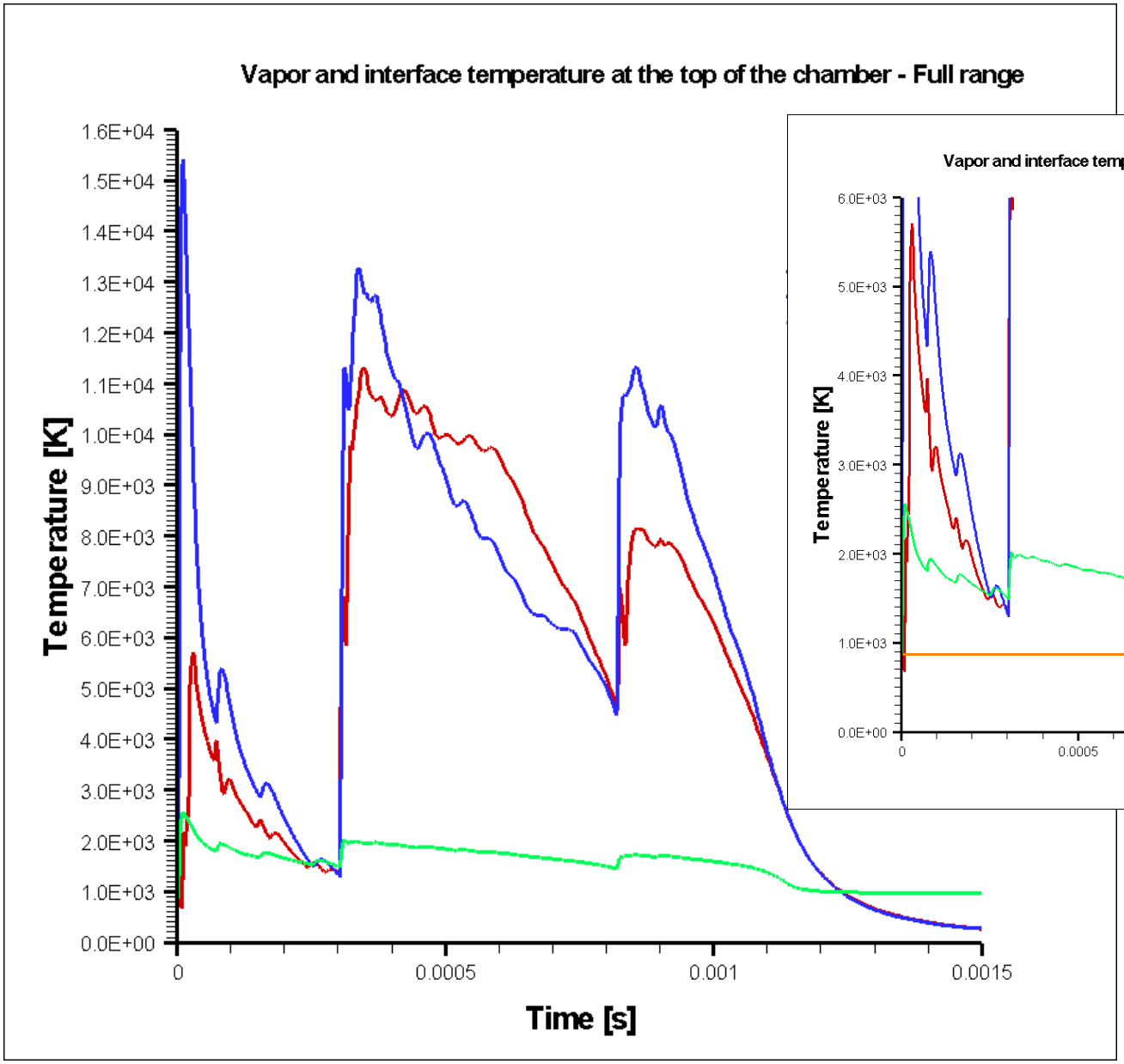
Temperature distribution - middle cells

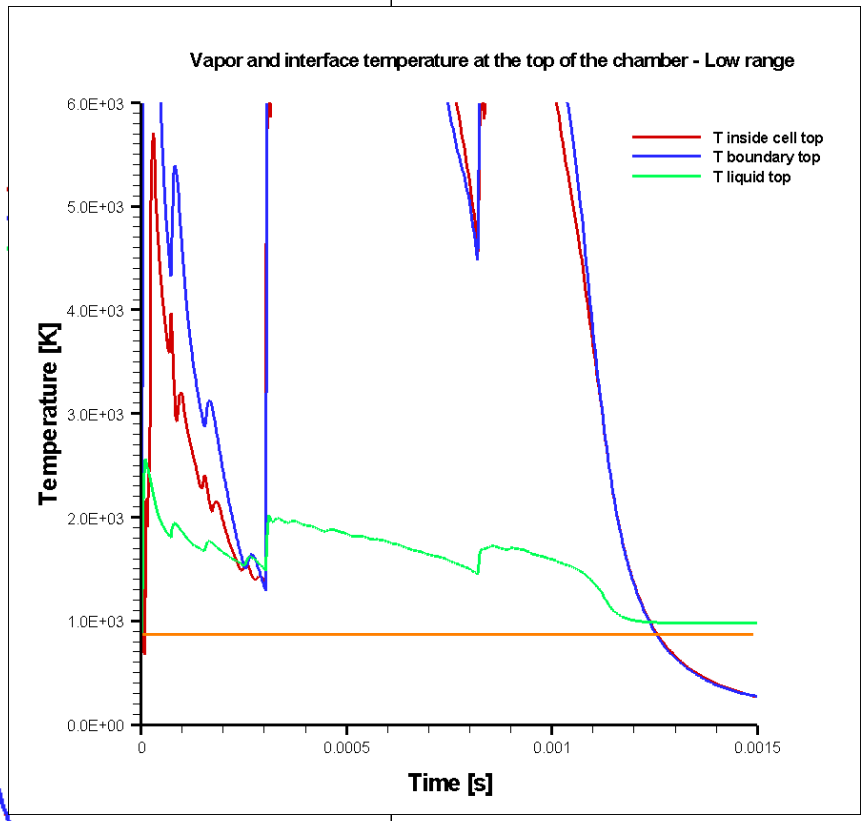




Gas temperatures evaluated by Tsunami fall below the imposed initial background temperature when remaining mass is low

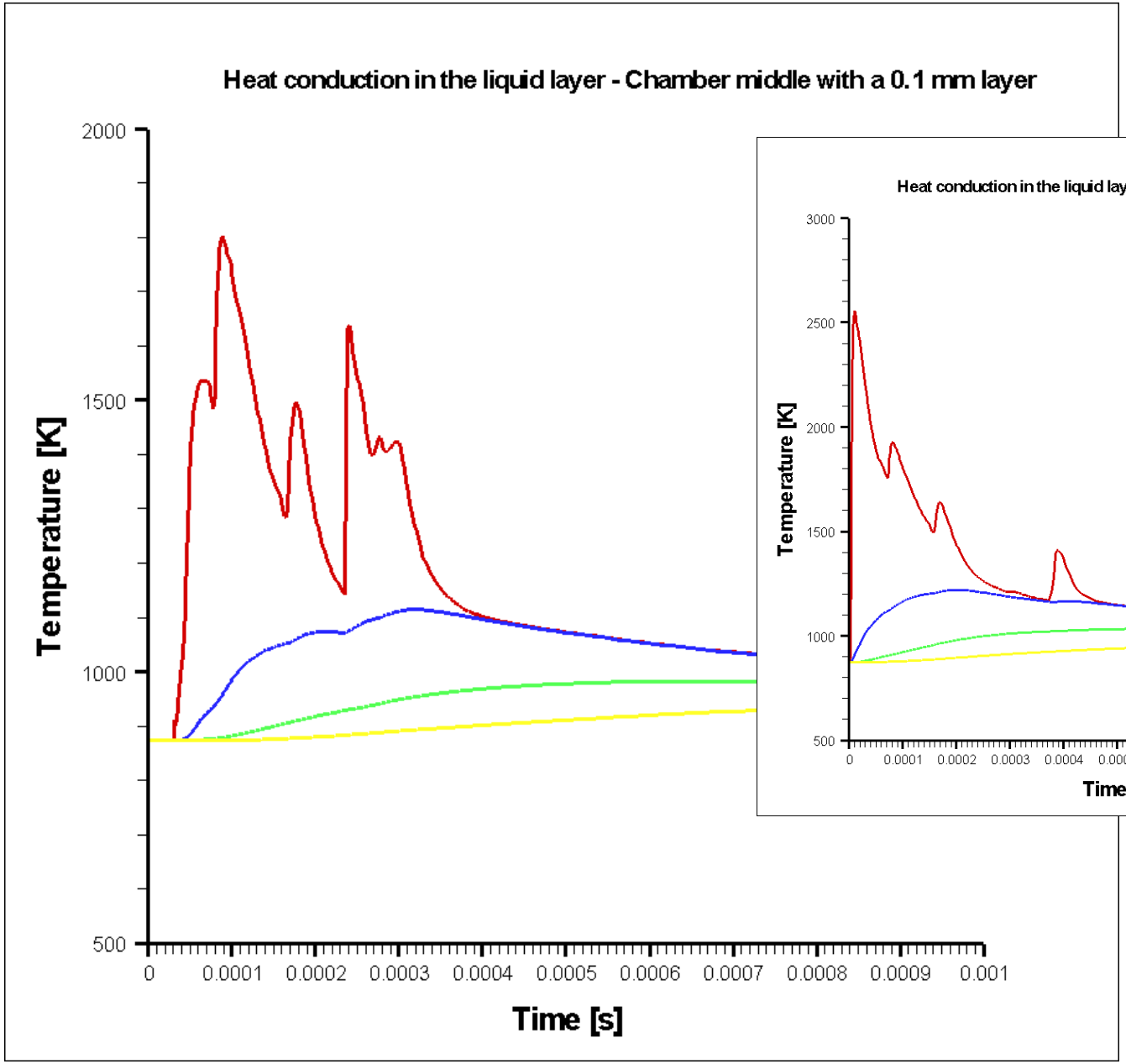
Temperature distribution - Top



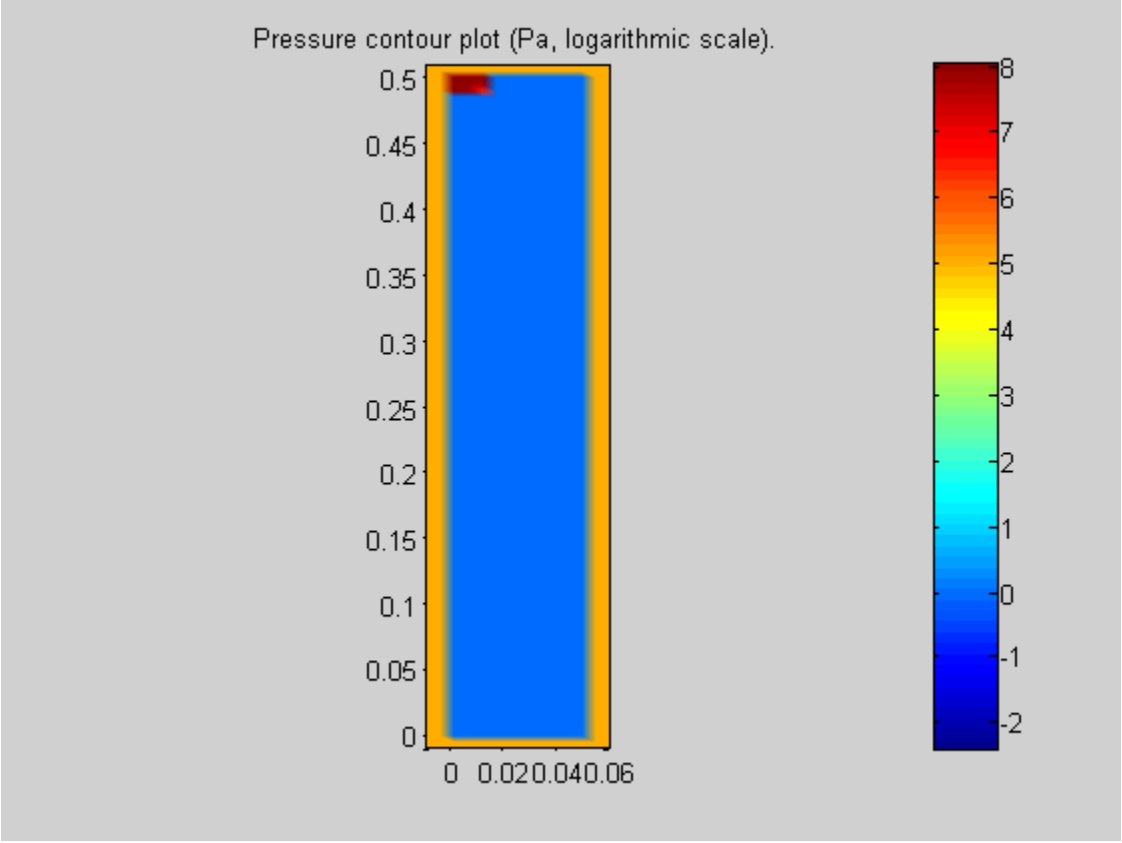


In the boundary cells at the top and bottom of the chambers the vapor interface T is higher then Tsunami evaluated temperature in the inner cells

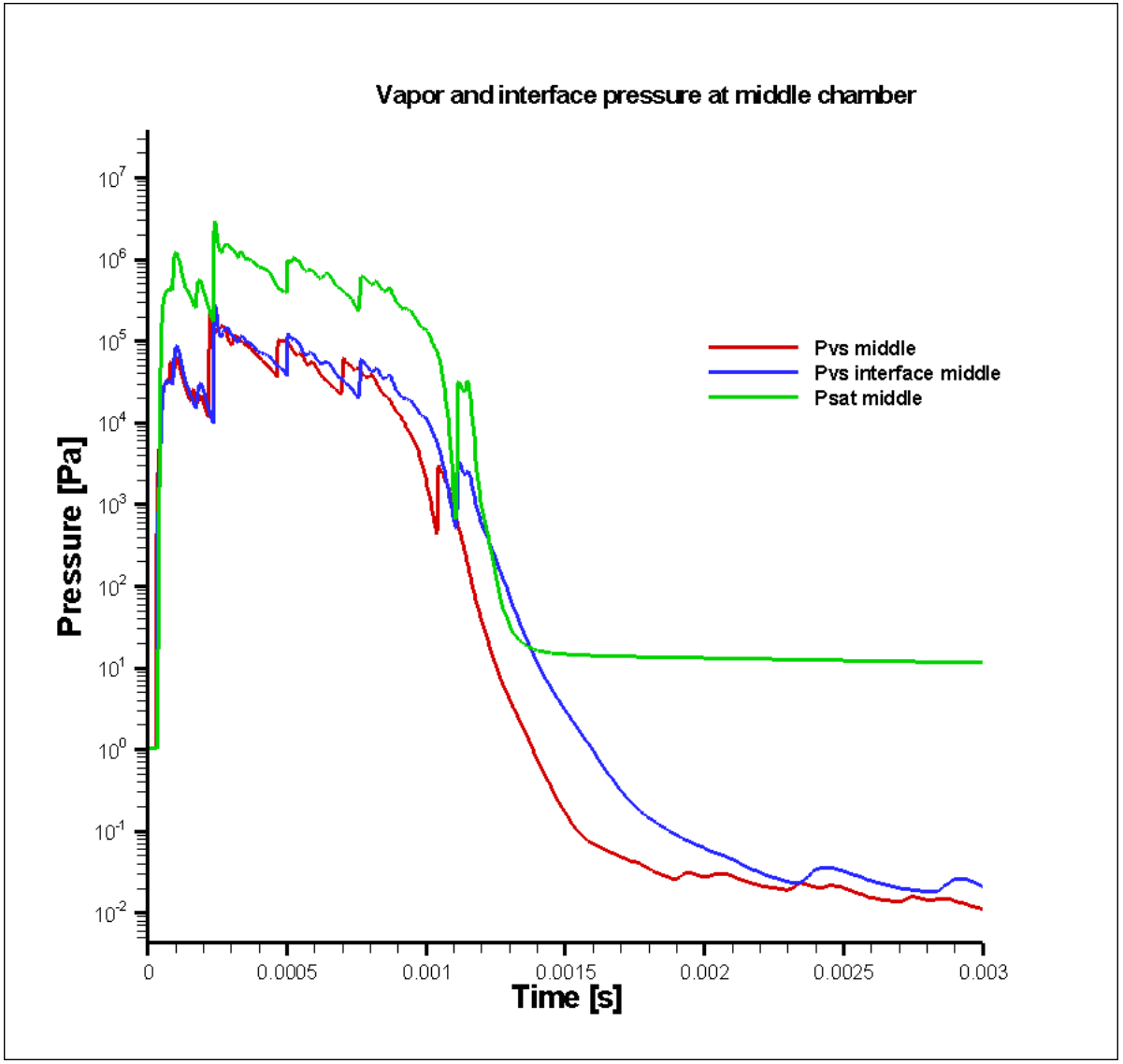
Heat conduction in the liquid layer



Pressure distribution in the 2-D axi-symmetrical numerical domain as a function of time for the reference case



Pressure distribution - middle cells



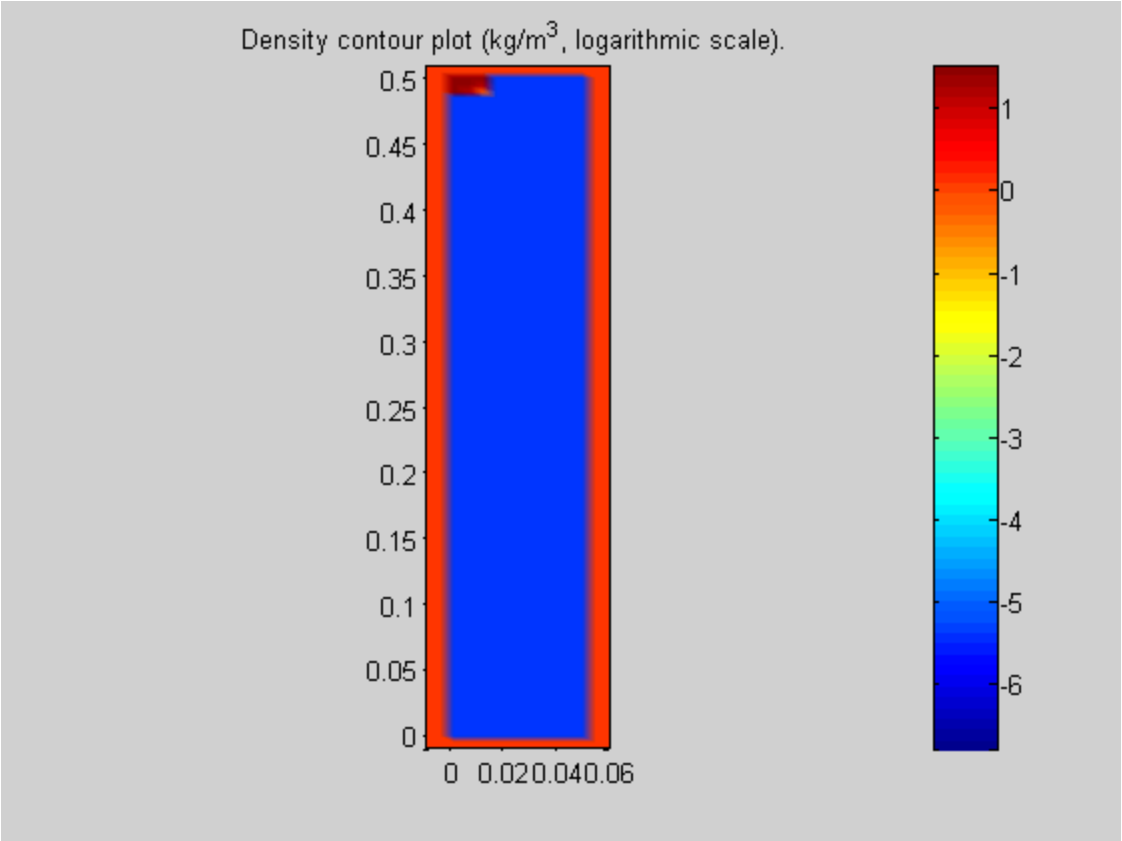
Liquid surface equilibrium assumptions not valid for transient condensation

Ohno fitted equation for flibe:

$$p_{sat} = \frac{101300}{760} \times 10^{\left(9.407 - \frac{10054}{T}\right)}$$

Ideal gas assumption for flibe overestimates vapor pressure during high temperatures initial transient

Density distribution in the 2-D axi-symmetrical numerical domain as a function of time for the reference case



Gas dynamics modeling in IFE liquid chambers

$$Kn = \frac{\lambda}{L} \cong 0.01$$

Continuum fluid regime

Hydrodynamic code Tsunami
HYLIFE - UCB (1979-2003)
NIF - LLNL, UCB (1994-1996)

solving Euler equation

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$$

$$U = (\rho, \rho u, \rho E)^T$$

$$F = (\rho u, \rho u^2 + p, \rho u E + p)^T$$

$$E = e + 1/2\ \rho u^2$$

with the eq of state

$$p = p(\rho, E)$$

Free molecular regime

Direct Simulation Monte Carlo method
HIBALL - Wisconsin (1989)
KOYO - Osaka Un. (2002)

solving Boltzmann equation

$$\frac{\partial(nf)}{\partial t} + c \cdot \frac{\partial(nf)}{\partial x} + F \cdot \frac{\partial f}{\partial c} =$$

$$= \int\int [f(c',x,t) f(v',x,t) - f(c,x,t) f(v,x,t)] \times g\sigma(g,\chi) d\Omega dv$$

by decoupling molecular motion from collisions:

$$F^*(c,x) = (1 - \Delta t D) F(c,x,0)$$

$$F(c,x,\Delta t) = (1 + \Delta t J) F^*(c,x)$$

Proposed extension to gas dynamics slip regime

Kinetic theory of gas dynamics on a diffused surface in dilute gas conditions:

- **references include older theoretical studies of Cuette flow conditions and newer numerical studies with DSMC methods (1988 - 2001)**
- **models are based on imposing a velocity and temperature slip to the gas near the surface to compensate for the difference in the velocity distribution of the particles approaching and leaving the surface**
- **DSMC simulation show model is valid for Kn < 0.1**

Proposed extension for Tsunami is based on Harvie and Fletcher study (2001) that explicitly include the mass flux in the velocity and temperature slip formulation:

$$v_i = v_0 - U\lambda\frac{\partial v}{\partial x} \quad \Rightarrow \quad v_l - v_0 = \lambda U\left[\frac{1+(1-f_m)(1-f_c)}{\Phi f_c + f_m(1-f_c)}\right]\frac{\partial v}{\partial x} \quad \Rightarrow \quad v_0 = -\frac{\lambda}{\Phi}\frac{\partial v}{\partial x}$$

$$\Phi = \frac{G^-}{G^+}$$

$$T_i = T_0 - U'\lambda\frac{\partial T}{\partial x} \quad \Rightarrow \quad U' = 9\gamma - \frac{5}{4} \quad \Rightarrow \quad T_l - T_0 = \lambda U'\left[\frac{2-f_c(1-\Phi)-f_t}{f_t + f_c(1-\Phi)(\gamma-1)}\right]\frac{\partial T}{\partial x}$$

$$f_t = f_c + (1-f_c)f_m$$

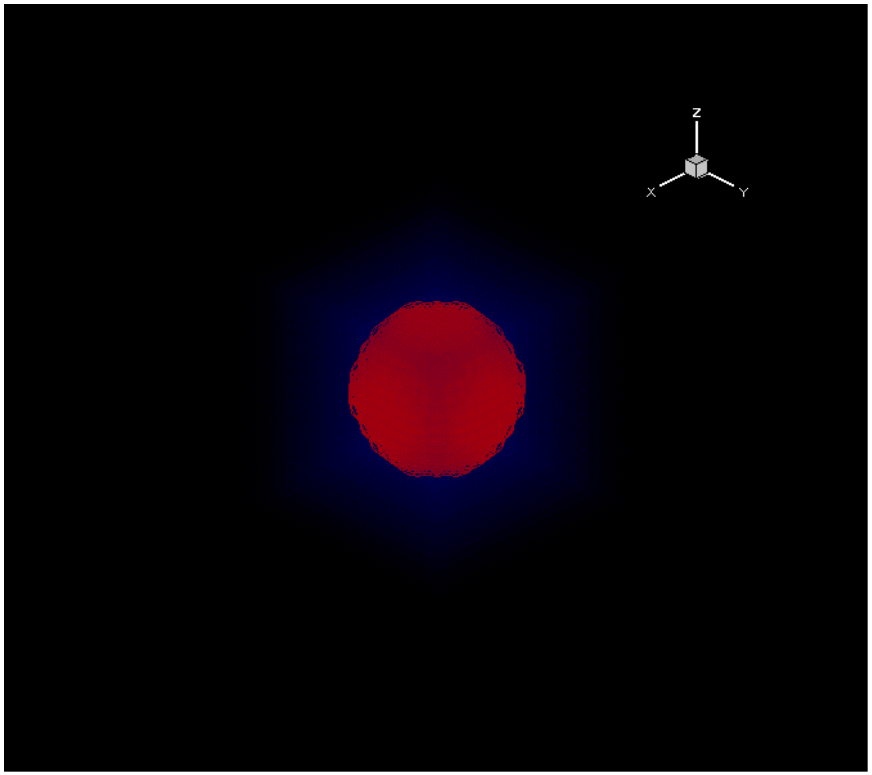
$$T_l - T_0 = 11.35\,\lambda\frac{\Phi}{1.4-0.4\Phi}\frac{\partial T}{\partial x}$$

Droplet Clearing in a Pressure Decay Field

Problem Definition: Droplet clearing represents another aspect of the chamber clearing issue. Droplets produced from the blast should be cleared away before the next shot.

Approach: Start with the development of an incompressible code for analyzing droplet heat and mass transfer with respect to a known pressure decay

Goal: Ultimately to couple the Tsunani code with the developed incompressible free surface heat and mass transfer code for chamber clearing evaluation



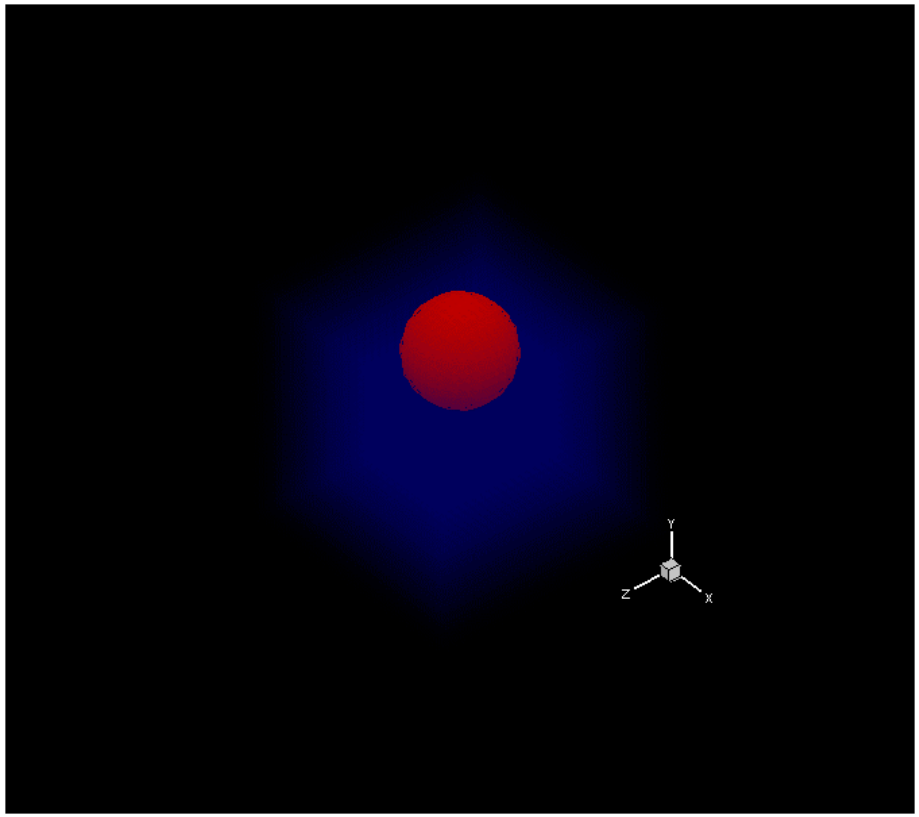
Movie: A hot droplet reacting to the cold surrounding environment

Droplet Heat Transfer and Phase Change with Truchas: Preliminary Evaluation

Truchas is a software program developed at LANL to simulate solidification manufacturing processes, most notably metal casting and welding operations.

Include models and algorithms for:

- Interfacial motion and heat transfer
- Properties varying with temperature
- Phase change
- finite volume method
- Simulations are fully 3 dimensional on unstructured grids.

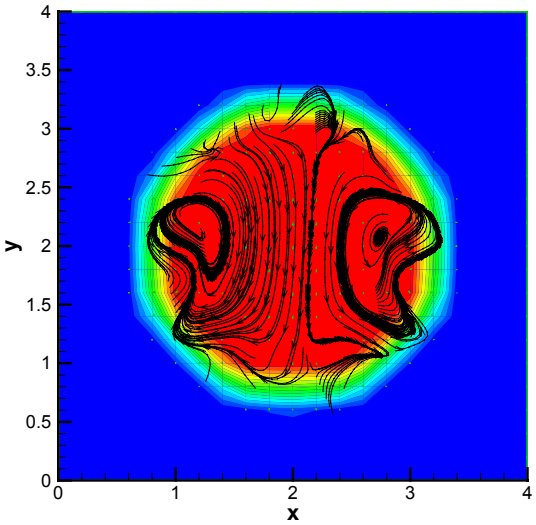


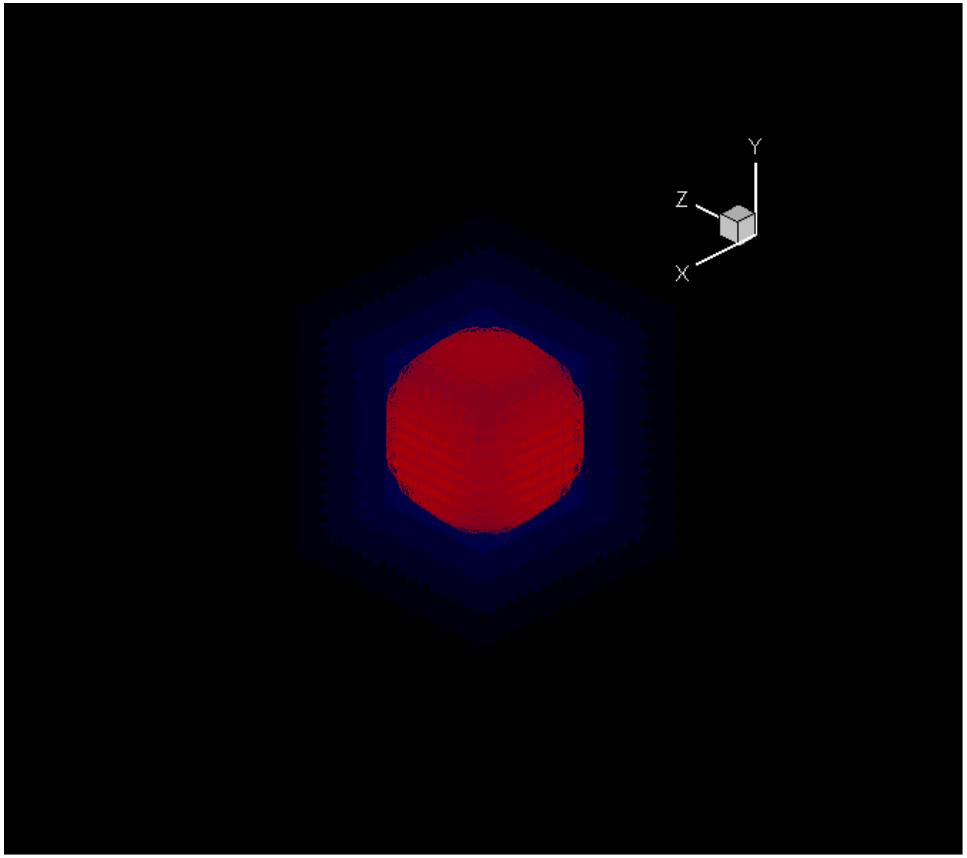
Movie: A hot droplet falling down through a cold environment

Internal circulation caused by the temperature difference is now employed in Truchas code through Boussinesq approximation

Buoyancy force

$$\Delta\rho g = \alpha\rho_o \Delta T g$$





Melting temp=723K
Bottom temp=723 k
Top temp=523 k
Initial temp inside droplet=735 k
initial temp outside droplet=723 k

Assumptions & Near Term Goal

The mass evaporated from the droplet into the surrounding pressure field will be discarded

Incorporate a time dependent temperature boundary condition (set at Tsat corresponding to saturated temperate as a function of known pressure decay)

Await approval from LLNL to modify Truchas code

The End