# Numerical Investigation of Microgravity Tank Pressure Rise Due to Boiling

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# Overview

- Objectives and Motivation
- TPCE/TP Description
- Modeling Approach
- Model Validation using TPCE/TP
  - Self-Pressurization
  - Boiling
- Predictions for the ZBOT experiment
- Conclusion

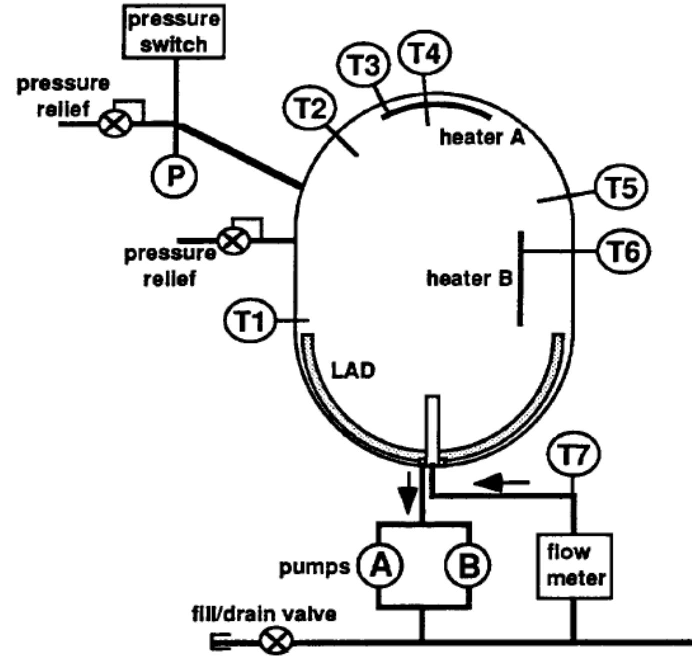
# Objectives and Motivation

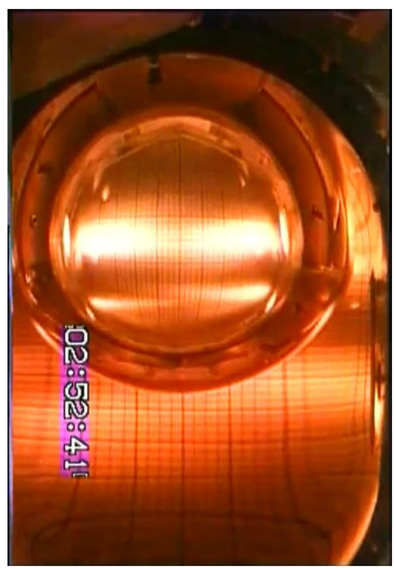
- NASA's missions depend on cryogenic fluid storage for fuel and life support systems
- During storage, heat can leak into cryogen tanks, causing pressurization
- Natural convection is weak in microgravity, so heat leaks can create superheated regions in the liquid, which can cause boiling. This can cause pressure spikes
- In order to control the pressure in a tank, it is necessary to be able to predict the magnitude of the pressure spikes

The goal of this work was to develop and validate a CFD model to predict the pressure rise in a tank due to boiling and use it to make predictions for the ZBOT experiment

# TPCE/TP Description

- The Tank Pressure Control Experiment: Thermal Phenomena (TPCE/TP) (Hasan et al., 1996) was used to validate the CFD model developed for this work
  - It was flown on the Space Shuttle Mission STS-52
  - 21 tests were run to study self-pressurization and pressure control by jet mixing
- A small-scale tank was filled to 83% with Freon 113
- 2 rectangular heaters represented heat leaks into the tank
  - The heater powers and temperatures were recorded
- Noncondensable gases were present in the tank
- Test 6 of the TPCE/TP experiment was used to validate the model
  - It used Heater A
  - The tank pressurized for a while before nucleate boiling occurred

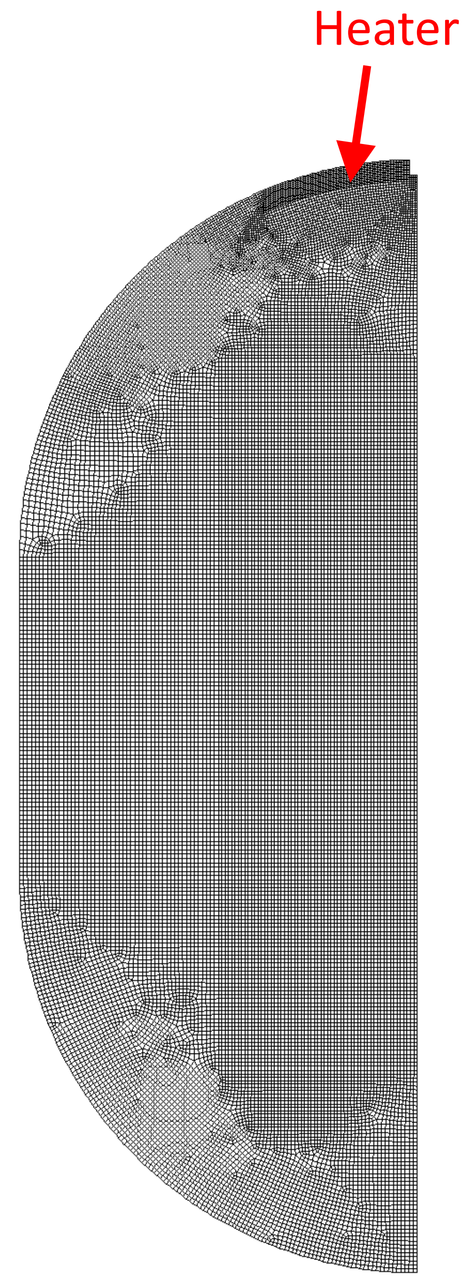




# Modeling Approach

- The tank was simplified to make an axisymmetric model
  - Heater A was modeled as a curved disk with the same area as the heater in the experiment
  - Heater B, the LAD, the nozzle, and the tank wall were neglected
  - Boiling is a 3D phenomenon, but many researchers (Dhir et al., 1999, 2002, 2007) have used axisymmetric models to represent this phenomenon with acceptable success
- The Volume of Fluid (VOF) model in Fluent v. 15 was used
  - A User-Defined Function (UDF) customized the VOF model to allow mass transfer
- The tank was meshed using an unstructured mesh of 28244 cells
- The fluid properties (obtained from the NIST Chemistry WebBook) were kept constant
- Contact angle of the fluid with the wall was set to 0°
- Heater temperature was applied as a boundary condition



# Mathematical Model

Continuity: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$

Momentum: $\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla P + \nabla \cdot [\mu(\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + \vec{F}_{vol}$

Energy: $\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\vec{v}(\rho E + P)\right) = \nabla \cdot \left(k_{eff} \nabla T\right) + S_h$

Volume of Fluid approach was used to track the interface between the phases:

VOF equations: $\frac{1}{\rho_q}\left[\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) = S_{\alpha_q}\right]$ , $\sum_{q=1}^{n} \alpha_q = 1$

Energy and temperature were defined as mass averaged scalars: $E = \frac{\sum_{q=1}^{n} \alpha_q \rho_q E_q}{\sum_{q=1}^{n} \alpha_q \rho_q}$

Properties: $\rho = \sum_{q=1}^{2} \alpha_q \rho_q,\ \mu_{eff} = \sum_{q=1}^{2} \alpha_q \mu_{eff\ q},\ k_{eff} = \sum_{q=1}^{2} \alpha_q k_{eff\ q}$

Natural convection modeled using Boussinesq model: $(\rho - \rho_0)g \approx -\rho_0 \beta (T - T_0) g$

Continuum Surface Force: $F_{vol} = \sum_{pairs\ ij, i<j} \sigma_{ij} \frac{\alpha_i \rho_i \kappa_j \nabla \alpha_j + \alpha_j \rho_j \kappa_i \nabla \alpha_i}{\frac{1}{2}(\rho_i + \rho_j)}$ , $\kappa = \nabla \cdot \hat{n}$

Implicit VOF time discretization: $\frac{\alpha_q^{n+1} \rho_q^{n+1} - \alpha_q^n \rho_q^n}{\Delta t} V + \sum_f \left(\rho_q^{n+1} U_f^{n+1} \alpha_{q,f}^{n+1}\right) = \left[S_{\alpha_q} + \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp})\right] V$

Explicit VOF time discretization: $\frac{\alpha_q^{n+1} \rho_q^{n+1} - \alpha_q^n \rho_q^n}{\Delta t} V + \sum_f \left(\rho_q U_f^n \alpha_{q,f}^n\right) = \left[\sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp}) + S_{\alpha_q}\right] V$

# Mathematical Model

Mass transfer was a volumetric source term (kg/m³*s): $S_{a_q} = \vec{\dot{m}} \cdot \vec{A_i}$ or $S_{a_q} = \vec{\dot{m}} \cdot \frac{1}{V_{cell}^{1/3}}$

Interfacial area density (1/m): $\vec{A_i} = |\nabla \alpha|$

For boiling, mass transfer was limited to high-temperature liquid: $T_{sh} - T_{sat} > threshold$

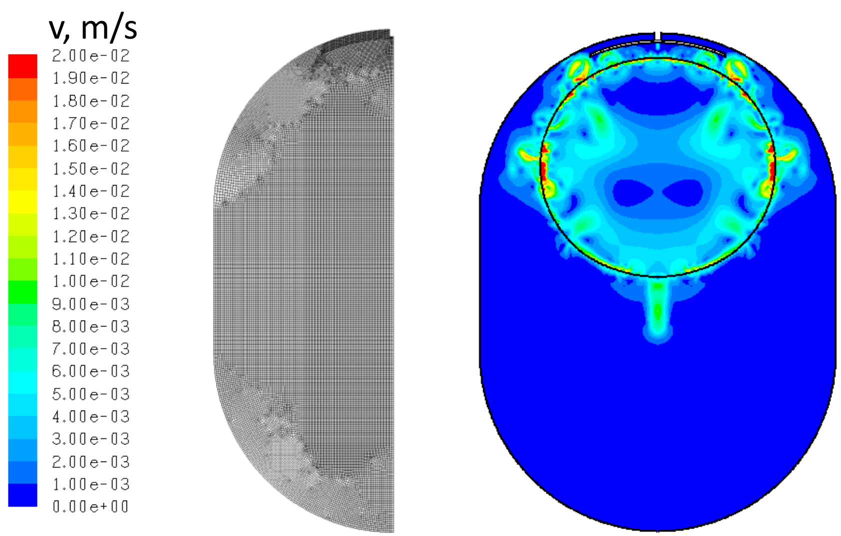
$\vec{\dot{m}}$ is a mass flux vector (kg/(m²*s))

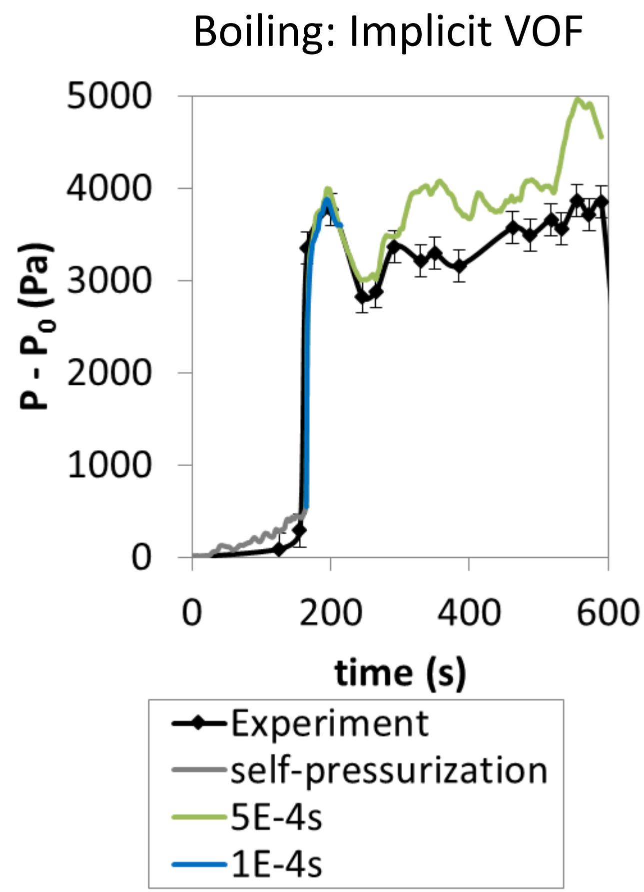
Schrage equation is based on difference in pressure: $\dot{m} = \sigma \sqrt{\frac{M}{2\pi R_u T_{sat}}} (P_{sat} - P_v)$

# Mesh and Time Step Independence

- Meshes with 1208 elements to 38141 elements, in different configurations, were tried
- Cases were run with no gravity and no mass transfer
- The mesh with the smallest spurious velocities was chosen for running the cases

28244 Elements

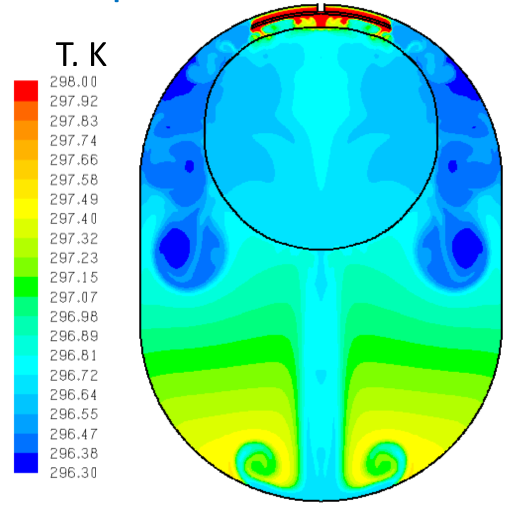


# Model Validation

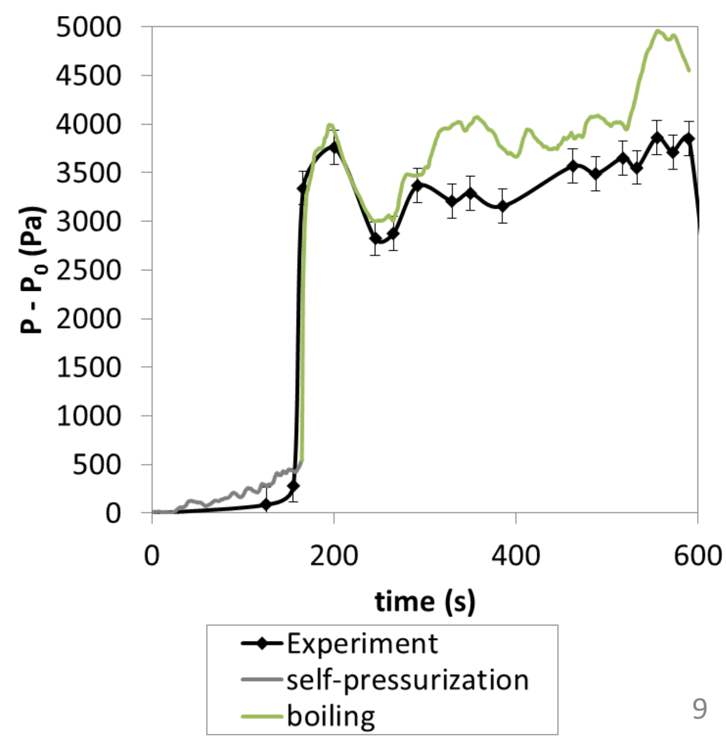
- The following parameters were studied for boiling:
  - Accommodation coefficients
  - Threshold superheat temperatures required for boiling

Initial Temperature Field for Boiling




## Best Case

- Threshold superheat temperature set to 3K
- Accommodation coefficient for boiling is larger than that for evaporation: $\sigma_b$ = 0.1, $\sigma_e$ =0.005
- Effect of noncondensable gas is captured by low condensation coefficient: $\sigma_c$ = 0.00001

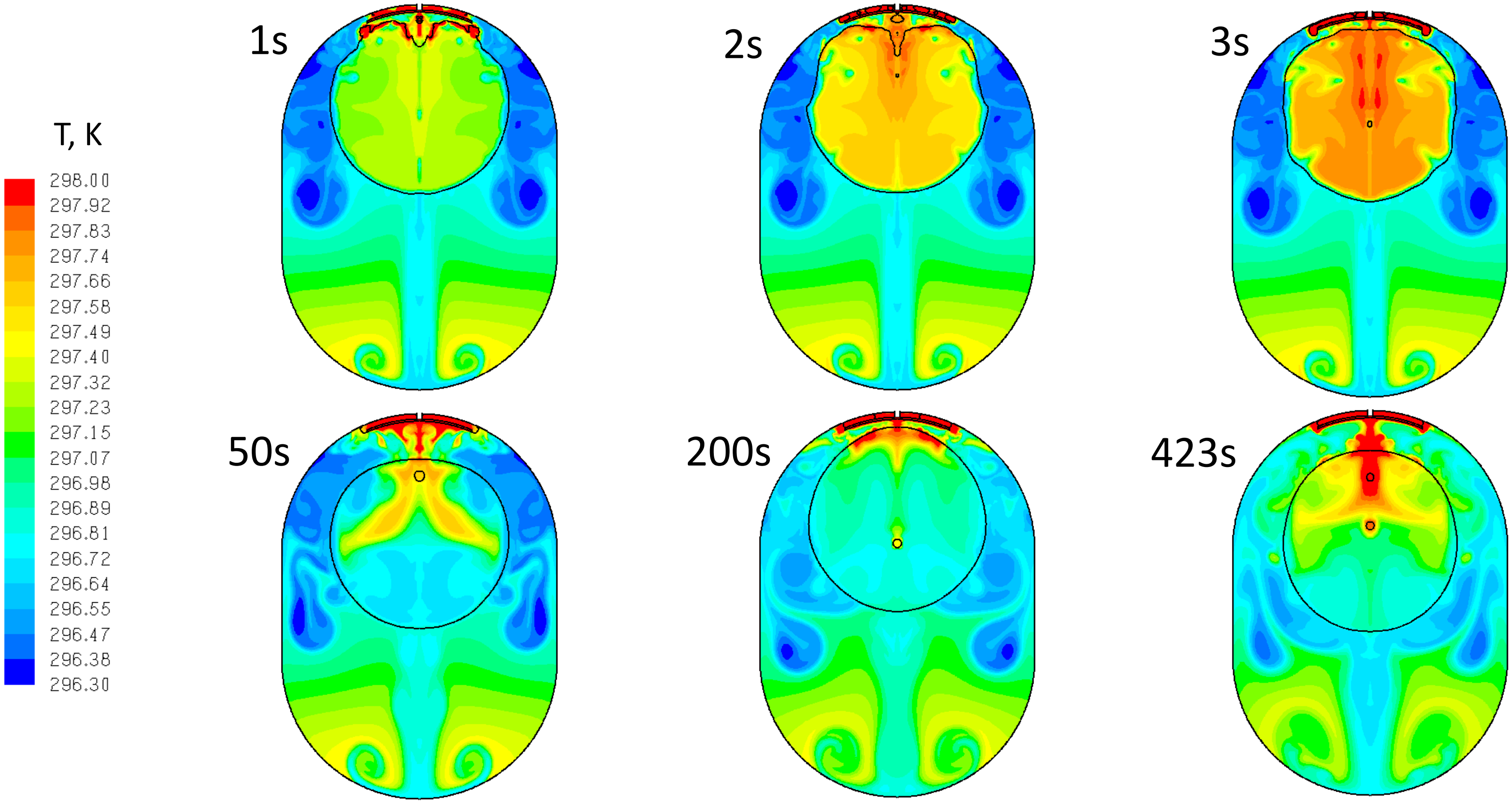



The time at which boiling started was a user-defined parameter

# Model Validation: Best Case

Implicit VOF, bounded second order time discretization, compressive scheme, PISO, threshold superheat temperature set to 3K

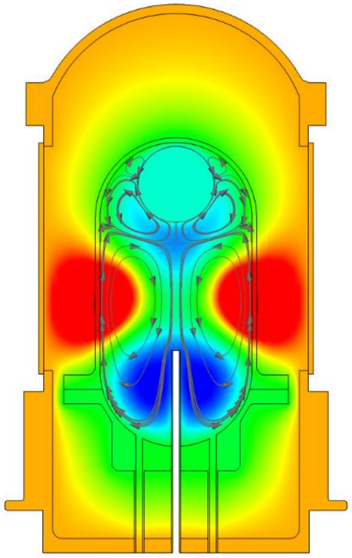
Temperature contours, seconds after boiling starts

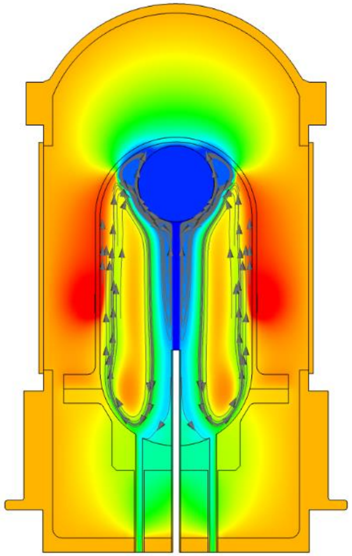



Behavior during boiling was similar to that of the experiment

# ZBOT Description

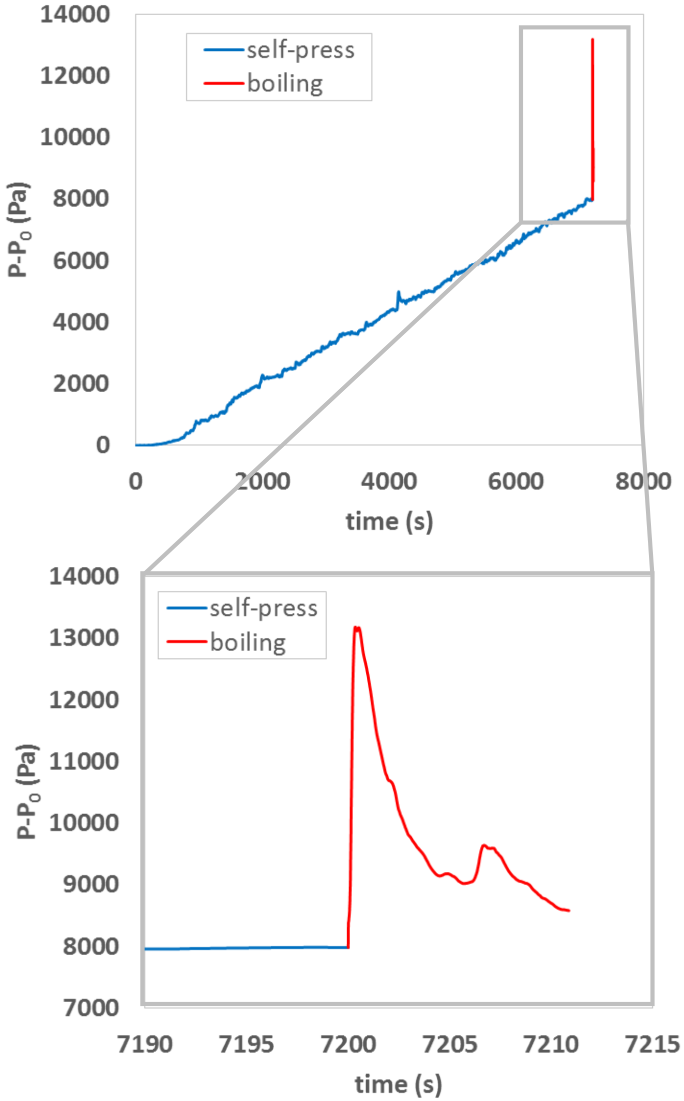
- Small-scale simulant fluid experiment, to study pressurization and pressure control in microgravity
  - Current pressure control strategies involve venting of fluid from tank
  - Zero Boil-Off strategy involves mixing/cooling of fluid to reduce pressure, eliminating need for venting
- CFD and analytical models being developed
- Microgravity data will be used to validate models
- Models will be used for full-scale tanks, and for optimization of ZBO technology



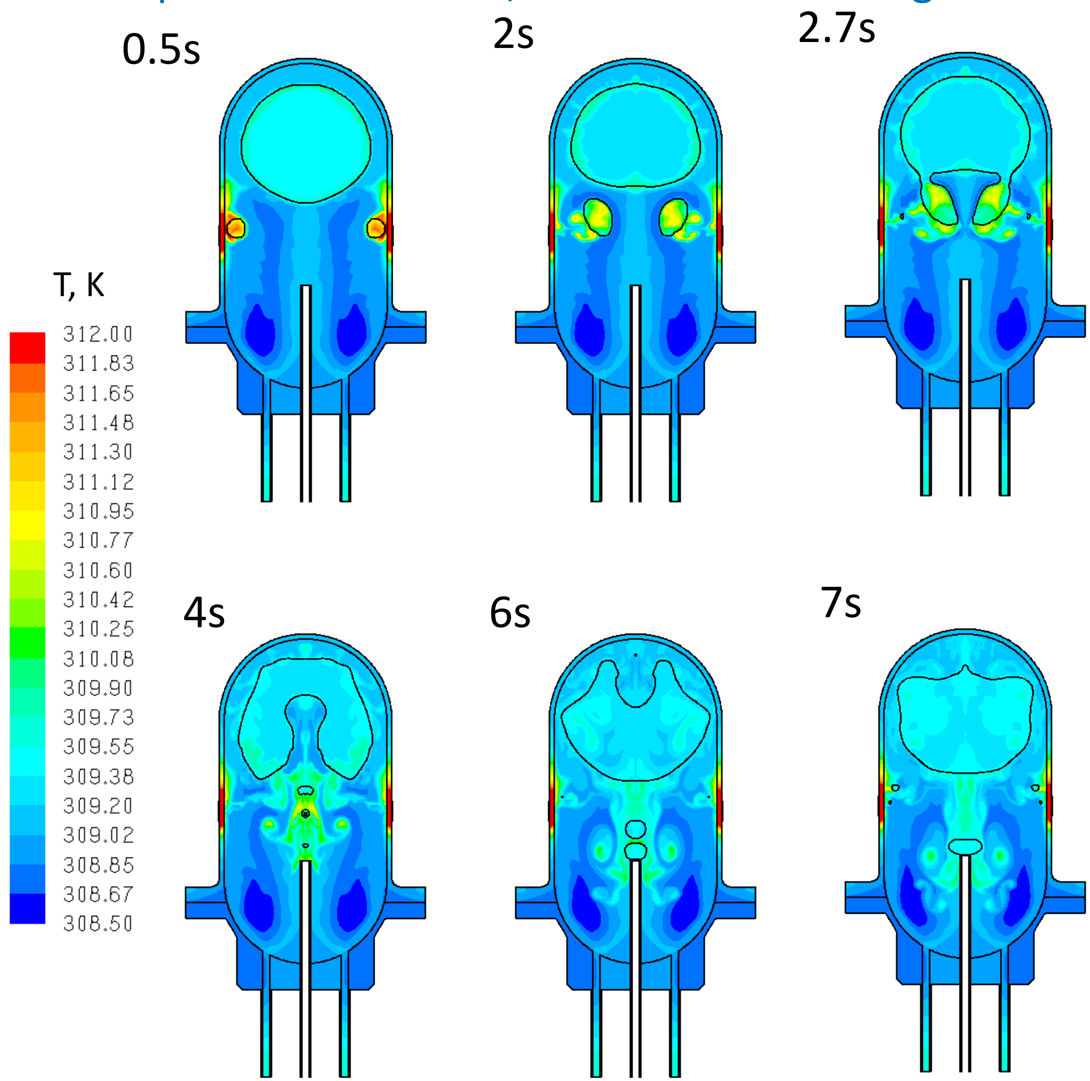


# Predictions for ZBOT

$\sigma_h = 0.1, \sigma_e = \sigma_c = 0.005$




Temperature contours, seconds after boiling starts



# Conclusion

- Have developed a model to predict the magnitude of the pressure spikes due to boiling in a tank in microgravity
  - Good results were obtained by manipulating the Schrage equation to use different accommodation coefficients for boiling and evaporation
- Model was used to predict pressure rise in ZBOT tank due to boiling
  - Should be able to contain the pressure rise for even the tests with the highest heat flux to be used
- Working on a sub-grid model to capture the physics better using equations applied via a UDF

# Backup Slides

# Numerical Implementation

- Time discretization schemes (Explicit with first order time discretization, Implicit with bounded second order time discretization)
- Pressure-velocity coupling (PISO, Coupled)
- Spatial discretization: Least-squares cell based
- Pressure: Body force weighted
- Density, momentum, and energy: Second order upwind
- Convergence criteria
  - Self-pressurization: $10^{-4}$ for continuity, $10^{-5}$ for the x- and y-velocities, and $10^{-7}$ for energy
  - Boiling: all variables converged to about $10^{-3}$ or better

# Numerical Parameters Studied

Time discretization schemes

    Explicit with first order time discretization

    Implicit with bounded second order time discretization

Pressure-velocity coupling

    PISO

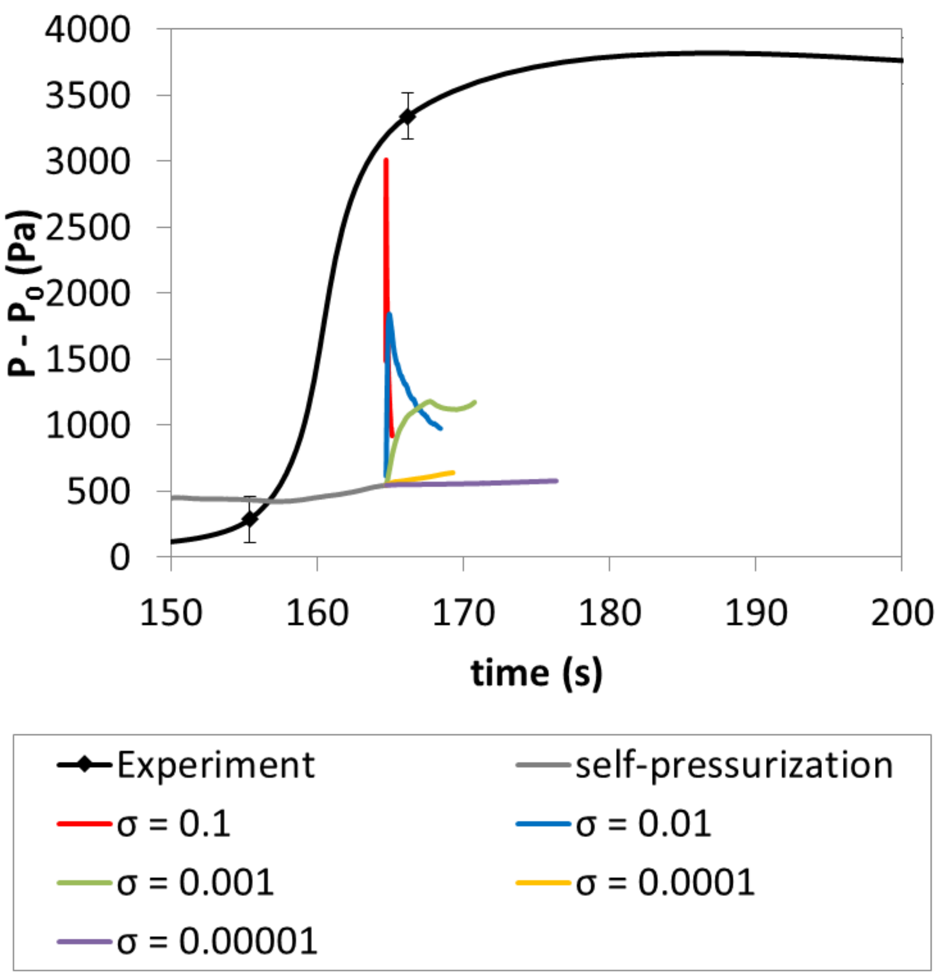
    Coupled

# Model Validation

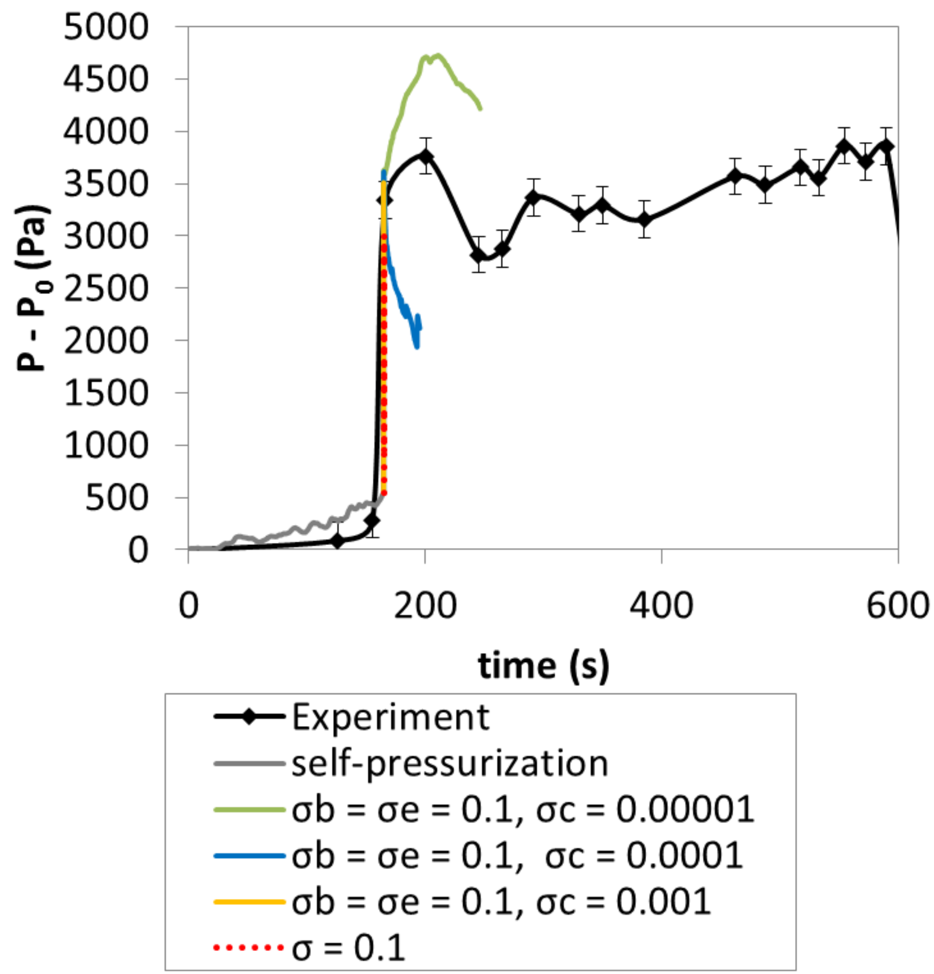
Explicit VOF, first order time discretization, geometric reconstruction

Threshold superheat was set to 3K

$\sigma_e = \sigma_b = \sigma_c$




$\sigma_e = \sigma_b \neq \sigma_c$

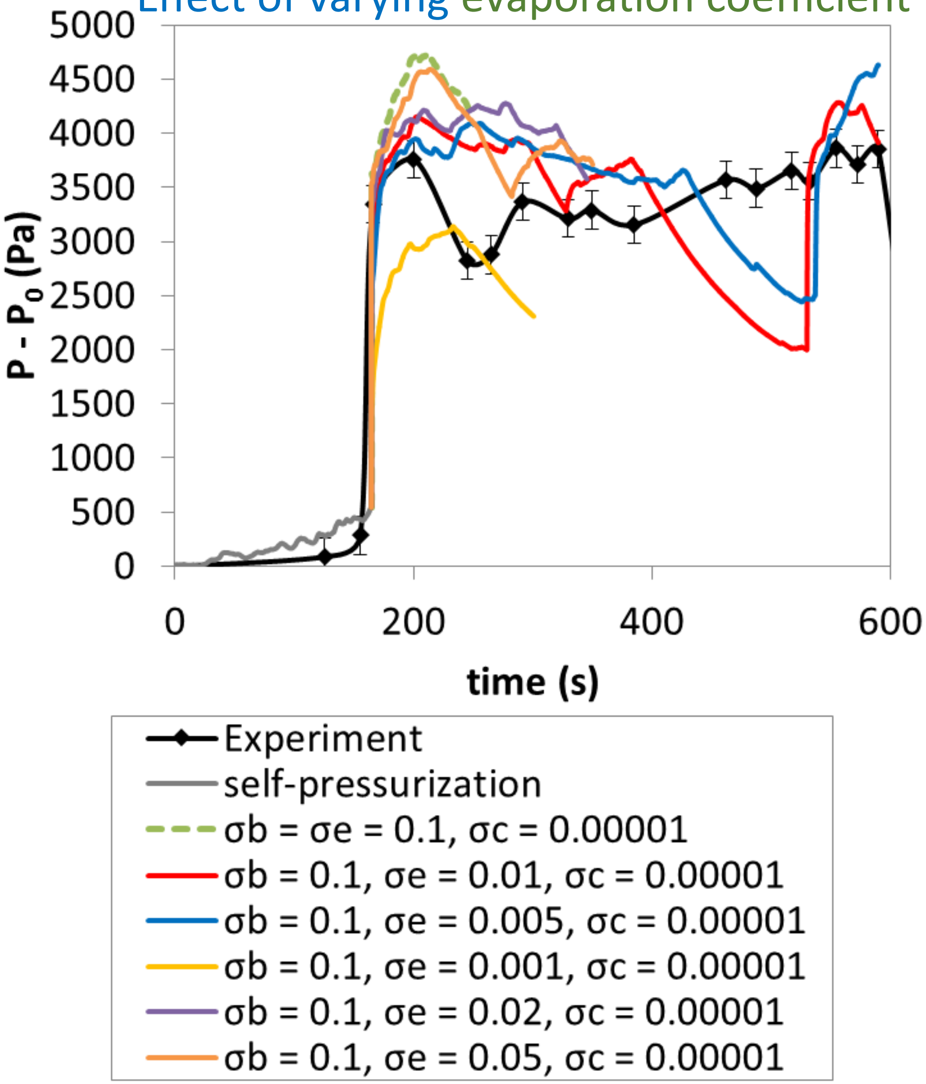


# Model Validation

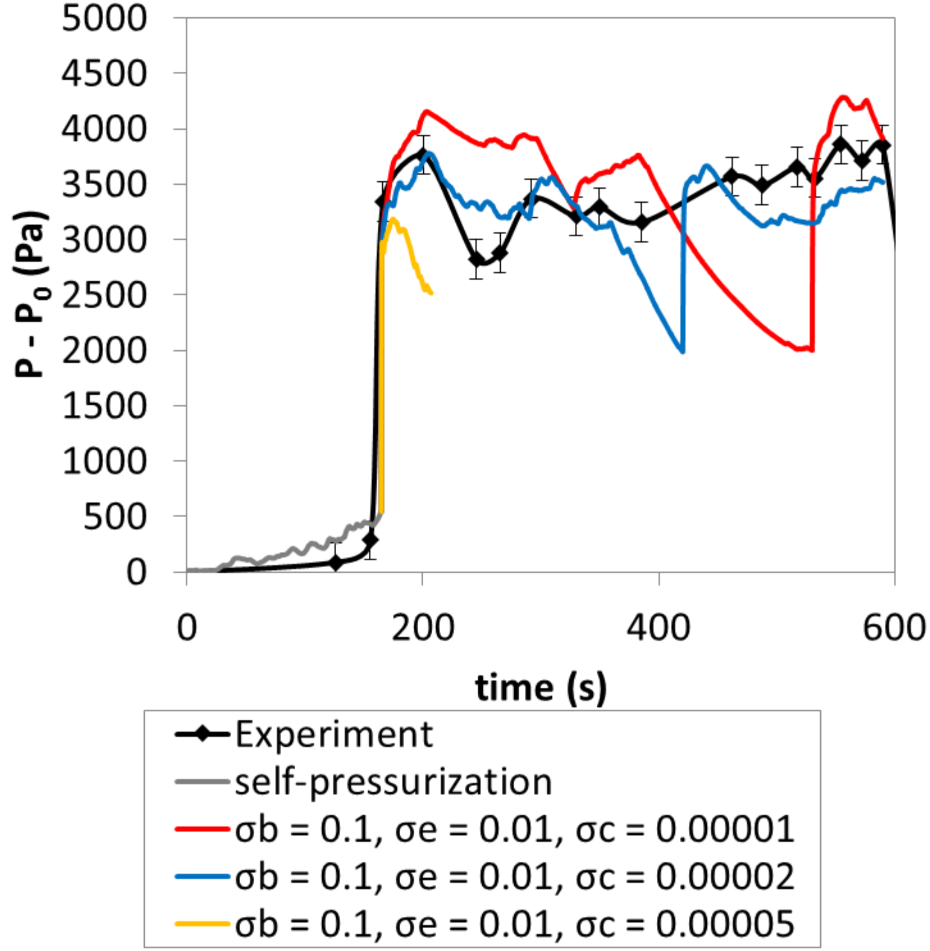
Explicit VOF, first order time discretization, geometric reconstruction

Threshold superheat was set to 3K

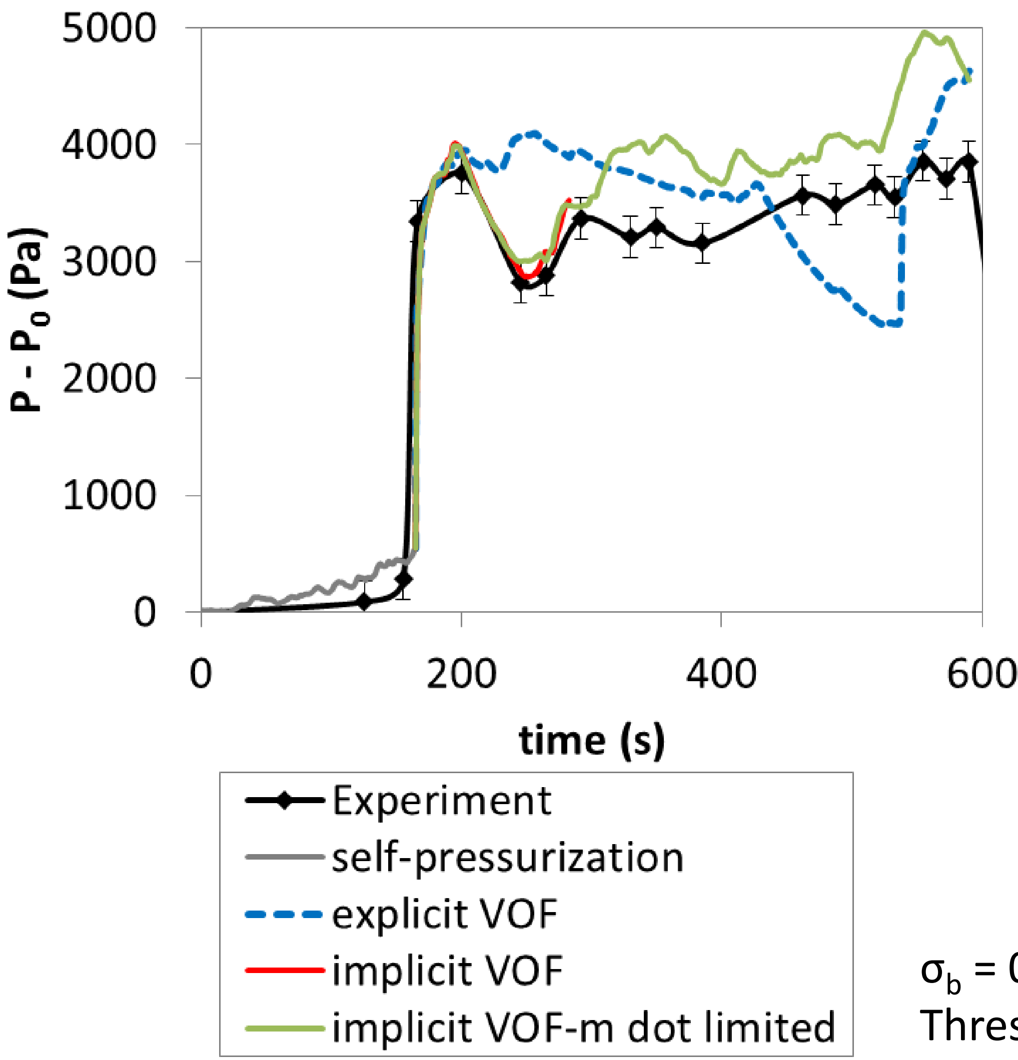
Effect of varying evaporation coefficient




Effect of varying condensation coefficient



# Model Validation




Explicit VOF, first order time discretization, geometric reconstruction

vs

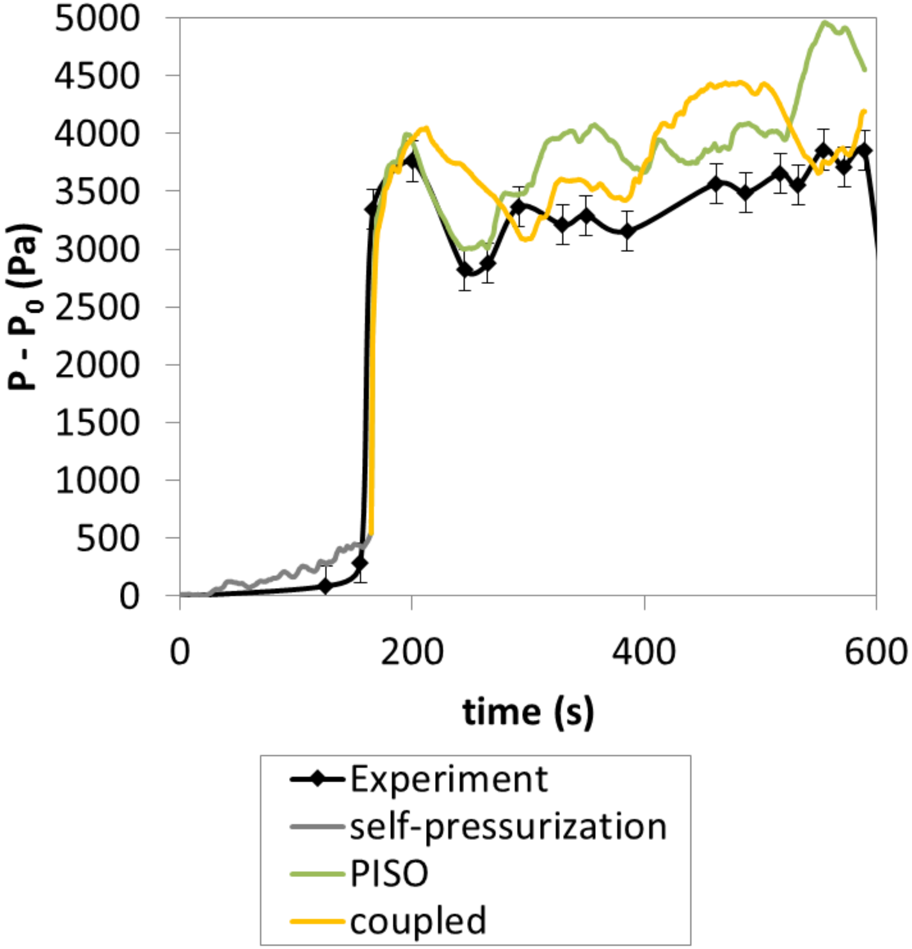
Implicit VOF, bounded second order time discretization, compressive scheme (allows larger time steps with more accuracy)

$\sigma_b = 0.1$, $\sigma_e = 0.005$, $\sigma_c = 0.00001$;
Threshold superheat was set to 3K

# Model Validation

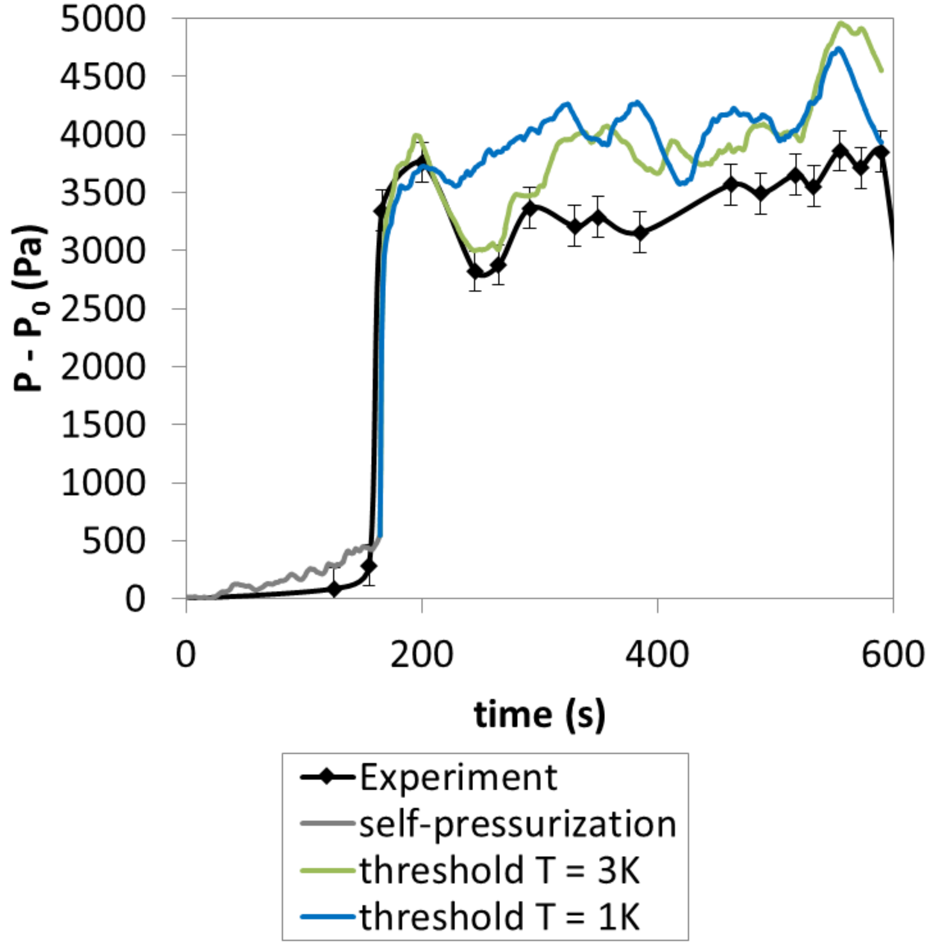
Implicit VOF, bounded second order time discretization, compressive scheme

Effect of pressure-velocity coupling




Threshold superheat was set to 3K

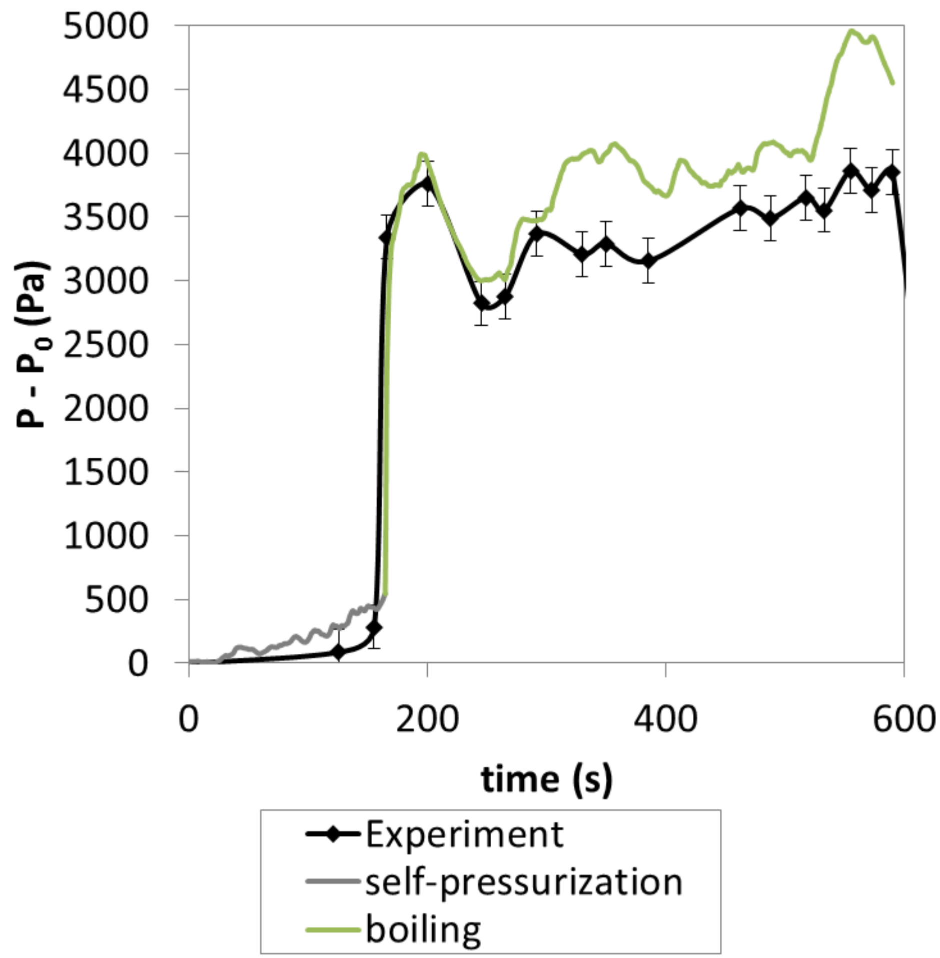
Effect of threshold superheat temperature




PISO

# Model Validation: Best Case

- Implicit VOF
- Bounded second order time discretization
- Compressive scheme for the volume fraction
- PISO pressure-velocity coupling
- Threshold superheat temperature set to 3K
- Accommodation coefficient for boiling is larger than that for evaporation: $\sigma_b = 0.1$, $\sigma_e = 0.005$
- Effect of noncondensable gas is captured by low condensation coefficient: $\sigma_c = 0.00001$



# Pressure-Velocity Coupling

- PISO
  - Pressure-Implicit Splitting of Operators
  - Segregated algorithm (solves the momentum equation and the pressure correction equation separately)
  - Recommended for transient flow calculations w/ large time steps
- Coupled
  - Solves the momentum and pressure-based continuity equations together

Sources: ANSYS Fluent v. 15 User's Guide and Theory Guide

# Volume Fraction Formulation

- Schemes used to calculate face fluxes at phase interfaces
- Both are used for cases with sharp interfaces (phases don't penetrate each other)

- Geometric Reconstruction
  - Available for explicit VOF scheme
  - Most accurate scheme in ANSYS Fluent
  - Gives a sharper interface than the Compressive scheme
  - Used to obtain time-accurate transient behavior

- Compressive
  - Available for implicit VOF scheme
  - "A second order scheme based on the slope limiter" (Fluent theory guide)

$$\phi_f = \phi_d + \beta \nabla \phi_d$$

where

$\varphi_f$ is the face VOF value

$\varphi_d$ is the donor cell VOF value

$\beta$ is the slope limiter value

$\nabla \varphi_d$ is the donor cell VOF gradient value

Sources: ANSYS Fluent v. 15 User's Guide and Theory Guide

# Various Schemes

- Body force weighted
  - Calculates the face pressure by assuming the "normal gradient of the difference between pressure and body forces is constant" (Fluent theory guide)
  - Works for cases with buoyancy
  - Recommended for cases with large body forces
- Least-squares cell based gradient
  - Gives second order discretization
  - About as accurate as node-based gradient and less computationally expensive for unstructured meshes
- Second order upwind
  - Provides better accuracy than first order (especially when the flow is not aligned with the mesh)
- Bounded second order time discretization
  - More accurate than first order implicit formulation
  - More stable than (but as accurate as) second order implicit

Sources: ANSYS Fluent v. 15 User's Guide and Theory Guide

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