# Development and Experimental Benchmark of Simulations to Predict Used Nuclear Fuel Cladding Temperatures during Drying Operations

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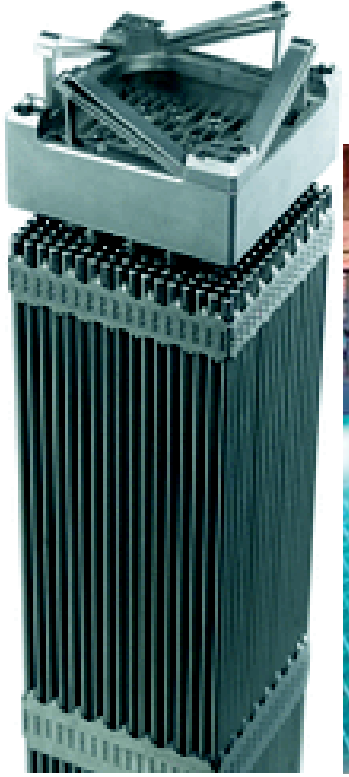
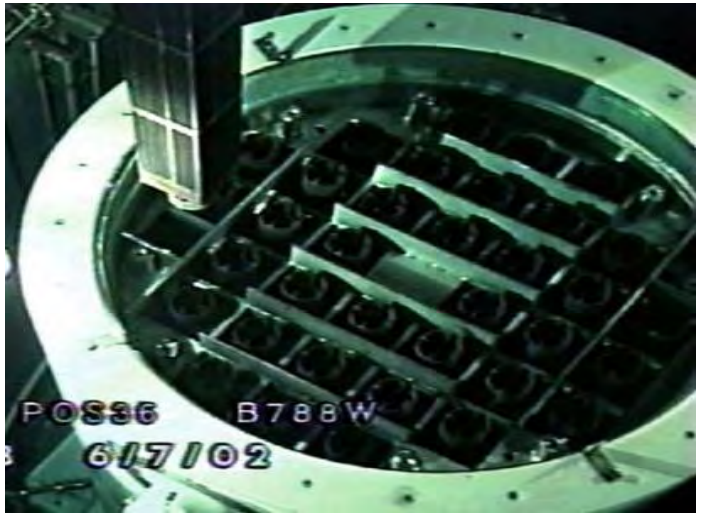
# Used Nuclear Fuel Assemblies





- Consist primarily of square arrays of zircaloy cladding tubes containing highly-radioactive, heat-generating $UO_2$ pellets and fission-product gases
- After removal from a reactor the fuel is stored underwater while its radioactivity and heat generation rates decrease
- After sufficient time the fuel is loaded into gas-filled canisters.
- Essentially all moister must be removed to limit corrosion and hydrogen/oxygen formation, before the canister is filled with helium gas and placed into storage or transport over-packs

# Moisture Removal

- Industry uses Vacuum Drying or Forced Helium Dehydration (force/natural convection)
- During vacuum drying the He gas is evacuated from the canister in stages, to pressures as low as 0.7 Torr (100 Pa) to vaporize and remove moisture.
  - The process continues until the canister can hold a 3-torr vacuum for 30 minutes (indicating very little water is still vaporizing)
- Vacuum drying "usually" takes
  - 12 to 24 hours for metal matrix baskets
  - 80 to 100 hours if Boral is used
  - Temperatures approach steady-state values
- Vacuum Drying is simple, but removing high-conductivity helium may raise cladding temperatures

# Cladding Temperature During Drying

- The cladding may experience its highest temperature during drying
  - This is the first operation when the fuel is removed from a water-cooled environment, and its heat generation rate is still relatively high
- If the cladding temperature exceeds certain limits (~400°C), it may develop radial-hydrides and become brittle after its temperature decreases during long-term storage.
  - The temperature limit depends on fuel burnup, and is the subject of research
  - Brittle cladding would reduce the fuel's suitability for future transport or processing, and should be avoided if possible.
- The <u>objective of this work</u> is to develop accurate computational methods to predict cladding temperatures during low-pressure drying
- This will allow efficient drying operation to be designed that safely maintain temperatures below required limits

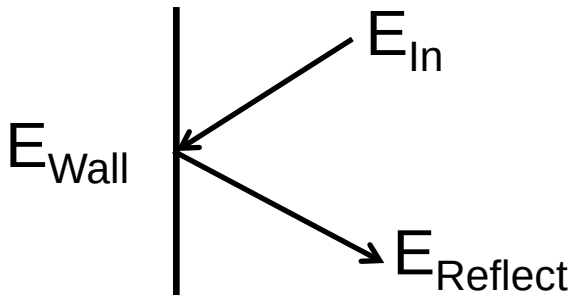
# Effects of Low Pressure on Heat Transfer

- Natural Convection
  - Gas motion is driven by the ratio of buoyancy to viscous forces, which is characterized by the Grashof number
    - $Gr = g\Delta TL^3\rho^2/\mu^2T_{Mean}$
    - Decreases significantly as the pressure and density $\rho$ decrease
  - Neglecting natural convection is justified
- Gas Conduction
  - Reducing gas pressure from 1 ATM ($10^5$ Pa) to 100 Pa reduces thermal conductivity by no more that 1%:
  - Neglecting conductivity change is justified

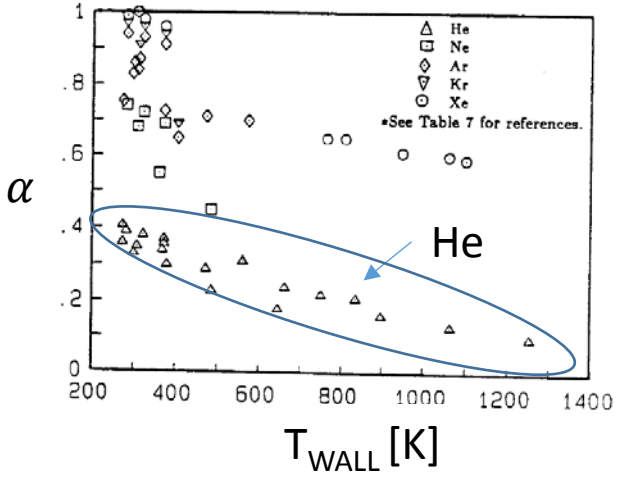
# Possible Gas Rarefication

- In a low pressure and density gas, individual molecules travel "considerable" distances before encountering other molecules
  - mean free path length: $\lambda = \frac{T\mu_0}{P}\sqrt{\frac{2k_B}{mT_O}}$ increases as pressure decreases
- In rarefied gases a molecule's speed may be significantly different from those surrounding it
- The gas may not act as a continuum
  - Transport properties ($\kappa$, $\mu$) are not functions of the <u>local</u> temperature and pressure alone
    - The Navier-Stokes and Fourier conduction equations rely on these properties
  - Gas speed and temperature at solid surfaces they encounter may not be the same as those of the surface
- Package vendors currently do not include rarefication effects when calculating clad temperatures during vacuum drying
  - Should they?

# Surface Thermal Accommodation




$$\alpha = \frac{E_{Reflect} - E_{In}}{E_{Wall} - E_{In}}$$




- As the pressure decreases molecular collisions with the wall become relatively more important compared with collisions with each other
- The Thermal Accommodation Coefficient $\alpha$ characterizes how the energy of a collection of molecules is affected when interacting with a wall, $0 \leq \alpha \leq 1$
  - Not important when the gas acts as a continuum
- From measurements of "engineering" surfaces
  - $\alpha$ primarily depends on <u>gas composition</u> and <u>temperature</u>
    - not wall composition or surface finish
  - For <u>dry helium</u> with $T_{WALL}$ = 25 to 400°C (300 to 670 K)
    - $\alpha$ ~ 0.4 to 0.2

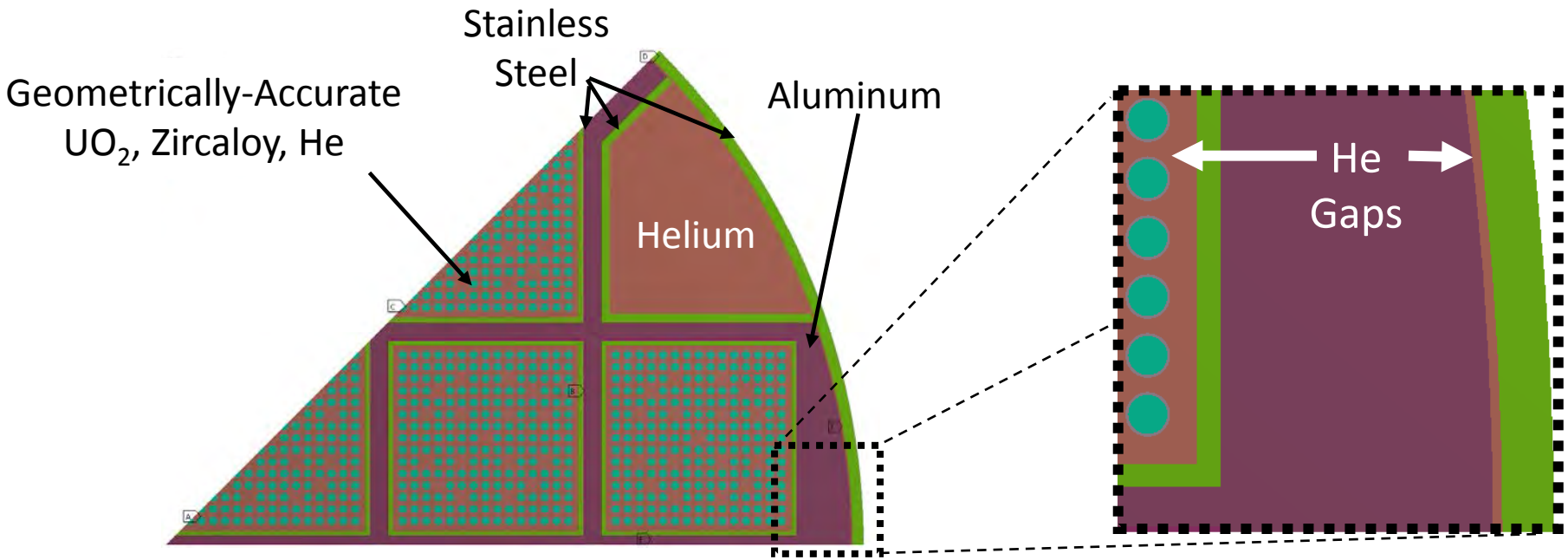
# When is an enclosed gas Rarefied?

- When the mean free path length is "large" compared to the enclosure characteristic dimension, $L_C$
  - Knudsen number $Kn = \frac{\lambda}{L_C}$ increases at gas becomes more rarefied
- For small $Kn < 0.001$ gas acts as a continuum
  - For $Kn > 0.001$ the Navier-Stokes and Fourier equations are not strictly valid
- Boltzmann Equation must be solved to calculate transport
  - Models transport by collisions of vast numbers molecules
  - Computationally intensive, especially for complex enclosures

# Rarefication Regimes

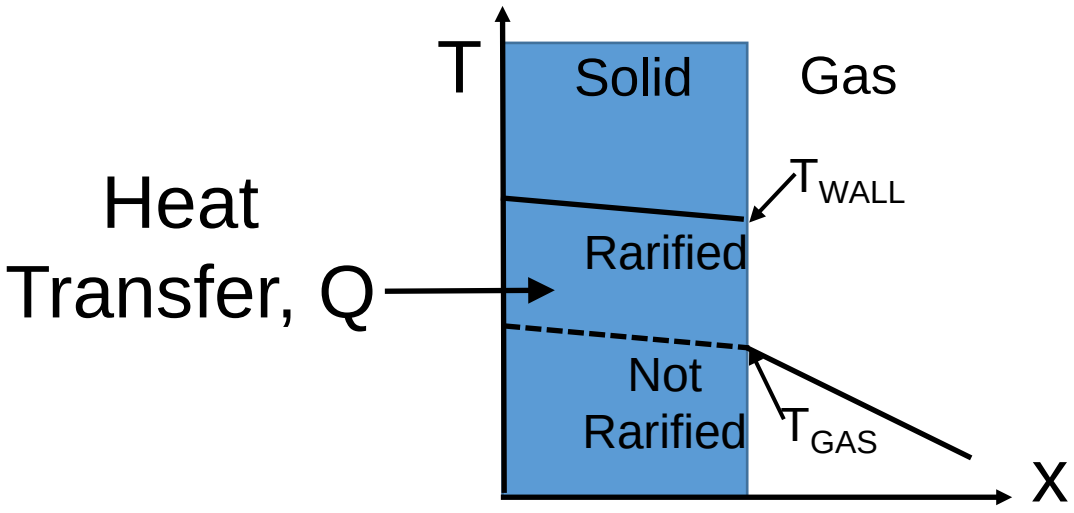
- $0.001 < Kn < 0.1$
  - At moderately low pressures (moderately high *Kn*) the continuum assumptions breaks down only at the walls
    - The gas temperature and velocity are not the same as the surface's
    - Known as "velocity slip" or "temperature jump" regime
  - Transport may be modeled using Navier-Stokes/Fourier equations <u>away</u> from the walls with special temperature and velocity boundary conditions <u>at</u> the walls
    - How to find those conditions?
- $Kn > 10$
  - At extremely low pressures molecules interact with walls but only rarely with each other
  - Known as "collisionless" regime, modeled using a simplified collisionless Boltzmann Eqn.
- $0.1 < Kn < 10$
  - In this Transition regime, the full Boltzmann equation is required to model transport (computationally intensive)
- Which regimes are relevant for vacuum drying?

# One-eighth Model of a Loaded Canister for 24 PWR Assemblies




- Each basket opening contains a 15x15 PWR assembly
- Is $0.001 < Kn = \frac{\lambda}{L_C} < 0.1$ ?
- Surface-to-surface spacing of helium filled gaps, $L_C$
  - Fuel region: 9.5 mm; Basket/canister gap: 2.3 mm
- $\lambda = \frac{T\mu_0}{P}\sqrt{\frac{2k_B}{mT_O}}$ (depends on gas temperature and pressure)
  - P = 400 Pa, 0.01 ≤ *Kn* ≤ 0.04
  - P = 100 Pa, 0.04 ≤ Kn ≤ 0.15 (*slightly inside* the transitional regime)

# Slip-Regime Temperature Conditions

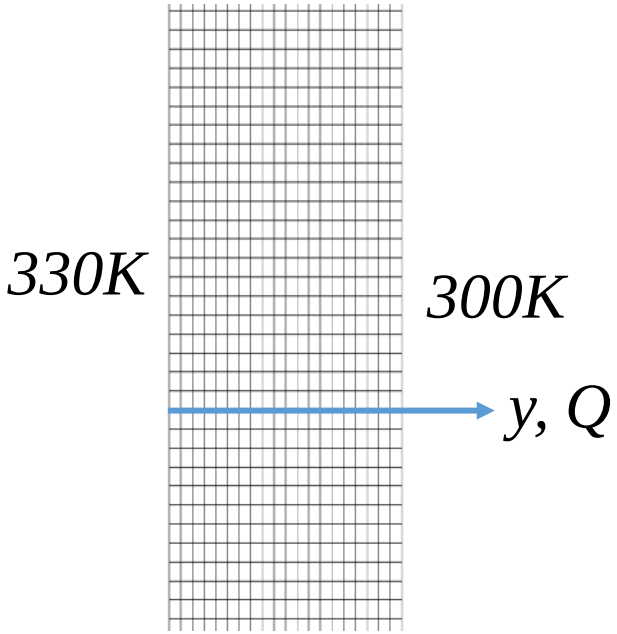


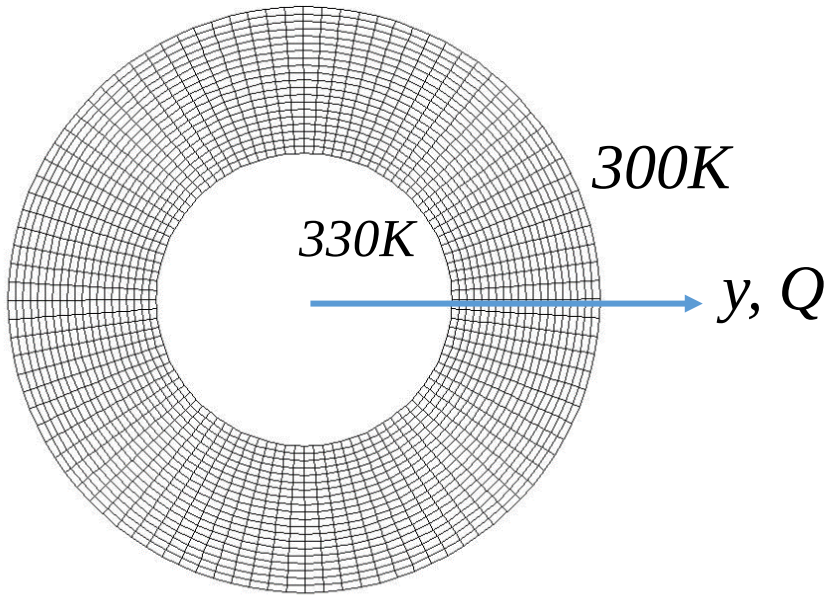

- Heat Conduction from a solid to a gas
- There is a temperature-jump (TJ) at the interface between a solid and rarefied-gas that increases with heat transfer rate Q
- By a dimensional argument: $T_{Wall} - T_{Gas} = \left(-\frac{dT}{dx}\right)\lambda\zeta_T = \left(\frac{Q}{\kappa A}\right)\lambda\zeta_T = QR_{TJ}$
  - $Q$ = Heat transfer; $\kappa$ = Gas conductivity; $A$ = Wall area
  - $\zeta_T$ = Temperature Jump Coefficient = ? (dimensionless, subject of research), expect it to:
    - Increases as $\alpha$ decreases, depend on gas properties
- $R_{TJ} = \frac{\lambda\zeta_T}{A\kappa}$ = Temperature-jump thermal resistance
  - Can be implemented in Fluent or other CFD codes

# How to find the Temperature Jump Coefficient, $\zeta_T$

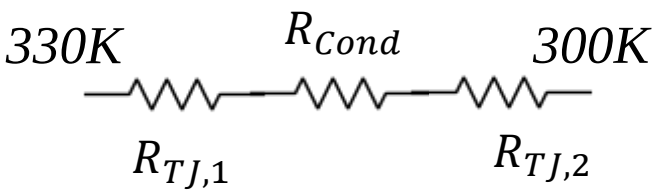
- ANSYS/Fluent has a built-in utility that uses $\zeta_T = 2\left(\frac{2-\alpha}{\alpha}\right)$
  - Temperature jump increases as thermal accommodation decreases
  - Not dependent on gas properties
- Lin-Willis [1972]: $\zeta_T = \frac{\sqrt{\pi}\gamma}{(\gamma+1)Pr}\left(\frac{2-\alpha}{\alpha} + 0.17\right)$
  - Dependent on gas properties; $\gamma = \frac{c_p}{c_v}$; $Pr = \frac{\mu c_p}{\kappa}$
- Others are also in the literature
- Which ones accurately reproduce Boltzmann equation simulation results in the slip-regime?

# Boltzmann Solutions across Simple Gaps



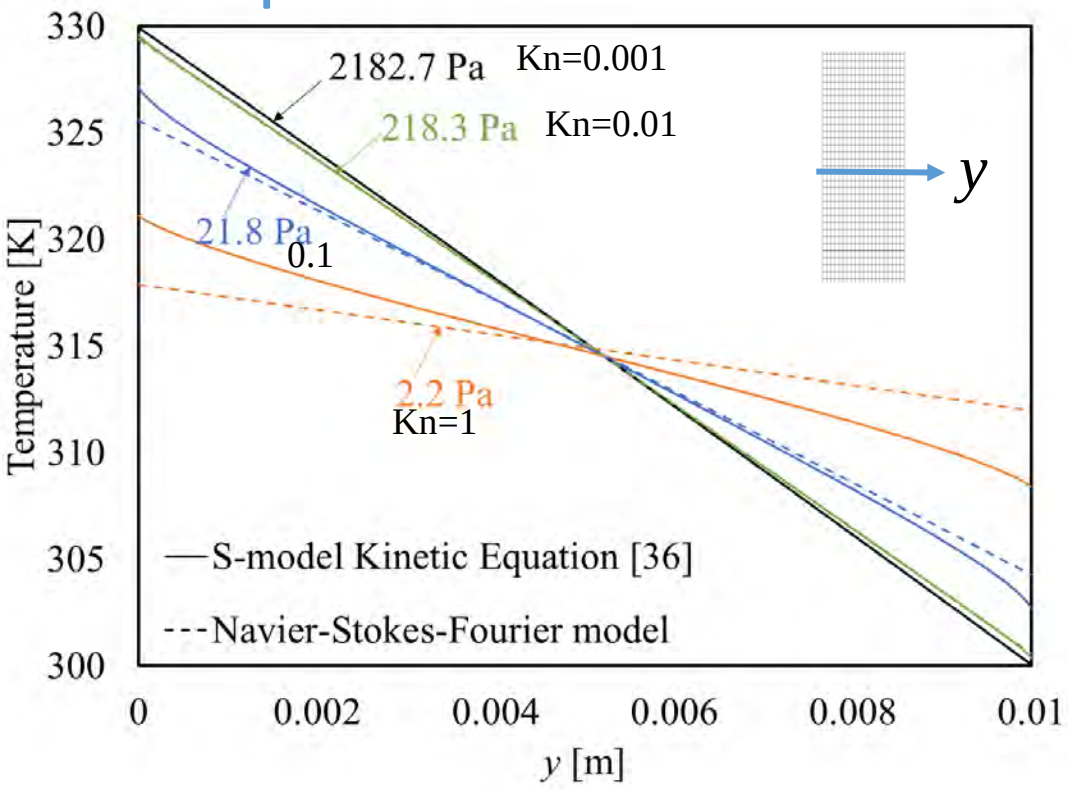



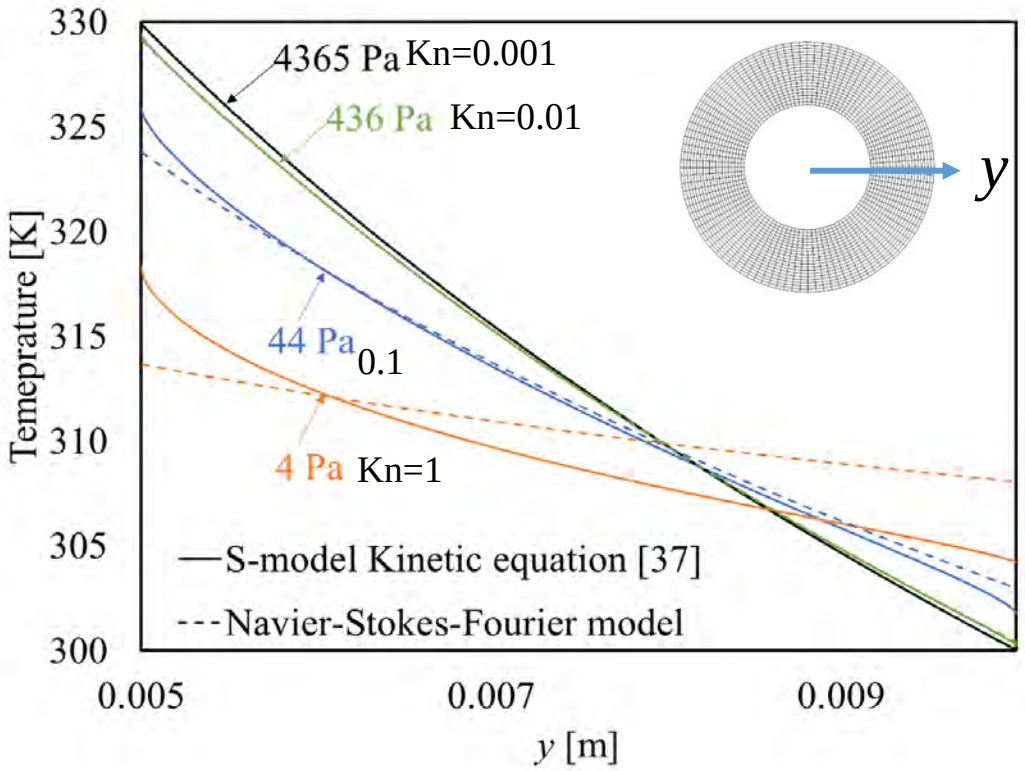

Resistance Model



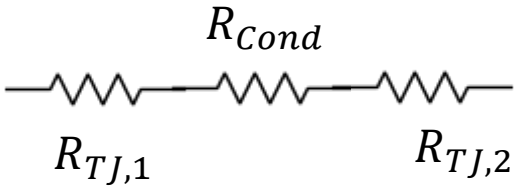

- Calculate conduction across helium-fill gaps between isothermal Parallel Plates and Concentric Cylinders with $\alpha$=1 using the Boltzmann equation.
  - In these "simple" geometries we (Ho and Graur from *Aix-Marseille*) use the Discrete Velocity (DV) method to find the temperature profiles and heat transfer from the Shakov model
- Compare to calculations using Fourier conduction within the gas and Lin-Willis temperatures jumps at walls

# Temperature Profiles for Different Pressures

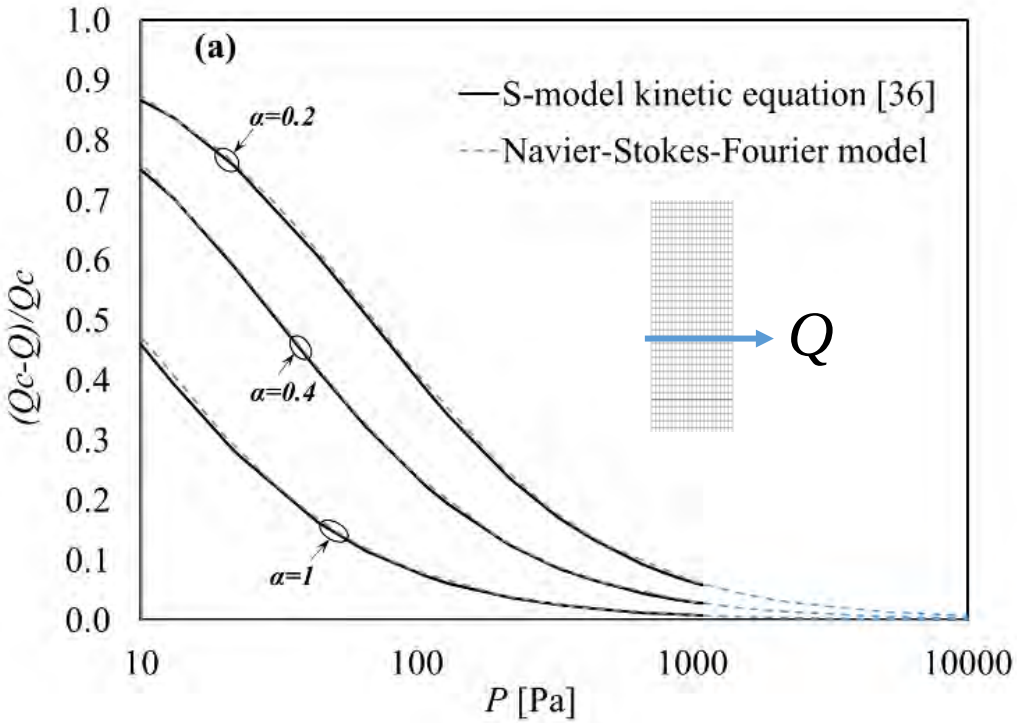


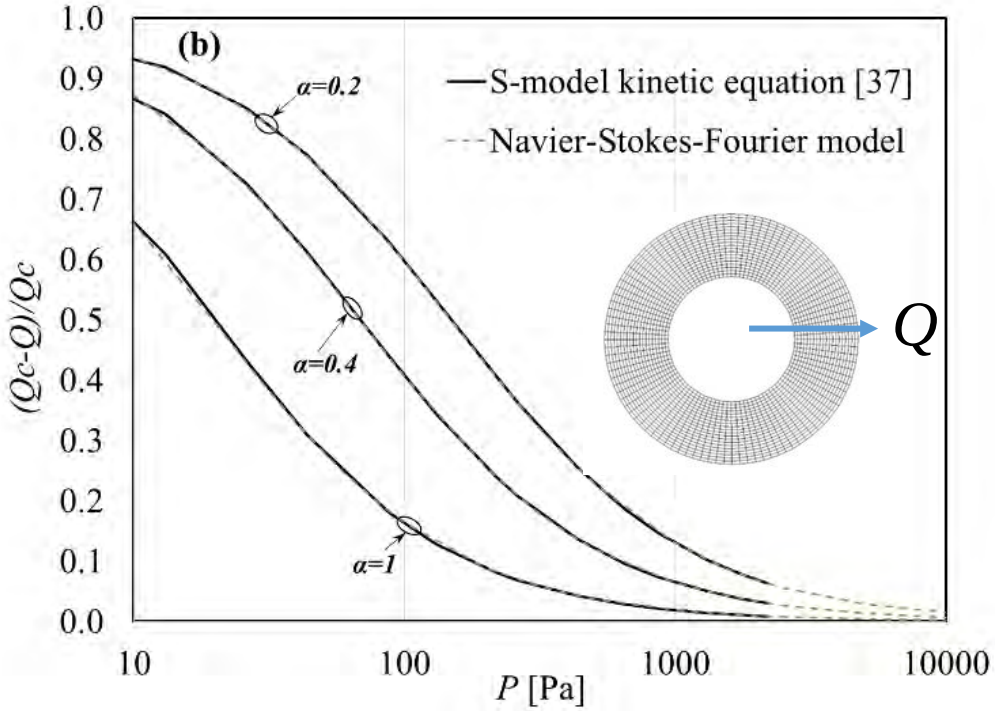




- Solid line are DV results using the Shakhov-method (S-method)
  - At low pressures observed Temperature Jumps at both boundaries
- Dashed lines are from Fourier Equation solution with the Lin-Willis temperature jumps
- Good agreement for Kn < 0.1 (slip and continuum regimes)



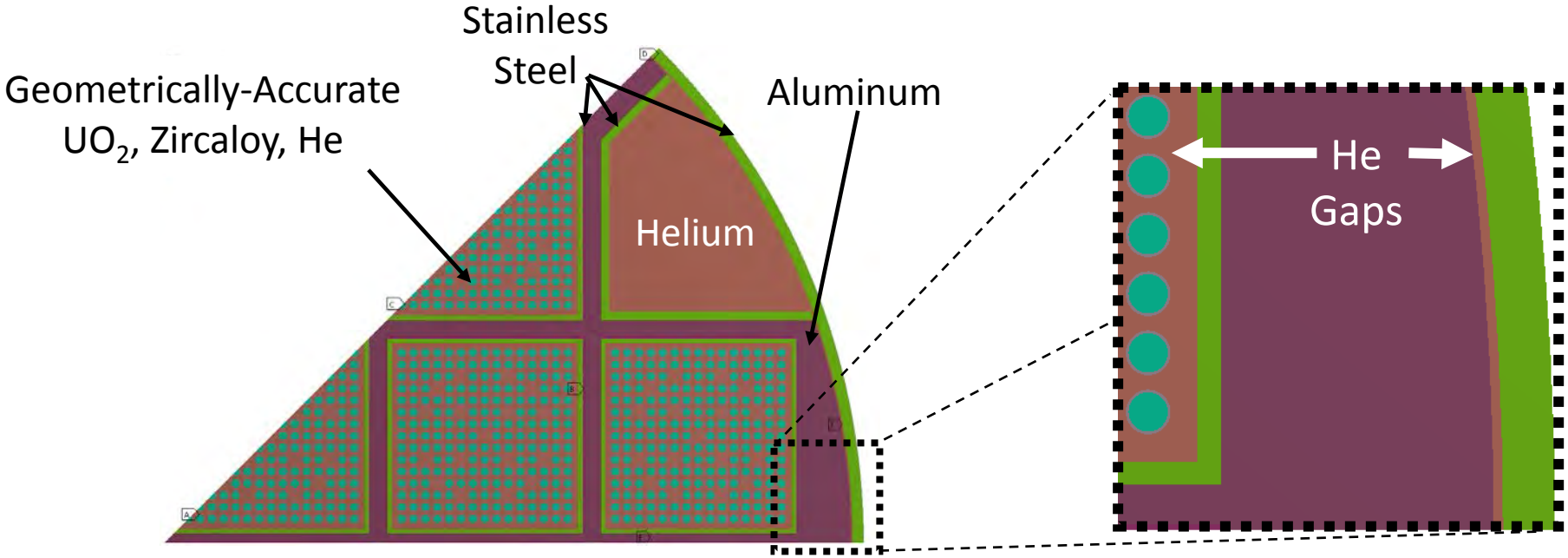
# Fractional Heat Transfer Reduction




- $Q_C$ = heat transfer from the hot to cold wall for continuum conduction
- Q = heat transfer for a given pressure and accommodation coefficient
  - Decreases as P and $\alpha$ decrease
- Lin-Willis model (dash lines) accurately reproduces the Shakov-model-calculated rarefied conduction (solid lines) versus pressure in helium for $\alpha$ = 0.2 to 1 and two simple gap geometries
- Implement the Lin-Willis thermal resistance in the CFD transfer canister model

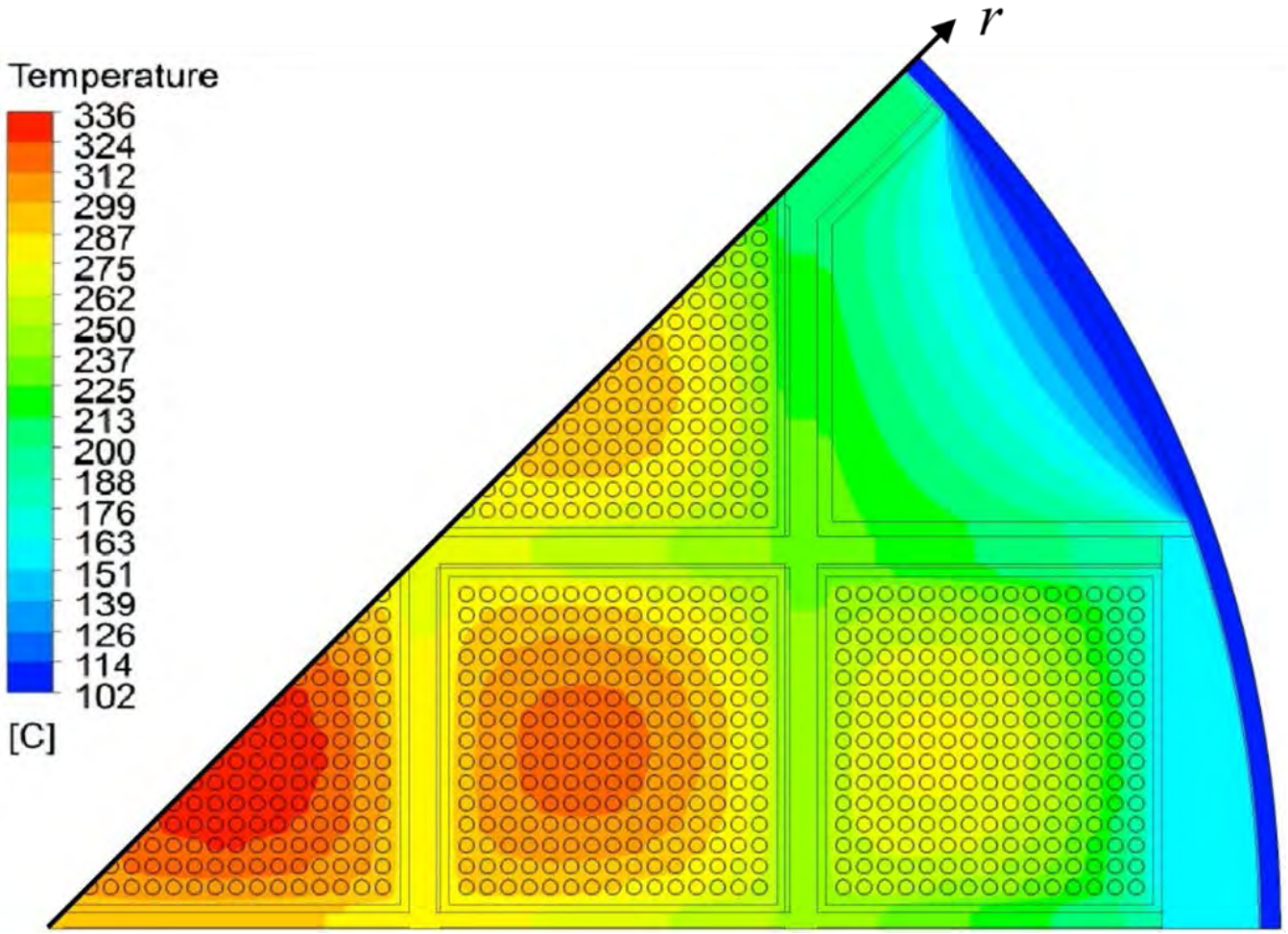
# Loaded 24 PWR Canister Model




- ANSYS/Fluent One-eighth Model of a TN24P
  - Symmetry on radial boundaries
  - 101.7°C on outer curved surface (conservatively simulates contact with boiling water)
  - Geometrically-accurate helium-filled regions in fuel and gap between basket and canister
- Heat Generation within the $UO_2$
  - Fourier Conduction within all solid regions
  - Surface-to-surface radiation across He-filled regions
- Lin-Willis temperature jump at gas solid interfaces $T_{Wall} - T_{Gas} = QR_{TJ}; R_{TJ} = \frac{\lambda \zeta_T}{A\kappa}$
  - $\lambda = \frac{T\mu_0}{P}\sqrt{\frac{2k_B}{mT_O}}; \zeta_T = \frac{\sqrt{\pi}\gamma}{(\gamma+1)Pr}\left(\frac{2-\alpha}{\alpha} + 0.17\right)$; Negligible at higher pressures

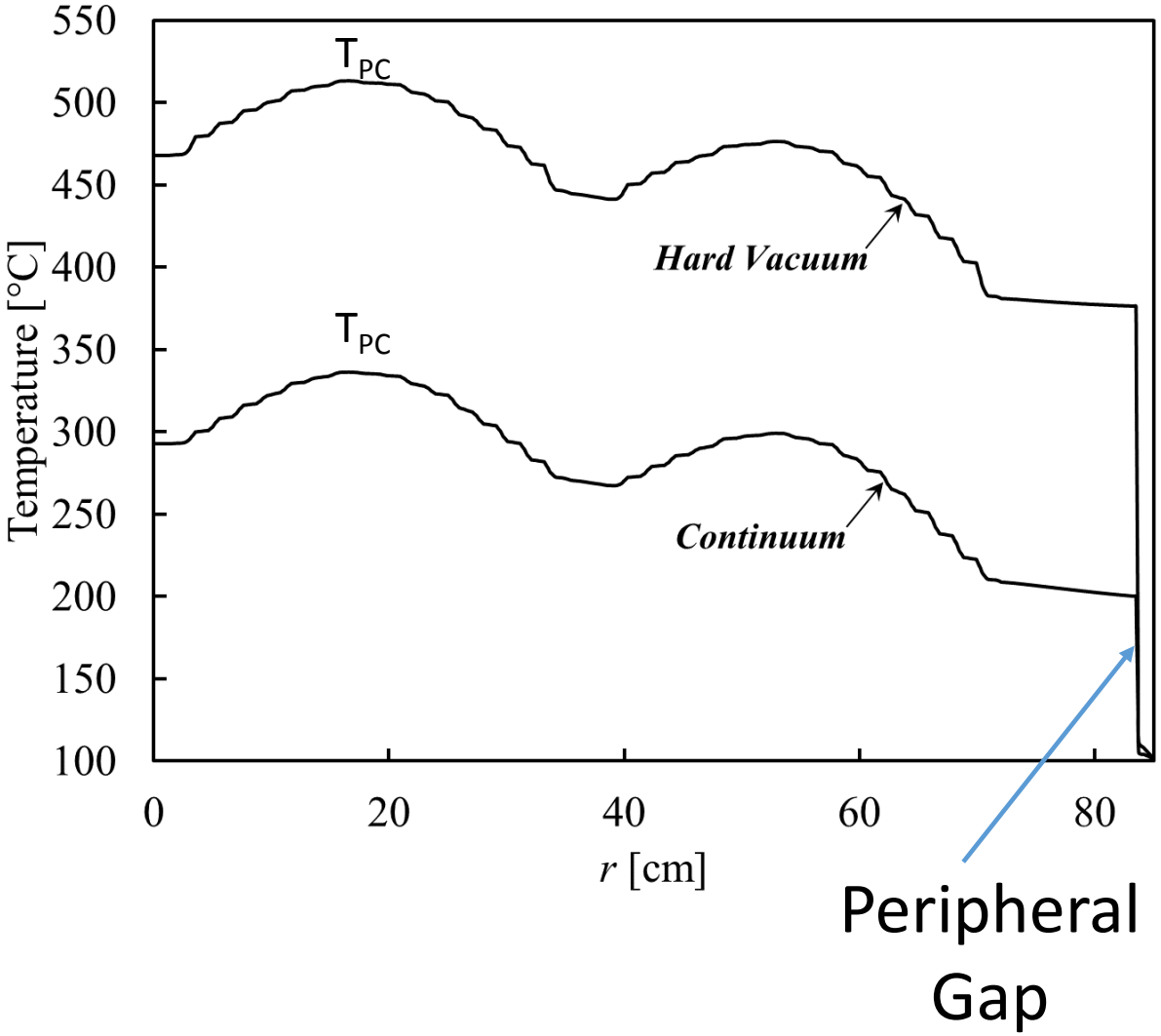
# Loaded Package Temperature Contours

- Atmospheric pressure
  - Continuum model
  - Neglect Natural Convection
  - $Q_F$ = 2290 W/assembly
- Local maxima in each assembly
- Hottest in centermost assembly
  - $T_{PC}$ = 336°C
  - Below 400°C even at this "high" heat generation rate
- r-axis
  - Traverses two assemblies, an aluminum rib and canister



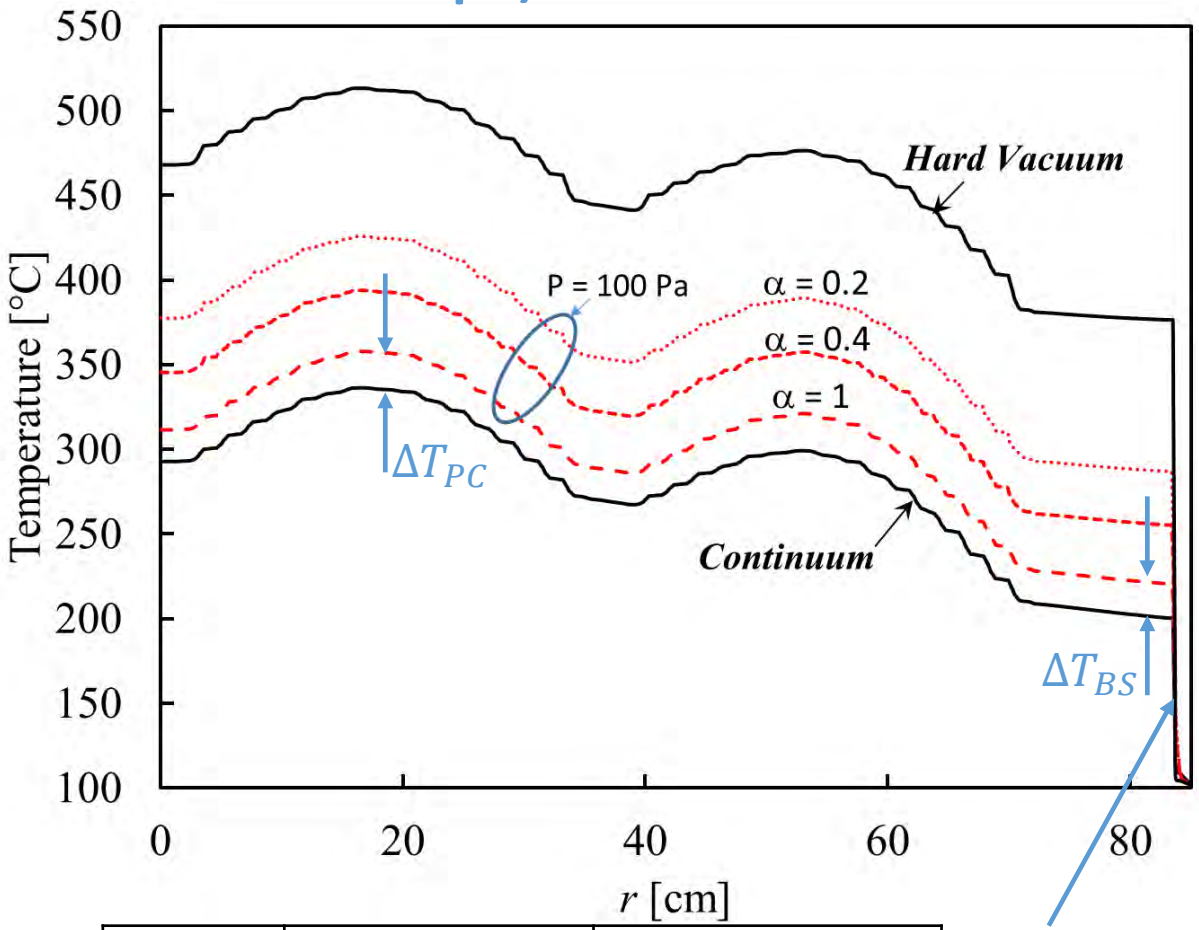
# r-axis Temperature Profiles

- Two Models
  - Continuum
  - Hard vacuum (no gas conduction)
    - Higher Peak Clad Temperature, $T_{PC}$
- Peripheral gap between basket rib and canister
  - Exhibits a very steep gradient due to
    - High heat flux
    - Low temperature (minimal radiation HT)
  - Major contribution to peak cladding temperature
  - This is the location where the main difference between continuum and hard vacuum profiles resides.
  - Radiation dominates in the high-temperature fuel regions (not dependent on gas conduction)



# Rarefied (Temperature Jump) Model

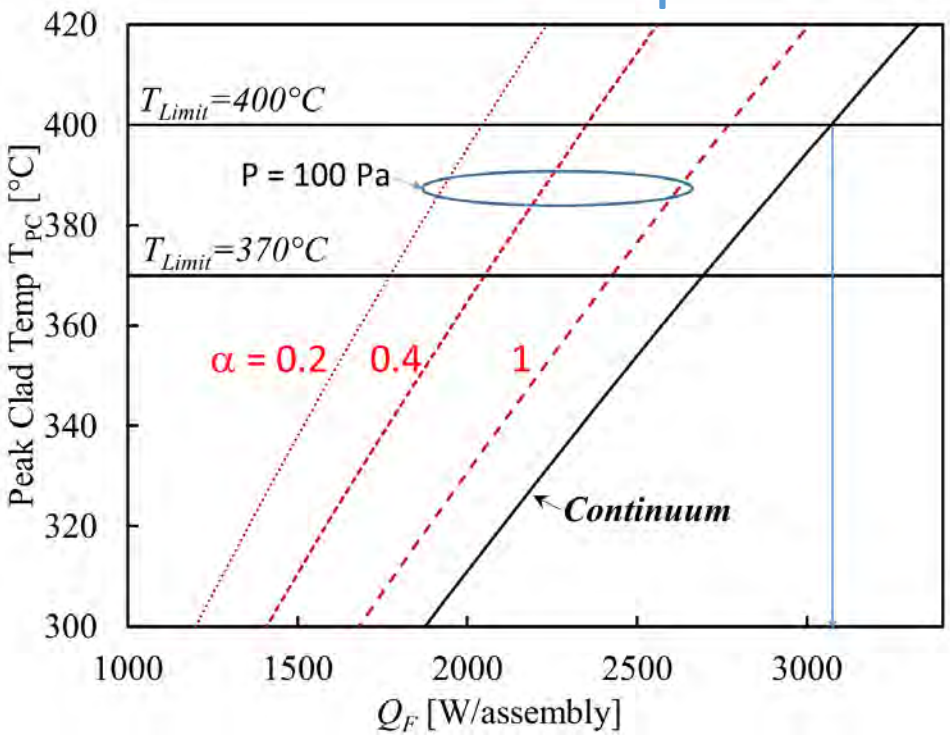
- Temperature-jump
  - *P*=100 Pa, *α =1, 0.4 & 0.2*
- $T_{PC}$ increases as α decrease
  - $\Delta T_{BS}$ = Temp. Diff at Basket Surface
  - $\Delta T_{PC}$ = Temp. Diff at Peak Clad
- The main difference between continuum and other profiles is in the peripheral gap
  - Heat flux from fuel rods is smaller
  - More radiation at fuel rods
- **To accurately determine peak clad temperatures, it is important to predict the effect of rarefication <u>within the peripheral gap</u>**
- **Hard vacuum model is overly conservative**




Peripheral Gap

| $\alpha$ | $\Delta T_{BS}$ [°C] | $\Delta T_{PC}$ [°C] |
|---|---|---|
| **1** | 20.2 | 21.5 |
| **0.4** | 55.0 | 57.7 |
| **0.2** | 86.7 | 89.5 |

# Peak Clad Temperature versus Assemble Heat Generation



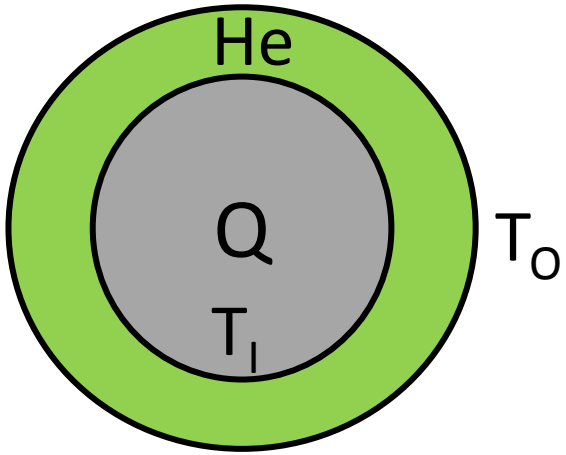

| | Continuum | P = 100 Pa | | |
|---|---|---|---|---|
| | $P = 10^5$ Pa | α=1 | α=0.4 | α=0.2 |
| Assembly Heat Generation Limit [W] | 3070 | 2769 | 2351 | 2043 |
| % reduced | --- | 10% | 23% | 33% |

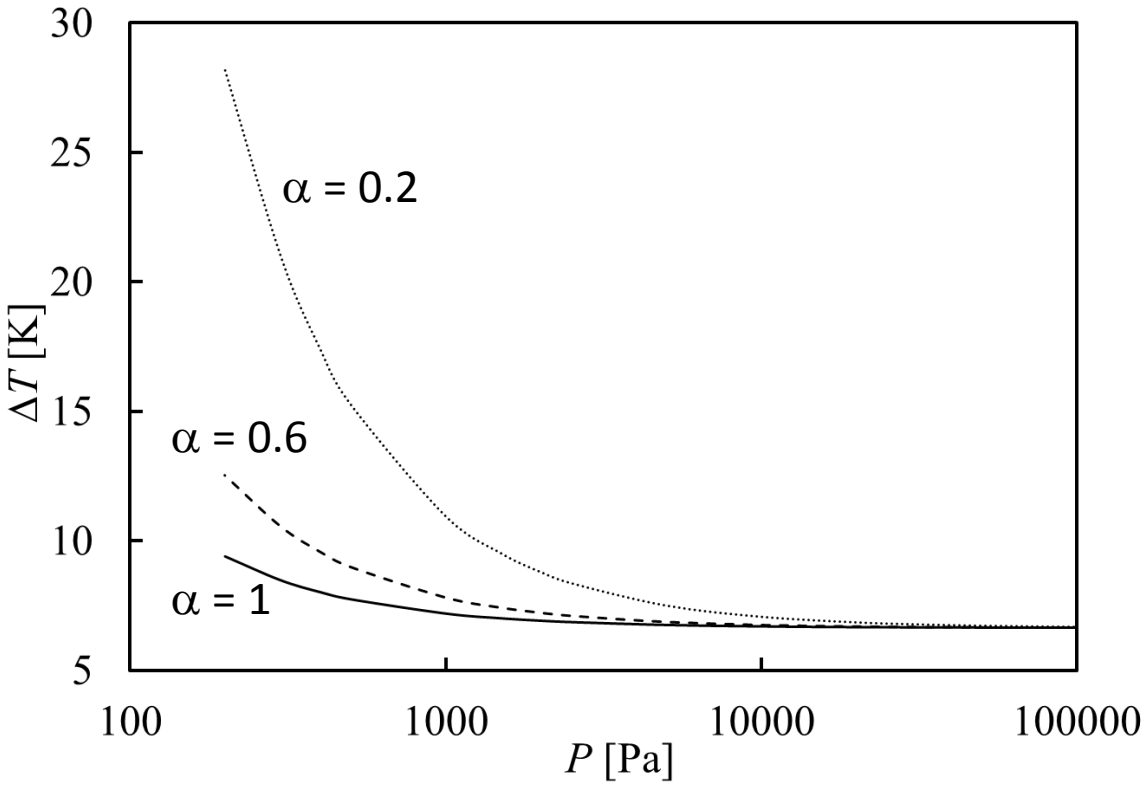
- Peak cladding temperature $T_{PC}$ increases as assembly heat generation rate increases
  - The assembly heat generation limit causes $T_{PC}$ to reach its limit (i.e. 400°C)
- Cladding temperatures increase, and the allowable heat generation rate decreases, as α (and pressure) decrease
  - By up to 33% compared to continuum conditions (for P = 100 Pa and α = 0.2)
- The limit temperature may be dependent on fuel burnup level
  - If the temperature limit is decreased by 30°C, then the limit heat generation rates decrease by another 13%

# Summary

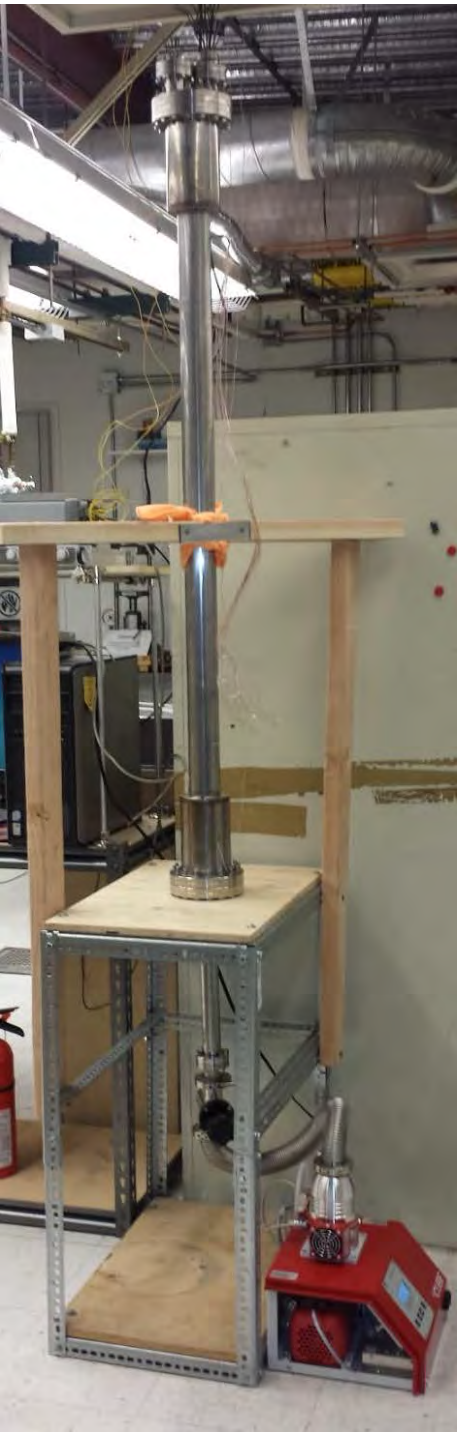
- To accurately determine peak clad temperatures, it is important to predict the effect of rarefication within the peripheral gap
- The hard vacuum model is overly conservative
- Depending on the drying pressure P, gas thermal accommodation coefficient $\alpha$, and limit temperature $T_L$ rarefication <u>can</u> affect
  - Cladding temperatures
  - The allowed assembly heat generation limit, and
  - The required underwater aging time
- Ongoing Work
  - Three-dimensional package model to accurately calculate
    - Temperature and vapor transport during
    - Vacuum Drying and Force Helium Dehydration (mixed forced and natural convection)
  - Measure thermal accommodation coefficients $\alpha$ for a He/stainless steel system.

# Thermal Accommodation Coefficient Measurement

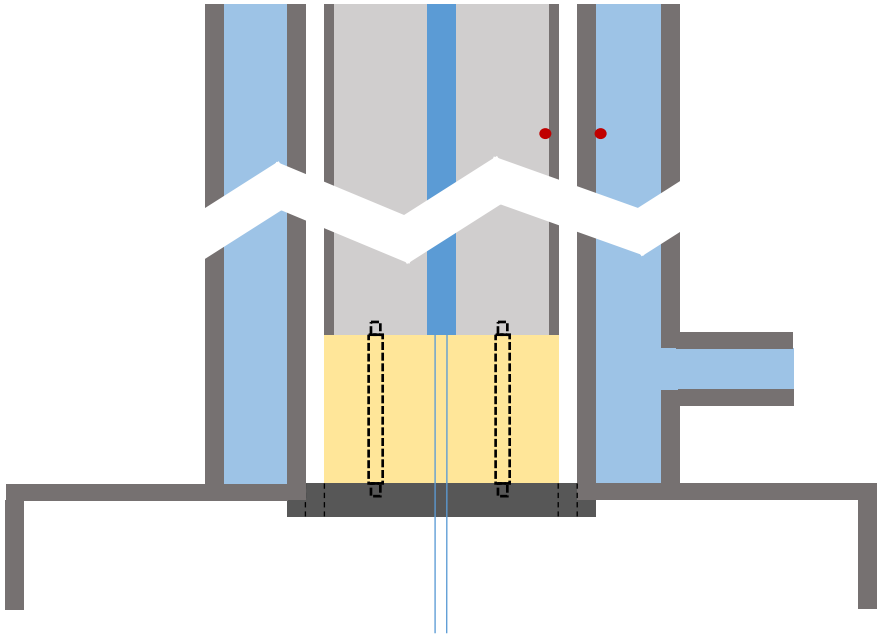


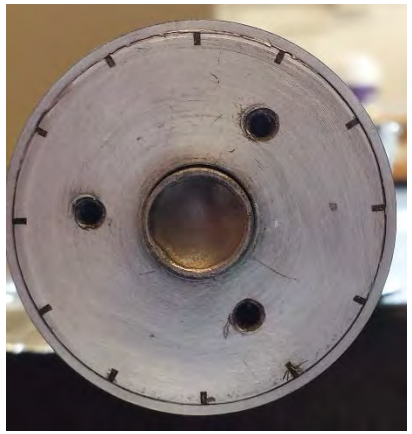




- Measure conduction heat transfer across an annular gap containing rarefied helium
- Control total heat generation rate dissipated by the inner cylinder Q (internal heater), the temperature of the outer cylinder $T_O$ (water jacket), and the helium gas pressure P (high purity dry He, vacuum pump).
- Measure the temperature of the inner cylinder $T_I$ for a range of gas pressures P
- Compare to predicted $T_I$ versus P results for a range of $\alpha$.

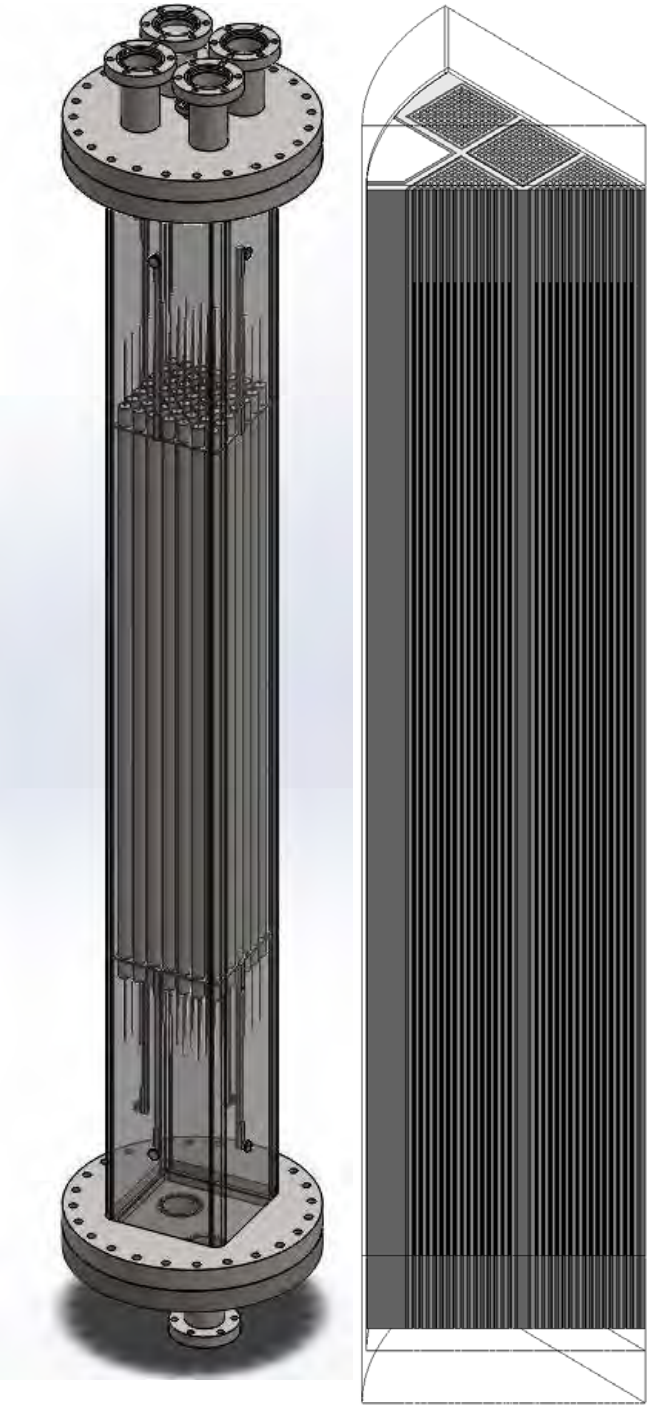


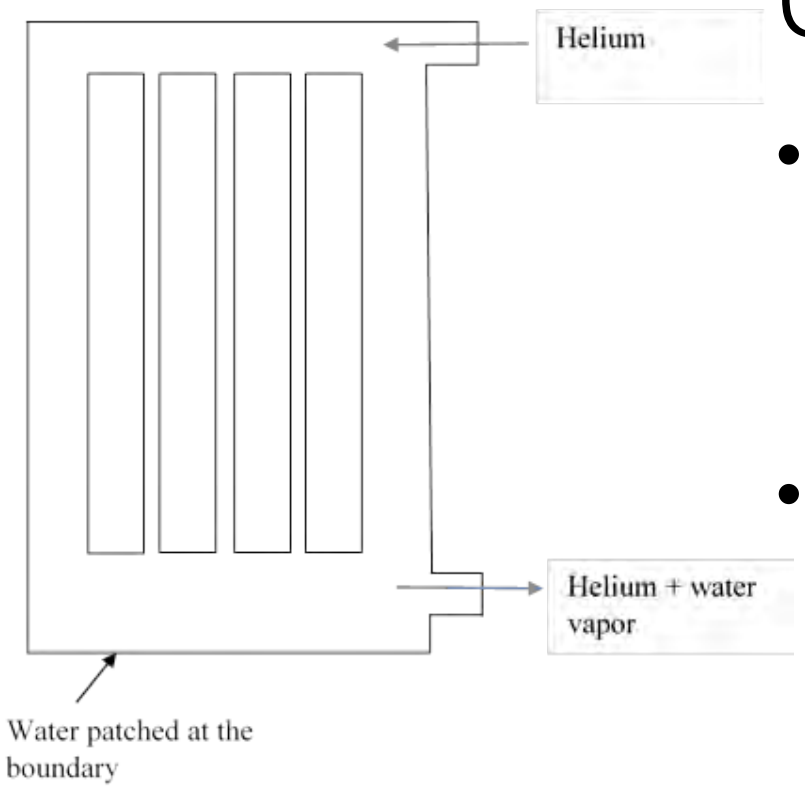
# Experiment Design





- To maximize the effect of rarefication on the inner cylinder temperature, minimize
  - Gap width (minimize conduction temperature difference relative to surface temperature jump, 1mm)
  - Outer surface temperature (to minimize radiation relative to conduction heat transfer)
  - End losses
    - Minimize inner cylinder diameter to length ratio
    - Insulate cylinder ends, minimize contact to outer shell
- Inner aluminum cylinder, surface thermocouples, centered electric heater, sheathed in 1-mm-thick stainless steel
- Vertical, sealed, water-jacketed enclosure, power and TC feedthroughs (data soon)






# Ongoing Work

- Enclosed 7x7 Square Array Experiment Design
  - Verify simulations for “complex” configuration
- Three-dimensional canister simulations for
  - Vacuum Drying
  - Force helium dehydration (mixed natural/forced convection)
- Vapor Transport
- Helium/Water vapor transport
  - Continuum and rarefied conditions

An UDF is used at the interface between water and helium for free surface evaporation and boiling. A layer of 2 cm of water is assumed to be present at the bottom of the canister in the beginning of the simulation. At t=0s the evaporation and the helium circulation is started, so no vapor at the beginning of the simulation.

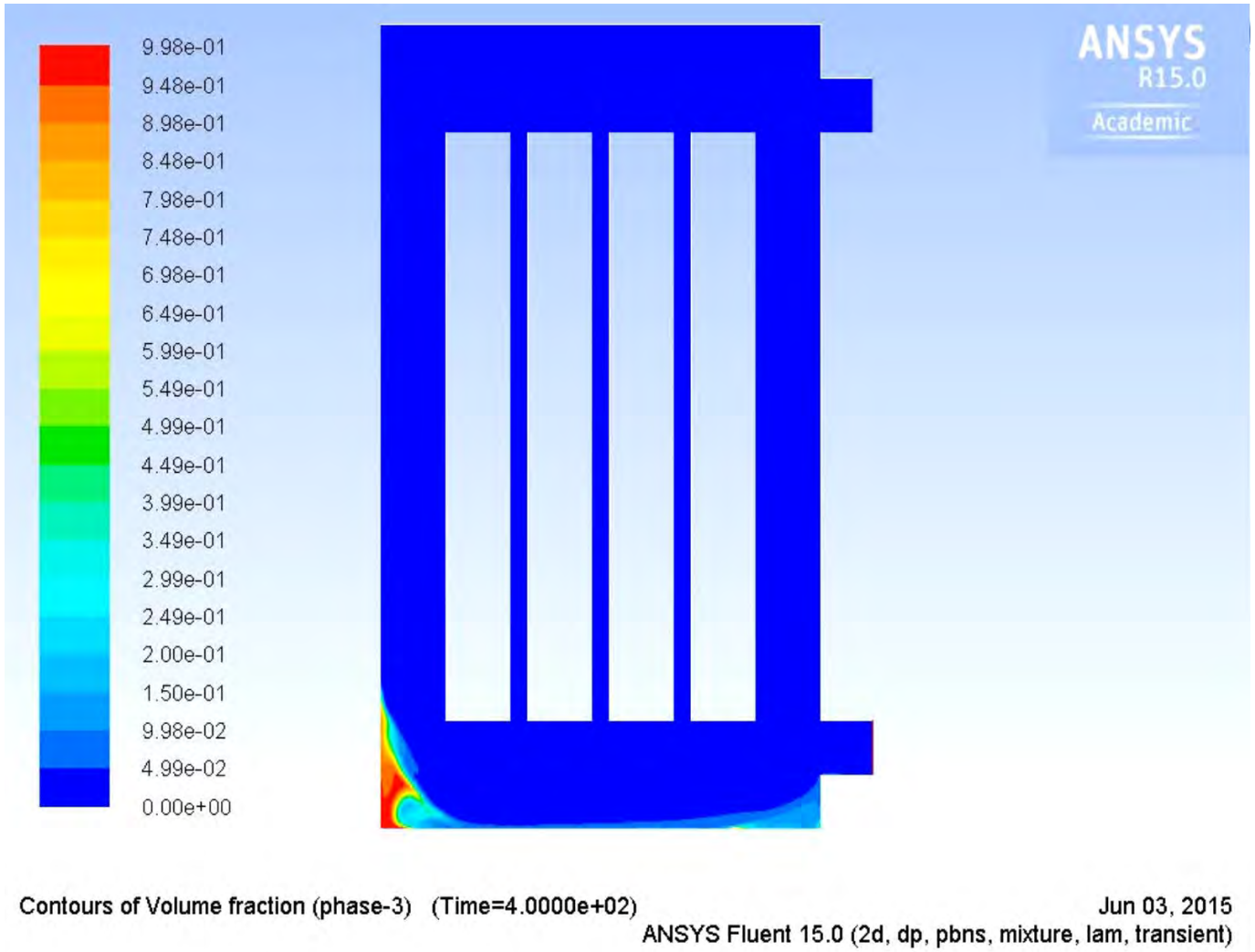



Fig. Contour of volume fraction of water vapor.

# Questions?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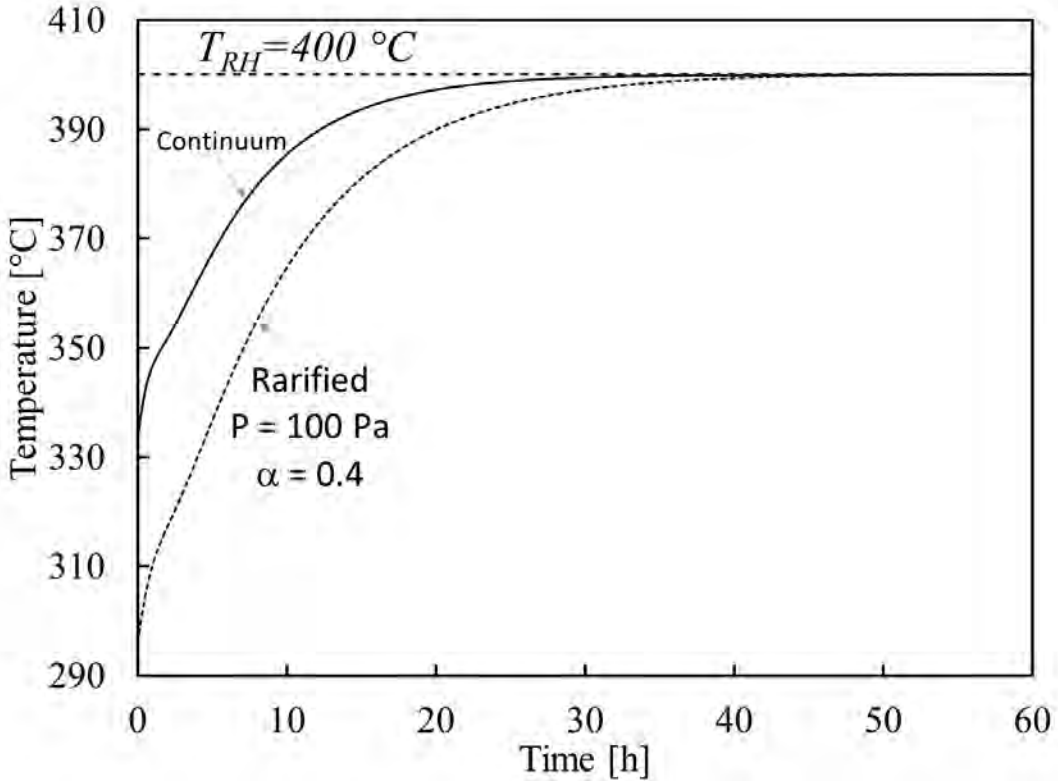
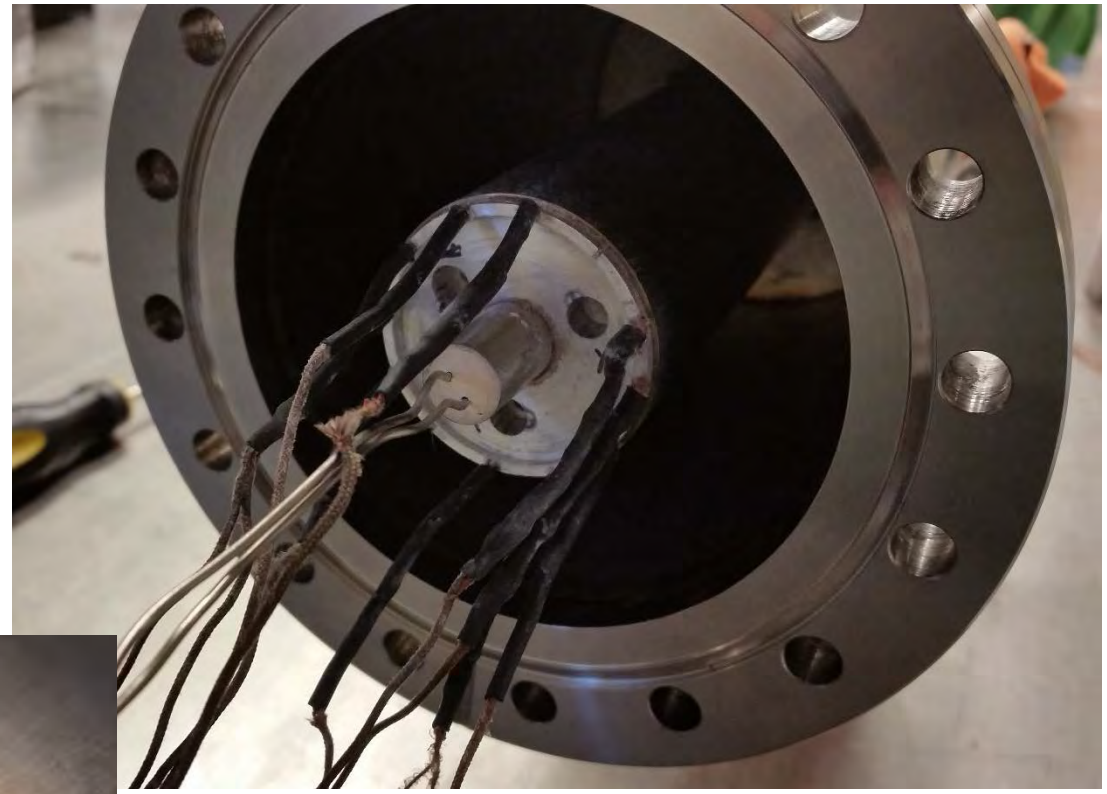
# Transient Simulations




- How long will it take the canister to reach steady state conditions
  - Initially assumed canister is filled with water and allowable fuel heat generation rate
  - Requires 24 to 35 hours to be within 2°C of steady state value