

# Flow Calorimetry Modeling With Heat Transfer Module

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**Introduction:** Our research group is conducting calorimetry of a metal hydride chemisorption reaction at high-temperature reaction conditions. The mass flow calorimetry setup used for this experiment measures heat output by determining the temperature gradient of water flowing around a heated (100W input) reaction chamber. The amount of energy released by the reaction can be calculated with the heat capacity of water and the flow rate. To increase accuracy of the measurement, heat losses not going to the flowing water must be minimized. Using the non-isothermal flow feature of the Heat Transfer Module, we modeled the heat-loss of our reaction vessel for insight on how to best thermally insulate our reaction chamber.

**Computational Methods:** The non-isothermal flow tool uses both the heat flow equation as well as laminar flow equations. Our model is 2D-axisymmetric and the geometry is shown in Figure 1:

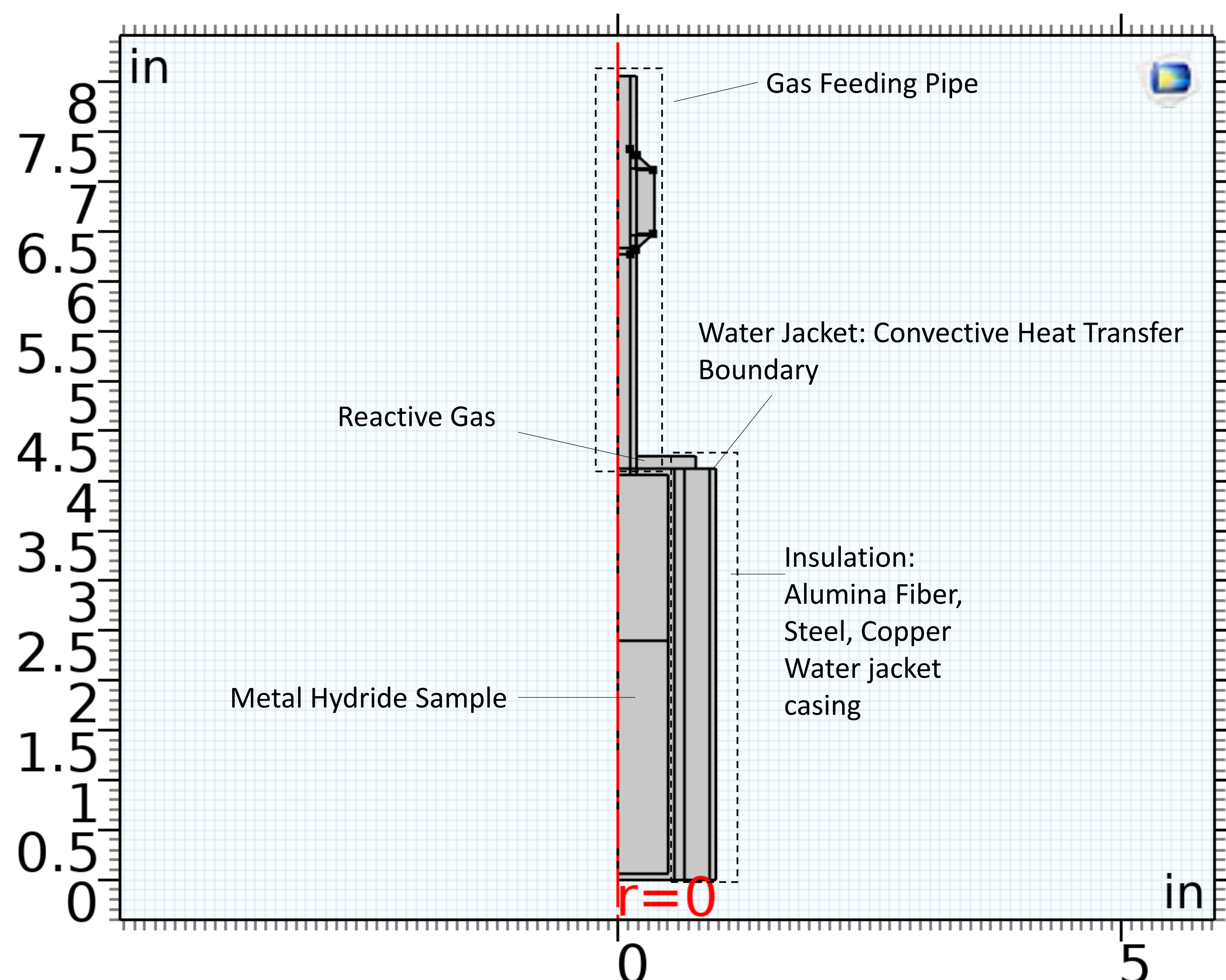


Figure 1: Geometry of mass flow calorimetry system

The boundary conditions were set as such:

1. 100W constant heat input
2. water jacket convective heat flow condition
3. gas convection out of the gas feeding pipe: outflow and outlet condition
4. surface-to-ambient radiation condition on outside surfaces

**Results:** We found that heat flux leaving the reaction chamber system was mostly due to conduction through the gas feeding tube. The resulting temperature distribution is shown in Figure 2.

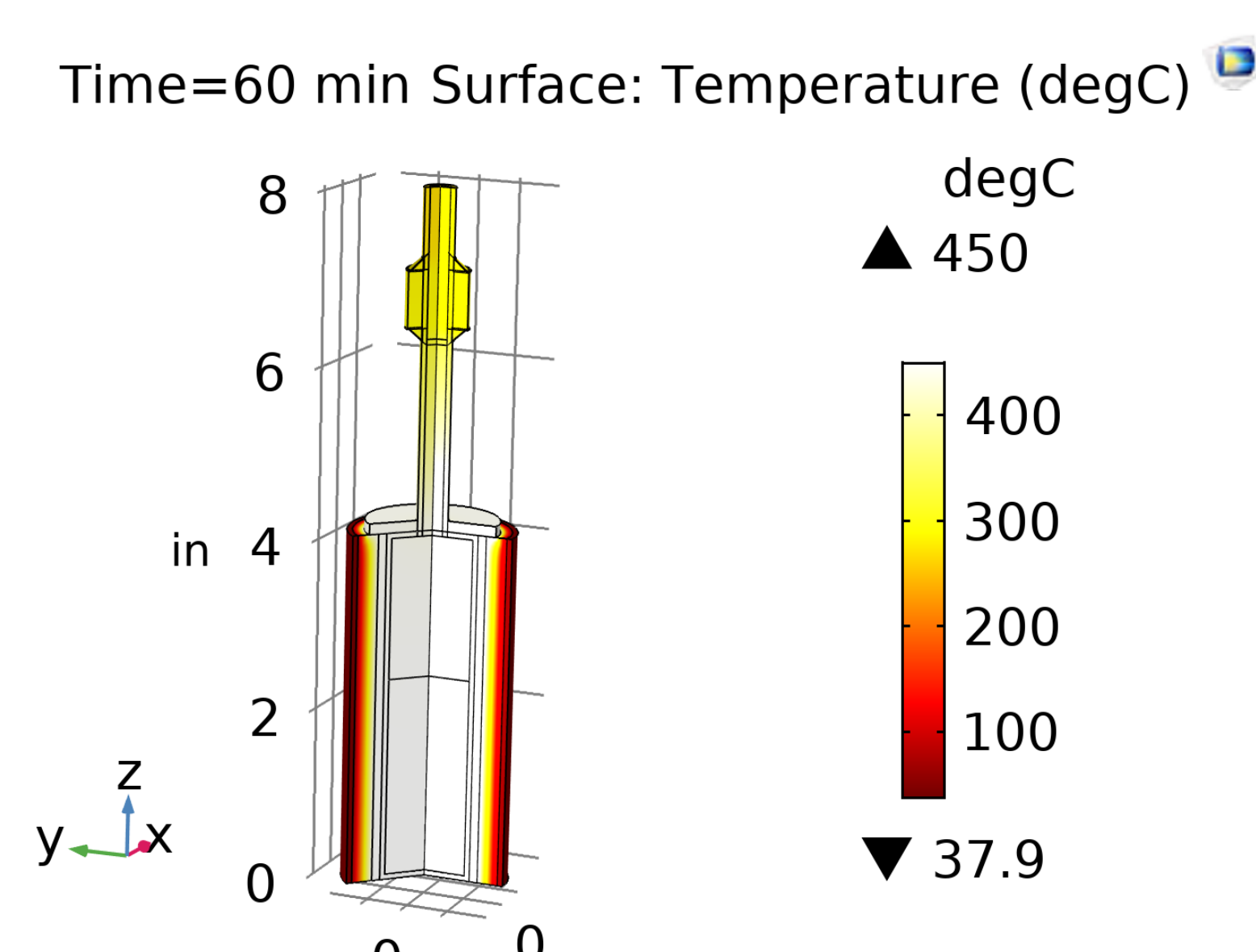


Figure 2: Resulting temperature gradient

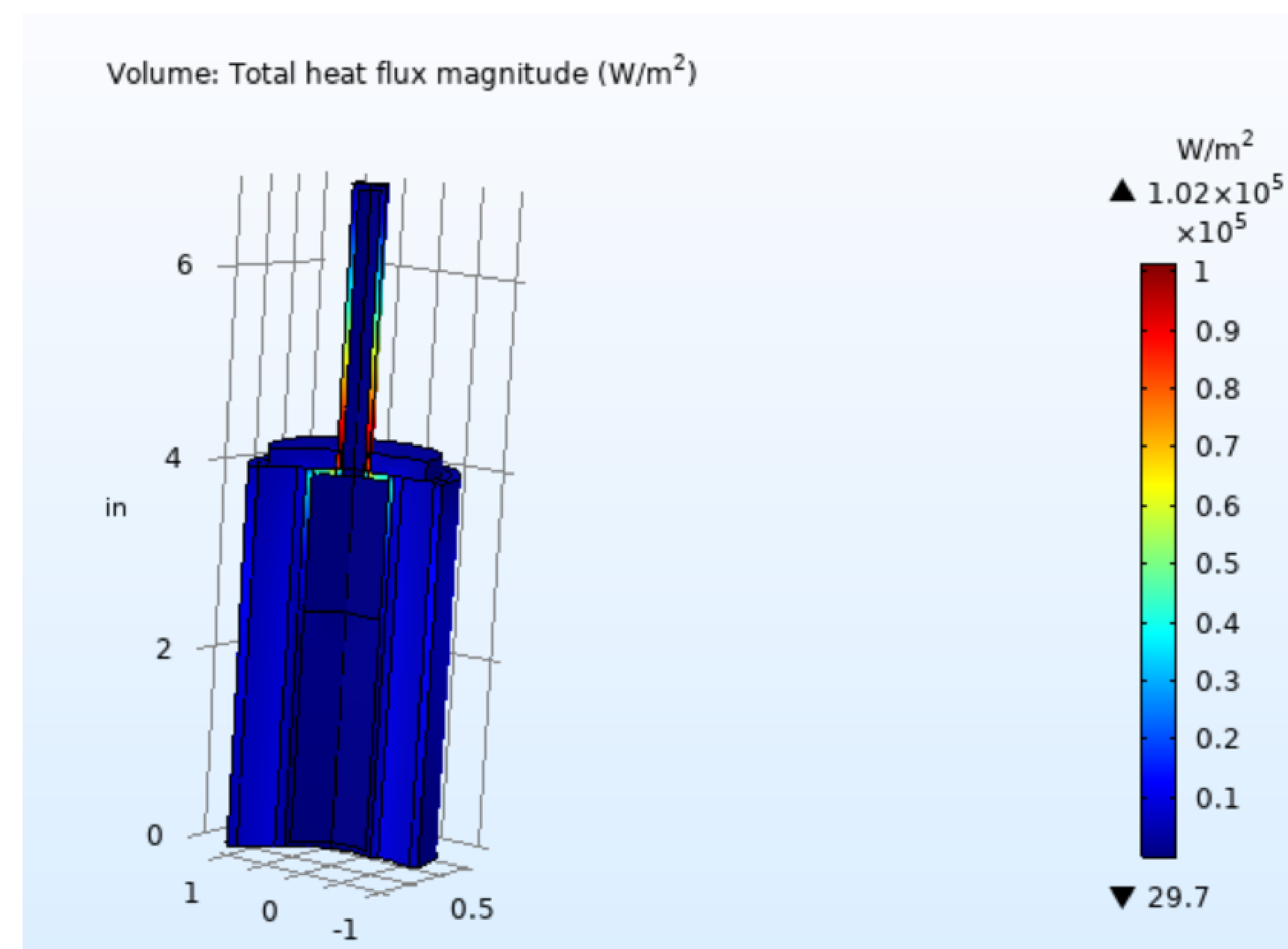


Figure 3: Heat flux gradient

To find quantitative power loss values, we integrated the heat flux shown in Figure 3 and 4 over the entire top portion of the reaction chamber, giving us power values.

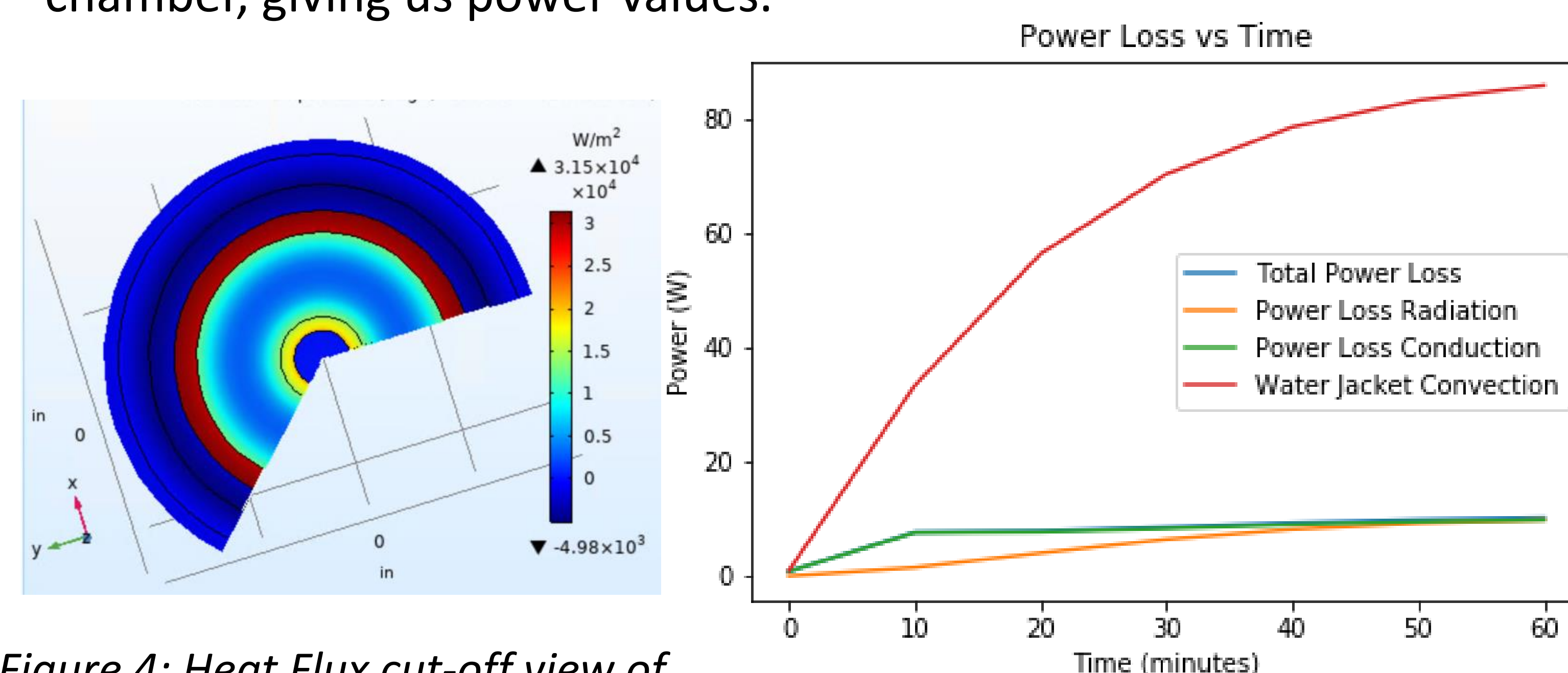


Figure 4: Heat Flux cut-off view of top flange

Figure 5: Power loss versus time in 1-hour interval

As seen in Figure 5, we see that the water jacket will convect 85W of power out of the system at  $t = 60$  minutes, with 10W of loss being from conduction through the gas feeding tube. The last 5W is due to radiation and convection.

**Conclusions:** According to this COMSOL model, the most significant source of heat loss and reduced accuracy in measurement was due to conductive losses through the gas feeding tube. We found that power loss due to surface-to-ambient radiation as well as convection of the reactive gas through the gas feeding tube was insignificant compared to conduction. Using this information, we can potentially reduce power loss by using a material for the gas feeding tube with a lower thermal conductivity, such as manganese. We can also use an insulating ceramic break made of Zirconia to slow down heat loss.