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Prediction of The TREAT Facility Power and Temperature of Sirius-2c Nuclear Propulsion Fuel Experiment

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ABSTRACT

This paper presents simulation results of the Sirius-2c full power experiment that was performed at the TREAT facility to support experiment modeling and transient analysis of the NASA-sponsored Sirius series of experiments for nuclear thermal propulsion applications. We presents a novel approach to predict the control rod motion and power of the reactor and the temperature of the specimen during transient experiments using the Griffin and Bison packages of the Multiphysics Object Oriented Simulation Environment (MOOSE). First, the model predicts the transient rod motion that results in the desired reactor power shape. Then, the temperature of the specimen is predicted based on the power deposited in the specimen. The prediction results are in good agreement with the measured reactor power and control rod position and over-predicted the specimen temperature which is mainly related to specimen surface emissivities. The reactor reaches a peak power of 80 MW and a specimen temperature of 2500 K and considering the right specimen emissivities the predicted temperature is in an excellent agreement with the measured values. This model can be utilized in helping and supporting the design and optimization a new experiments that are going to be irradiated in the TREAT facility.

Keywords: Predictive Model, TREAT, NTP, Sirius

1. INTRODUCTION

The National Aeronautics and Space Administration (NASA) is collaborating with Idaho National Laboratory (INL) to design experiments and test nuclear materials for nuclear thermal propulsion (NTP) applications at the Transient Reactor Test Facility (TREAT). The current series of experiment is named the SIRIUS experiments. The SIRIUS experiments aim to test candidates for NTP fuel at prototypical NTP conditions including rapid power and temperature ramps, hot fuel temperatures for significant periods of time, and intense radiation fields. TREAT's capability for executing shaped transients (i.e., transients with tailored control rod motion) allows to test nuclear fuel samples under the aforementioned conditions [1, 2].

Shaped transients are distinguished from natural and clipped natural transients. In natural transients, the transient control rods are withdrawn at the beginning of the transient and then remain stationary until potentially inserted when power clipping is desired. In contrast, shaped transients use control rod motion throughout the transient to shape the power with the goal of accomplishing desired sample power and temperature ramps. Shaped transients give NTP designers more flexibility to examine the performance of the fuel specimen performance near operational conditions. The design of shaped transient experiments is supported by modeling and simulation (M&S) at INL prior to execution of experiments. The goal of M&S

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in this case is to determine the control rod motion as a function of time that leads to a desired power and temperature profile experienced by the specimen.

The Multiphysics Object Oriented Simulation Environment (MOOSE) [3] is utilized to perform neutronics and thermal analysis of the shaped transient experiments at TREAT. The analysis includes predicting the reactor power, control rod motion, and specimen temperature as a function of time. The tools within MOOSE used for the analysis of the SIRIUS experiments are the fuel performance code BISON [4], the neutronics analysis tool Griffin [5], and sensitivity analysis using the stochastic tools module of the MOOSE framework [6]. Recently performed analysis includes the SIRIUS-1(calibration) [7], Sirius-1, and Sirius-3 experiments [8]

The ultimate objective of this work is to develop a multiphysics model that will be able to predict control rod movements to achieve desired time-dependent conditions in the fuel specimen. To this end, the multiphysics model needs to be able to predict reactor power from control rod motion, specimen power from reactor power, and experiment temperature from experiment power. A predictive transient model of the TREAT facility has been developed to provide a prediction the axial control rod movement to achieve a demanded power shape [9, 10]. This paper presents the developed predictive transient model of the TREAT facility and its application to Sirius-2c full power experiment.

2. METHODS & MODELING APPROACH

2.1. Sirius-2c Model

The Sirius-2c fuel element specimen is a cylindrical fuel element made of ceramic fuel in a ceramic matrix (CERCER). The ceramic fuel is uranium nitride (UN) and the matrix material is zirconium carbide (ZrC). The composition of the CERCER fuel is given in Table I. The specimen is positioned within a molybdenum flask, with three tungsten rods positioned within the flask. Springs wrap around the tungsten rods that position two tungsten hold-down rings that sandwich the a small cylindrical specimen.

Table I. Table of pellet composition.,

Parameter	Value
Density $[g/cm^3]$	8.048
UN $[wt\%]$	65.257
ZrC $[wt\%]$	34.873
^{235}U Enrichment $[wt\%]$	19.92

The Sirius-2c thermal model is depicted in Fig. 1. It includes: the fuel element specimen, the hold-down rings, the tungsten hold-down rods, the molybdenum flask, the zirconia liner and the capsule are all modeled. A number of simplifications were made to the model:

- omitting the molybdenum flask studs,
- simplification of the hold-down ring geometry by removing the irregular interior opening and adding several circular holes that conserve surface area and material volume,
- replacing the pips that are inserted into three coolant channels in the specimen with cylinders that are in contact with the specimen at the top and bottom portions of the coolant channels,
- omitting the springs around the tungsten rods that hold the specimen and hold down rings in place,
- assuming the inner flask surface to be a smooth cylinder.

The dimensions and material density for the various elements used in to model Sirius-2c experiment are given in Table II. The thermal properties for uranium nitride, tungsten, zirconia, and titanium are taken

from reference [11] and thermal properties of zirconium carbide are taken from reference [12]. The thermal properties for molybdenum are taken from reference [13]. All of the material thermal properties are dependant on the material temperature, and the expressions to calculate the thermal properties are provided in the cited references. A static gas of 97% argon and 3% hydrogen by volume as detailed in [14] surrounds the fuel specimen, the top and bottom hold down rings, the tungsten rods, the interior and exterior of the flask and zirconia liner. The properties of the gas are obtained from reference [15].

Table II. Table of components and dimensions.

Component	Inner Diameter [cm]	Outer Diameter [cm]	Height [cm]	Material	Density $[g/cm^3]$
Specimen	0.312	1.288	1.27	UN-ZrC	8.048
Flask	2.858	3.683	6.75	Molybdenum	10.22
Liner	3.81	4.445	6.76	Zirconia	5.638
Capsule	4.691	5.963	6.76	Titanium	4.5
Hold-Down Rods	-	0.3175	6.76	Tungsten	19.254
Hold Down Ring	0.3124	2.54	0.16	Tungsten	19.254

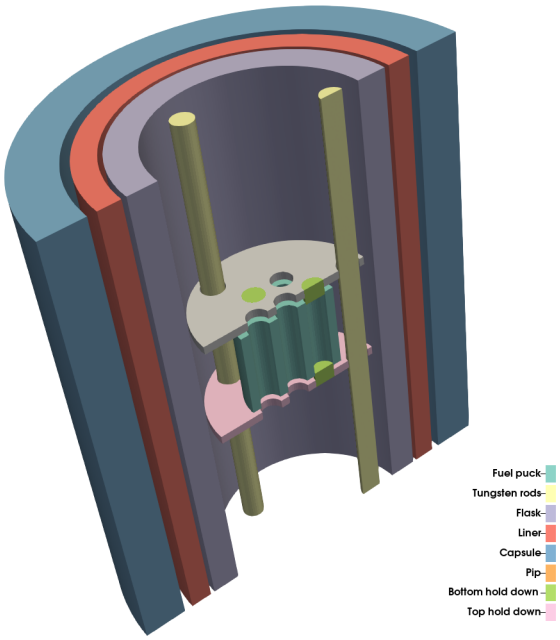

Figure 1. Depiction of the current Sirius-2c model for thermal analysis

In the thermal model, the heat conduction in all solid parts of the domain was considered including the heat conduction in the gas. Also, radiation heat transfer between the specimen, hold down rings, tungsten rods, and flask is modeled using the net radiation heat transfer method as described in Ref. [16]. The reactor temperature is imposed as a time dependent Dirichlet boundary condition on the outside of the capsule with temperature values supplied by the adiabatic core temperature model. The natural convection in the capsule was not directly modeled even though it might be as large or larger than thermal conduction through the cover gas. Therefore, the gas thermal conductivity was adjusted to twice its value for the baseline calculations. However it is expected for the radiation heat transfer to play the major role for high power experiments. The fission power density in the specimen P_{sp} is assumed to be uniform and it is determined using the

reactor power and the power coupling factors [17]. The power coupling factors are computed using Serpent steady-state eigenvalue calculations. The specimen power can be computed using the following relation:

$$P_{\text{sp}} = \rho_{\text{sp}} C_f(T_r, z_t) P_r \times 10^3, \tag{1}$$

where ρ_{sp} is the specimen density, $C_f(T_r, z_t)$ is the coupling factor as a function of core temperature T_r and control rod position z_t, P_r is core power and 10^3 is a conversion factor to ensure P_{sp} is in SI units.

2.2. Analysis Methodology

The Sirius-2c analysis is performed using a predictive transient model of TREAT that combines several constituent models to provide the power and temperature predictions. The model consists of three main parts: (1) data generation model, (2) predictive transient model, and (3) temperature predictive model. A schematic diagram of the calculation workflow and exchanged parameters of the coupled predictive models are shown in Figure 2.

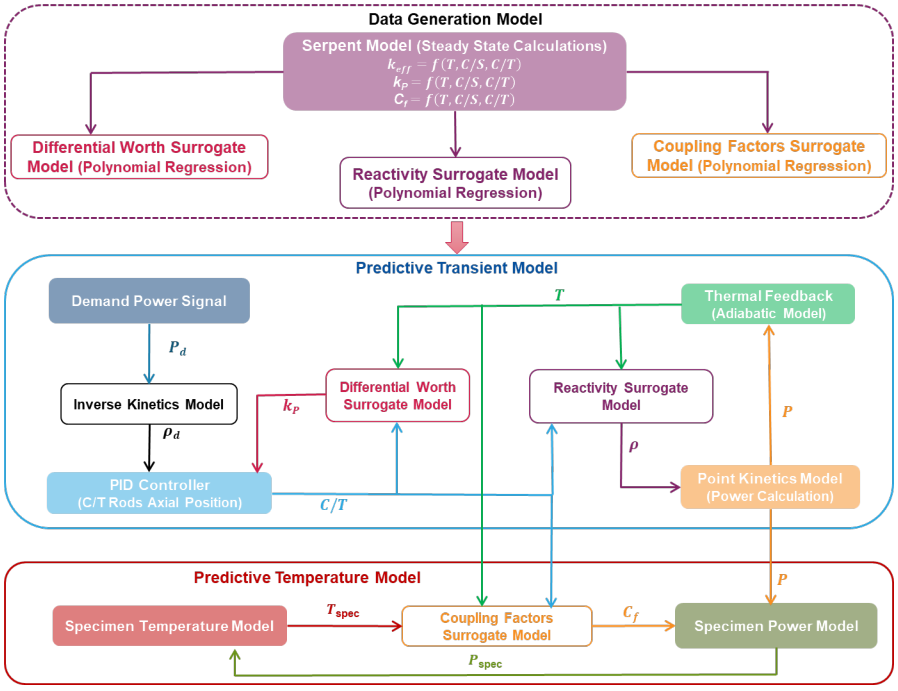

Figure 2. Predictive transient model of the TREAT facility.

The predictive power model can be executed in *forward* and *inverse* mode. The forward mode computes the power as a function of time given the control rod motion as a function of time. The inverse mode computes the control rod motion as a function of time given a desired power as a function of time. The forward model has been developed before the inverse model and is explained in detail in Ref. [9]. The inverse model is explained in detail in Ref. [10].

The data generation uses a Serpent full core model of the TREAT facility (including experiment vehicles and specimen) to calculate the system's total reactivity, differential rod worth coefficients, and the specimen power coupling factors as a function of the reactor average temperature, control rods axial positions, and the specimen average temperature. MOOSE's stochastic tools module uses polynomial regression to create an efficient surrogate model from this data. The developed models include:

- A full core Serpent model of the reactor core and irradiated specimen providing the necessary data sets to train developed surrogate models.
- A surrogate model that performs polynomial regression of the tabulated data that computes the differential rod worth coefficients for given axial control rod positions and fuel average temperature.
- A surrogate model that performs polynomial regression of precalculated steady state eigenvalue data set using the Serpent code to predict the reactivity introduced in the system given the core average temperature and the axial control rod positions.
- A surrogate model that performs polynomial regression of coupling factors computed by Serpent as a function of the predicted axial position of the control rods, the reactor average temperature, and specimen average temperature.

The inverse mode of the power prediction model is provided with the desired power signal. The power signal is converted into an equivalent reactivity signal using inverse kinetics. During the simulation of the transient, a PID controller is used to adjust the control rod position at each time step to the reactivity demand. This calculation requires to subtract the amount of feedback reactivity from the reactivity demand signal to obtain the amount of reactivity that must be provided by the control rods. The model couples the several components to obtain the reactor axial rod positions and total power during the transient experiments along with fuel average temperature as listed below:

- An inverse kinetics model that converts the demand power signal into a reactivity demand signal given the kinetics parameters and time step size.
- A surrogate model that performs polynomial regression of tabulated data based on Serpent calculations to predict the differential rod worth coefficients for given axial control rod positions and fuel average temperature.
- A proportional controller that determines the equivalent reactivity of the control rod axial position movement to the calculated demand reactivity signal.
- A surrogate model that performs polynomial regression of precalculated steady state eigenvalue data set using the Serpent code to predict the reactivity introduced in the system given the core average temperature and the predicted axial position of the control rods.
- An adiabatic thermal feedback model that calculates the reactor's average temperature given the heat deposited in the system at each time point.
- A point kinetics model that calculates total power and the delayed neutron precursor concentrations given the predicted reactivity introduced into the system at each time point.

The predictive temperature model of the specimen relies on the data provided by the predictive transient model to predict the specimen power and temperature. It utilizes the below listed models:

- A surrogate model that performs polynomial regression of precalculated coupling factors using the Serpent code given the predicted axial position of the control rods, the reactor average temperature, and specimen average temperature.
- A power conversion model that calculates the power of the specimen based on predicted coupling factor and the reactor total power.
- A thermal conduction model that calculates the specimen temperature using a detailed bison model of the specimen and given the specimen power.

3. PREDICTED RESULTS

This section presents a comparison of computational results of the predictive models for the Sirius-2c full power test with experimental results. The reactor power evolution and shape were selected to achieve a desired temperature ramp of the specimen. These predictive transient models can be utilized to study future experiments and help in achieving the desired outcome

3.1. Reactor Power & Control Rod Motion

Using the predictive transient model, the motion of the control rods in the axial direction was determined based on a demand power signal. As discussed in the previous section, this model relies on a point kinetics model coupled to an adiabatic thermal feedback model and connected to surrogate models that utilize pre-generated reactor data. Figure 3 shows the predicted power (red dashed line) along with demand power signal (red solid line) and measured power (black solid line). Also, the figure shows predicted transient control rod motion during the transient (green dashed line) compared with the measured control rod motion (black dashed line) along with the predicted reactor average temperatures (blue solid line). The predicted power was in close agreement with the measured power. Slight difference and delays were observed but these are due to differences in the predicted and the measured axial control rod motion. Nevertheless, the model was able to provide a blind prediction of the axial movement of the control rod and the power evolution that is in good agreement to the measured values taking into account all sources of uncertainties.

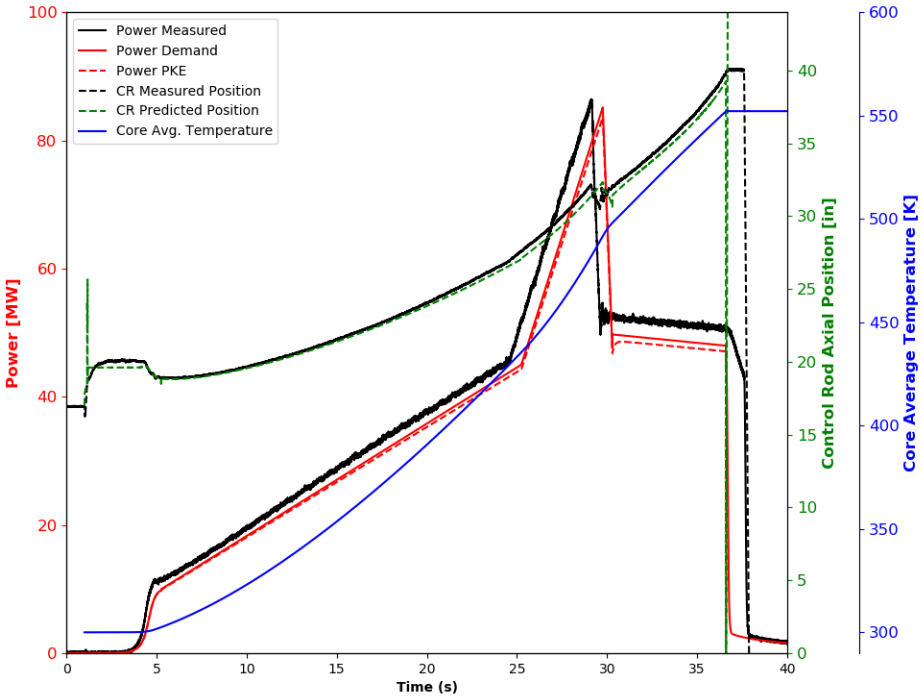

Figure 3. Comparison of predicted and measured power and axial control rod position of the Sirius-2c full power experiment.

3.2. Specimen Temperature

Using the power evolution calculated by the predictive transient model a prediction of the specimen temperature was made using the predictive temperature model presented in Figure 2. The specimen power was calculated by estimating the specimen coupling factor as a function of the reactor temperature and control rod position to provide a heat source for thermal conduction calculations of the Bison model. In addition, an uncertainty analysis was performed using latin-hypercube sampling implemented in MOOSE's stochastic tools module with 45 samples. The uncertainty quantification's goal was to investigate the impact of parameter uncertainties on the uncertainty of the temperature predictions. The parameters used in the

current parametric study can be classified into three categories: material thermal properties, power and coupling factors, and specimen geometry. However, the uncertainty from the geometry of the specimen was not considered in this analysis and each parameter was perturbed within ±10% of its nominal value. Figure 4 shows four curves originated from MOOSE uncertainty quantification model results along with measured value of the specimen temperature.

- TC-1: the temperature measured by thermocouple 1.
- Avg. predicted temperature: the average of all the sampled temperature trajectories.
- Best estimate: the temperature trajectory obtained with the best estimate parameter values.
- Min/Max predicted temperature: the minimum/maximum observed over all samples in the UQ at any given simulation time.

The predicted temperature evolution depicted in Figure 4 shows a good match with measured value during the power ramp region ($t = 0$ and $t = 28$ s), but overestimates the temperature at the plateau region ($t = 28$ and $t = 38$ s). After initiation of shutdown of the reactor ($t > 38$ s), the temperature is overestimated, but it decays at a similar rate as the measured value. The mismatch of the temperatures in this region is a direct consequence of not matching the measured temperature plateau (i.e. the cool down tail starts at a higher temperature).

The predicted temperature evolution indicates that the total power deposited in the specimen volume is overestimated, or the heat loss rate of the specimen is underestimated, or both. The specimen power relies on the reactor total power (which is very well predicted with predictive transient model) and the power coupling factors that relies on the Serpent model and it is not very sensitive to the temperature change of the specimen. However, the main heat loss mechanism of the specimen that is considered in the thermal model is radiative heat transfer which strongly depends on the surface emissivities.

In the current design, the values of the emissivities are not provided as an exact values rather than relying on values provided by scarce literature references for each material. These values depends greatly on chemical composition, geometrical structure, surface roughness, and machining of the specimen surfaces. In the current temperature predictive model, the fuel, tungsten, and molybdenum emissivities were selected to best knowledge of the analysts and available reported values in the open literature with values of 0.75, 0.29, and 0.1, respectively. A separate study was conducted on the specimen emissivities and it was found that the fuel emissivity has less impact on specimen temperature compared to the tungsten and molybdenum which surrounds a large portion of the specimen.

Much closer agreement between measured and predicted temperatures for the plateau and cool down tail regions was obtained after adjusting the emissivities The adjusted temperature predictions are shown in Fig. 5. For these results, the fuel and molybdenum emissivity was fixed at 0.75 and the tungsten emissivity was varied from 0.1 to 0.9. Similar temperature evolution was observed when varying the molybdenum emissivity while fixing the tungsten emissivity.

Other factors may contribute to the prediction of the temperature evolution is related to the modeling assumptions made which can be summarized as:

- All energy released in the specimen is assumed to be prompt. A delayed contribution would lead to a different specimen heat source as function of time.
- The delayed response of the thermocouple due to its thermal capacity and thermal contact to the specumen was not considered in the model.
- Underestimating radiative heat transfer due to uncertainties in the emissivities and the geometric simplifications, specifically in the hold-down rings. The simplified geometry obstructs a larger portion of the solid angle than the actual geometry which could decrease net radiation transfer from the top and bottom of the specimen.

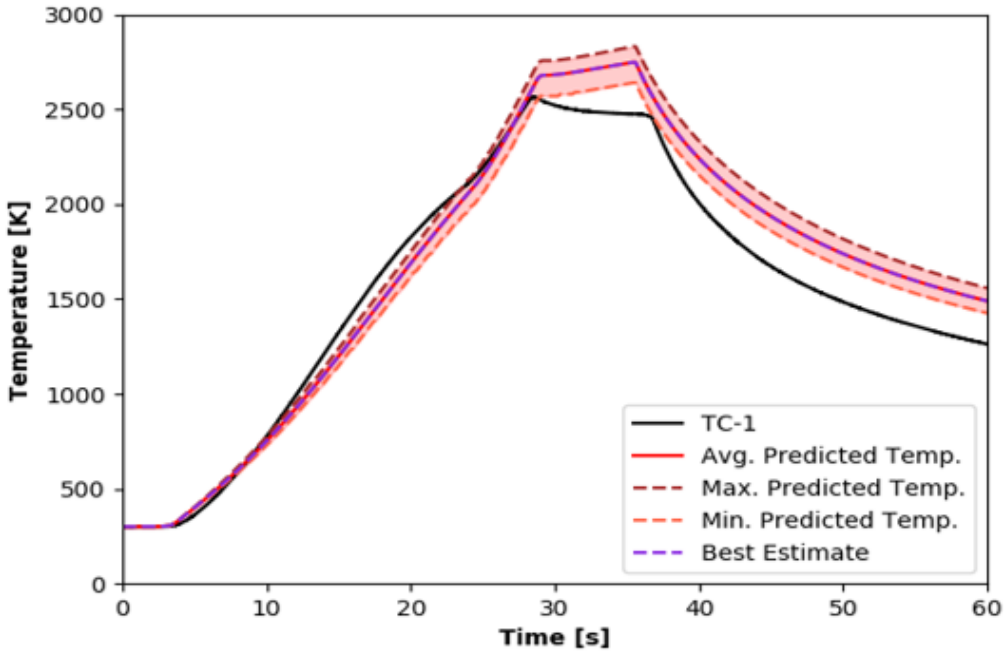

Figure 4. Comparison of predicted and measured temperature profile of Sirius-2c full power experiment during transient and after reactor shutdown.

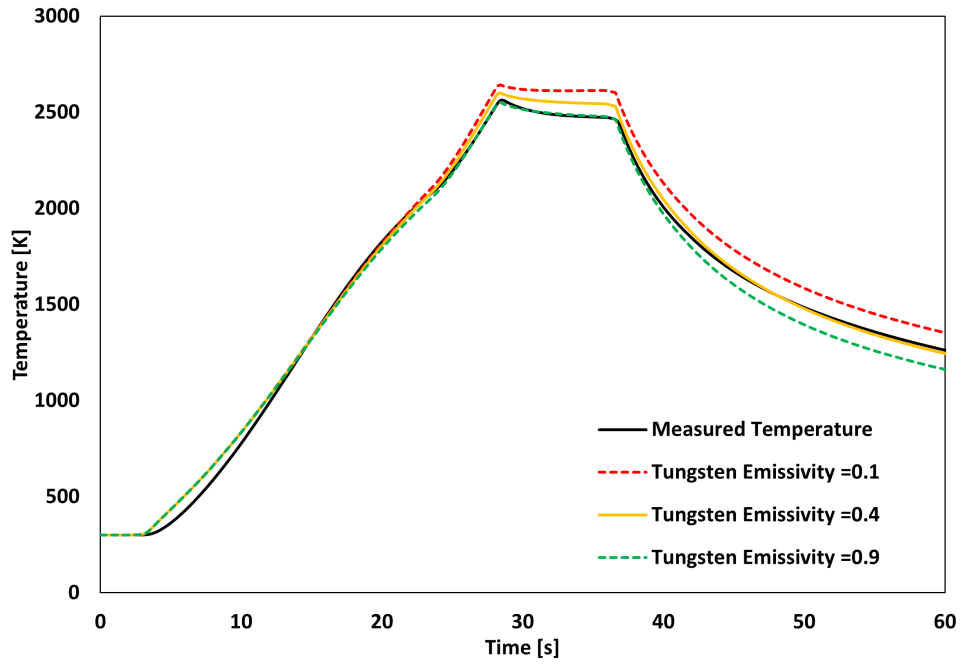

Figure 5. Impact of the surface emissivity on the predicted temperature profile of Sirius-2c full power experiment.

- Conduction or convection heat transfers were not considered, but it is less likely to have a significant impact because radiative heat transfer is dominate especially at temperatures above 2000 K.
- The differences in the as-designed and as-built specifications of the experiment could explain some of differences.

4. SUMMARY

In this work a predictive transient model of the TREAT facility was presented and applied to the Sirius-2c full power transient that is part of the SIRIUS experiment series. The model consists of three components: (1) data generation model relies on a full core Monte Carlo model, (2) predictive transient model, and (3) temperature predictive model. The predictive transient model used to determine the axial control rods motion of TREAT to reproduce a desired power signal and it relies on point kinetics model, adiabatic feedback model, and surrogate models for reactivity and control rod position prediction. The temperature predictive model is used to calculate the fuel specimen temperature and it relies on the predicted power evolution reactor and heat conduction model.

The predicted control rod motion and reactor power results agreed with measured values of the Sirius-2c full power experiment. The initial prediction of the specimen temperature ramp showed significant discrepancy at the plateau temperature and after shutdown region of the temperature ramp. By performing uncertainty evaluation on the current model, it was found that this large difference is related to underestimating of the heat loss rate which is very sensitive to the emissivities of the specimen surfaces. By fixing the fuel and molybdenum emissivity at 0.75 and varying the tungsten emissivity or fixing the fuel and tungsten emissivity and varying the molybdenum emissivity a good agreement of the calculated temperature evolution with measured values was observed. Further improvements of the predictive transient model will be included in the future with more validation and testing.

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