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Changing the World's Energy Future

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A Predictive Transient Model of the TREAT-SIRIUS Experiments

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To support experiments modeling and transient analysis of the NASA-sponsored SIRIUS experiments in the Transient Reactor Test Facility (TREAT), an innovative predictive transient model has been developed to simulate various transient experiments. The developed model is based on a new approach that utilizes steady-state Monte Carlo calculations along with a surrogate model based on polynomial regression to determine the core reactivity. The reactivity is supplied to a point kinetics model that determines the reactor power, and it is coupled to an adiabatic feedback model to determine the fuel average temperature. In this work, the newly developed model is introduced along with validation test results considering SIRIUS-1 experiments at different power levels. The initial test results show a very good agreement with experimental data at different power levels, which indicates that the model can be used to predict the power of future transient tests.

I. INTRODUCTION

The National Aeronautics and Space Administration (NASA) considers using a nuclear reactor to heat a gas to provide the required thrust to eject a rocket into outer space [1]. The system is called Nuclear thermal propulsion (NTP) and will replace chemical rockets. The NTP system is designed to reach its full power state from zero power state in less than a minute, which results in a large increase in fuel temperature ($\sim 3000\text{K}$) from cold conditions in a short period of time. This will create a very harsh environment that requires developing nuclear fuel and structural materials that can withstand these extreme operating conditions [2]. Currently, NASA is collaborating with Idaho National Laboratory (INL) to design and test such materials at the Transient Reactor Test Facility (TREAT) under prototypical conditions. TREAT allows material testing under rapidly changing power, as a result the temperature and the accompanying intense radiation fields [3].

A series of experiments are being designed and performed at the TREAT facility for testing NASA's NTP fuel materials known as SIRIUS. The main objective of the SIRIUS experiments is to examine the performance of candidate NTP fuel materials when it is subjected to high-temperature ramps and high-power rates under large irradiation fields that can be exposed to in a similar NTP system operation [4].

These transient tests are being evaluated at INL in advance to make an assessment of the test based on the desired outcome using the multiphysics object oriented simulation environment (MOOSE) [5]. This includes thermal analysis of the SIRIUS experiments [6] with the fuel performance tool BISON [7] and neutronics evaluation of the transient tests using the neutronics analysis tool Griffin [8]. However, the coupled calculations were not performed yet to provide a full predictive evaluation of the test to be performed. The ultimate goal of the analysis

performed by INL is to develop a predictive multiphysics model. This model will be able to predict the desired control rod movement to (1) achieve a desired reactor power trace, (2) achieve a desired specimen power deposition trace, and (3) achieve a desired specimen temperature trace.

In this work, a predictive transient model of the TREAT facility has been developed in an innovative way that leverages an existing Monte Carlo model of the TREAT facility for steady-state calculations, a surrogate model obtains core total reactivity via polynomial regression, a point kinetics model that calculates the reactor output thermal power, and an adiabatic thermal feedback model computes the core average temperature. This model will be coupled to a fuel thermal analysis model to perform fuel performance analysis in the future. However, this model should be tested and validated against experimental data before performing coupled calculations. This paper provides details of the developed model along with validation test results using SIRIUS-1 and 3 transient tests.

This paper is organized as follows: Section II provides a brief description of the TREAT facility, while Section III discusses the developed Monte Carlo model along with the control rod worth validation tests. Also, a parametric study on the reactivity worth change of the control rods is performed at the end of the section. Section IV discusses the predictive transient model and its four components and data generation procedure along with governing equations. In Section V, validation test results are presented for the SIRIUS-1 experiment at different power levels and the SIRIUS-3 test for the full power experiment. Finally, conclusions, summaries, and future work are provided in Section VI.

II. TREAT FACILITY DESCRIPTION

The operation of the TREAT facility was started in 1959 at INL and was specifically designed to test materials under transient conditions ranging from mild to severe accident conditions [9]. After being shut down for 24 years, the operation of TREAT was resumed for further testing in 2018 [10]. TREAT is a thermal, heterogeneous test facility with large inherent negative temperature feedback, central experiment irradiation position, and several rapid control and shutdown mechanisms [11]. The fuel is made of highly enriched uranium (HEU) elements dispersed in a graphite matrix. The graphite acts as a heat sink, and it resulted in having a strong negative temperature feedback since the fuel and moderator are forming a homogeneous mixture. The reactor is air-cooled and mainly used for post-transient heat removal. The TREAT core consists of a 19 by 19 square lattice, as shown in Fig. 1 [12]. Radially, the reactor core is surrounded by 61 cm thick graphite reflector and concrete shielding.

The fuel element pitch is approximately 10.16 cm with an

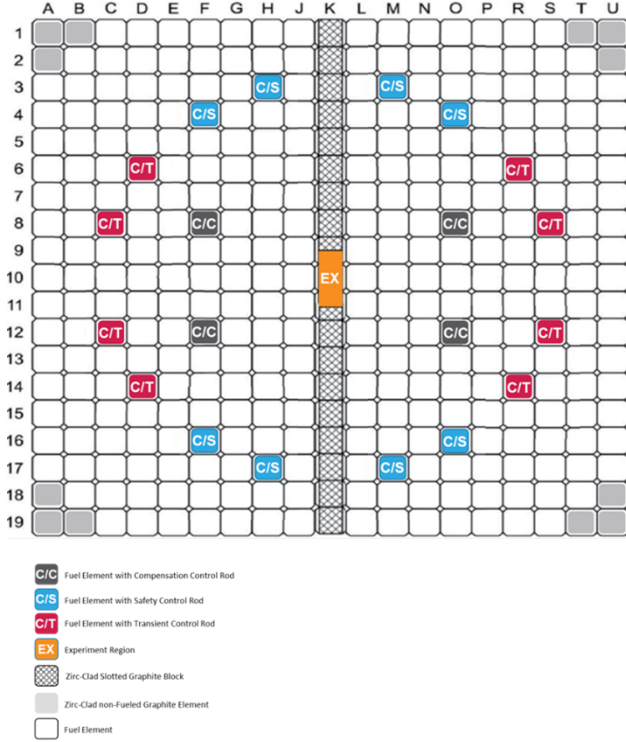


Fig. 1. Radial configuration of TREAT core region.

octagonal shape near the element corners to form air-cooling flow channels between elements. The fuel element length is approximately 255 cm. Detailed description of the reactor can be found in reference [13]. The TREAT facility is equipped with three reactivity control mechanisms made of boron carbide, namely compensation control (C/C), control shutdown (C/S), and transient control rods (C/T). The radial location of each control rod set is shown in Fig. 1. Each set is composed of four-rod drives, and each rod drive incorporates two control rods. The C/C rods are very close to the experiment location, but they are at a fully withdrawn position during the transient experiment. The C/C rods are used to shut down the reactor safely. The C/T rods are partially inserted into the active core region, and they are being withdrawn continuously during the transient so that they will yield the desired reactivity insertion upon the end of the transient. The C/S rods are partially inserted into the active core region to make the reactor critical prior to the transient and to compensate for the initial withdrawal of the C/T rods and they remain at a fixed position during the transient [12].

III. TREAT SERPENT MODEL

In this work, a TREAT full-core Serpent [14] model based on the data from the BATMAN report [12] is used. The model was developed initially in 2015 for minimum critical core analysis [15] of TREAT and followed by several improvements as discussed [16] [17] [18]. Figure 2 shows a radial view of the Serpent model used in this work. The model consists of a 19 by 19 array of standard fuel elements, and control rod elements, slotted elements, and dummy elements in the

core corners, central irradiation location of experiments, reflector region surrounding the core, biological shield made of concrete surrounding the reflector, and a thermal column [19].

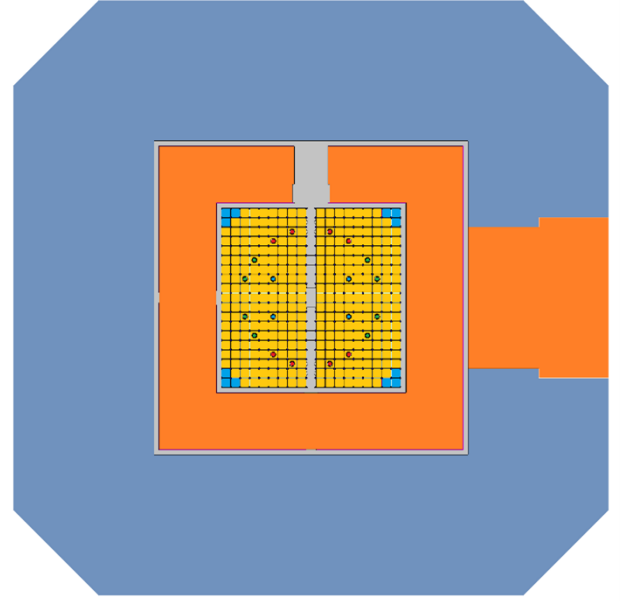


Fig. 2. Radial view of TREAT Serpent model showing fuel elements (yellow), graphite (orange), air (grey), and biological shield (blue).

III.A. Control Rod Worth Validation

In order to have a good predictive transient model of the TREAT controlled transient experiments, it needs to be validated against experimental data, especially control rod worth which should be in good agreement with the measurement. For this purpose, the measured reactivity worth of the C/S control rods was simulated with the current Serpent model. The measurement of the control rod worth was performed with the control rod swap method, in which the reactor is made critical with one control rod fully inserted and a second one fully withdrawn, while the remaining control rod positions are adjusted to make the reactor critical. During the experiment, the fully inserted rod is withdrawn gradually, and the resulting positive reactivity is compensated by inserting the fully withdrawn rod to return to a critical state. The reactivity is measured using the reactor stable period technique or using the inverse kinetics technique (via a reactivity meter that converts the measured neutron signal directly into reactivity). The calculated reactivities are compared with the measured values at each movement of the C/S-4 rod, as shown in Fig. 3, and the integral rod worth comparison is shown in Fig. 4. The calculated results show a good agreement with measurement, and most of the points are within statistical uncertainty of the calculations, however, the measurement uncertainty at the time of the experiment was not provided.

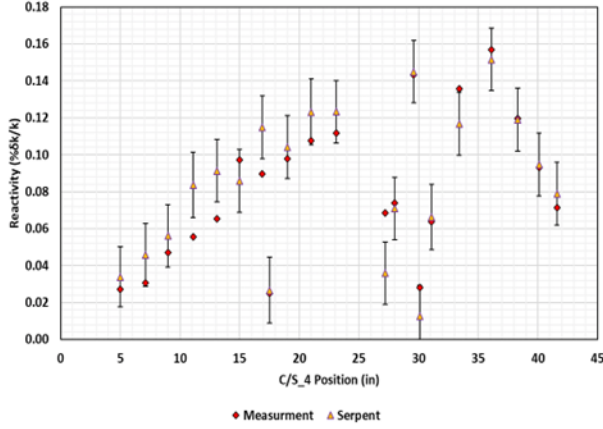


Fig. 3. Comparison of measured and calculated reactivities at different axial positions of C/S-4 rod.

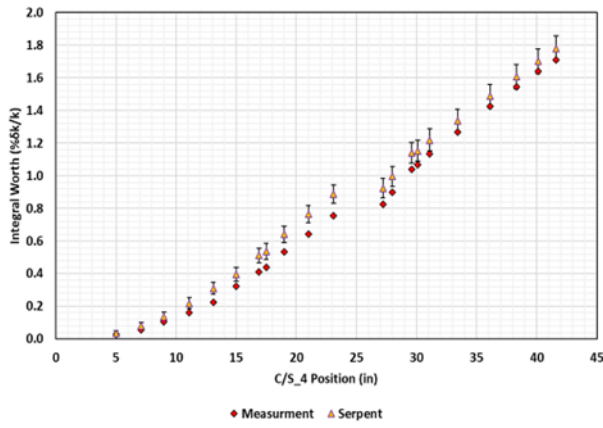


Fig. 4. Comparison of measured and calculated integral worth of C/S-4 control element.

III.B. Reactor Parametric Study

In the previous subsection, the integral worth of the C/S-4 rod was presented for a single state point, where the other control rods are fixed at a certain height, and the reactor was at zero power, so there is no temperature feedback involved. In the TREAT facility, there are three sets of control rods, as discussed in the previous section, and the axial position of these control rods will result in a redistribution of the neutron flux within the core, and it would alter the leakage fraction as well. Also, increasing the fuel temperature will significantly impact the control rod reactivity worth due to large negative feedback. In order to demonstrate the significance of temperature, control rod positions and their effect on the integral worth of the desired control rod, the integral worth of the C/T rods was calculated considering different fuel average temperatures ranging between 294K – 700K, and several C/S rods axial positions ranging between 20” to 58”. The integral rod worth map of the C/T rods presented in Fig. 5 shows a significant change in rod worth between 11-16 % $\delta k/k$. The control rod worth is enhanced at higher temperatures and increased penetration of the other control rods into the core.

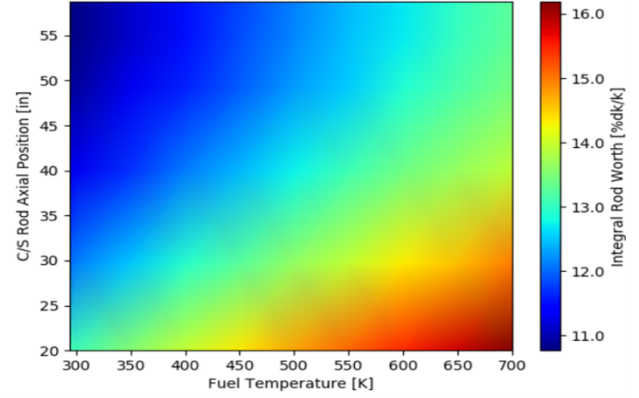


Fig. 5. Change of C/T rods integral worth as function of fuel temperature and C/S rods axial position.

Furthermore, the fuel temperature feedback coefficient was calculated considering several C/S rods axial positions ranging between 20” to 58” and C/T rods axial positions ranging between 0” to 40”. The temperature feedback coefficient map provided in Fig. 6 shows that it became less negative at higher temperatures and increased axial control rod positions with a value ranging between -28 pcm/K and -18 pcm/K.

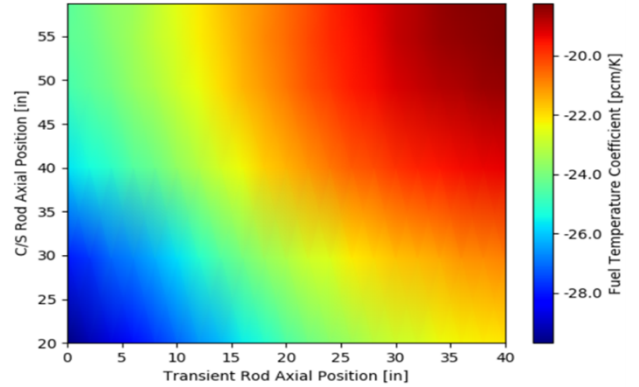


Fig. 6. Change of fuel temperature feedback coefficient as function of C/T and C/S rods axial positions.

These results indicate that the control rod worth and fuel temperature feedback coefficient are quite related. However, to explain this significant change in these two parameters, further analysis was performed to demonstrate the changes in the neutron spectrum and core leakage at different states of the core. Figure 8 shows the neutron spectrum at different fuel temperatures and C/T axial positions. Increasing the fuel temperature results in hardening the neutron spectrum, increasing the chance of non-fission absorption reaction rate, and increasing the neutron leakage, which results in a large shift in the neutron spectrum. On the other hand, the insertion of the control rods into the core will enhance the leakage rate as well as the non-fission absorption reaction. The changes in the neutron spectrum at different combinations of fuel temperatures and C/T axial positions are presented in Fig. 7. It can be clearly seen that a reduction in the thermal peak and increasing the fast neutron peak at higher temperatures and

more insertion of the control rods. Also, Fig. 8 provides the leakage fraction map of the neutrons from the core region, which clearly shows higher leakage fractions at higher temperatures. Also, the leakage fraction peaks at 15" of the C/T rod height due to neutron flux redistribution, especially the peak region to the bottom of the active core.

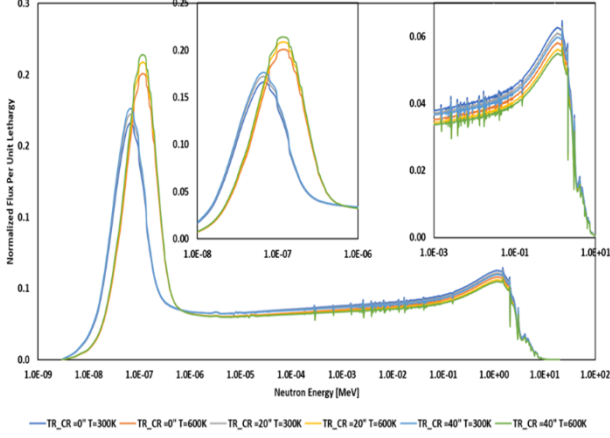


Fig. 7. Change of neutron spectrum at different fuel temperature and C/T rods axial position.

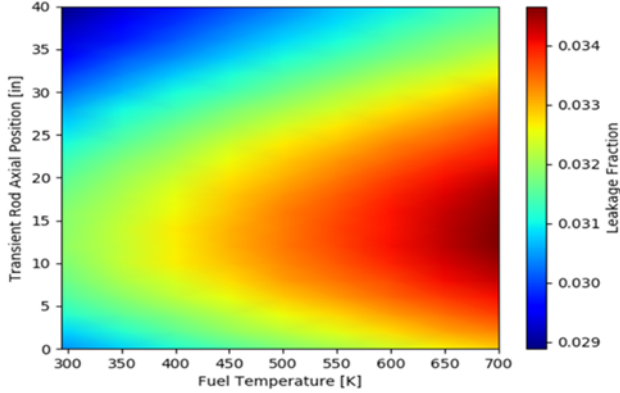


Fig. 8. Change of core leakage fraction as function of fuel temperature and C/T rods axial position.

IV. METHODOLOGY

A transient model has been developed based on the coupling of high-order (Monte Carlo eigenvalue calculations) and low-order (point kinetics equation) solutions to perform the transient calculations. The PKE drives the solution during the transient by updating the power magnitude. While the steady-state eigenvalue calculations are required at each time step to update the total reactivity and provide problem kinetics parameters. The PKE used in the current model are provided in Eq. (1) and Eq. (2). The detailed derivation of the PKE can be found elsewhere [20].

$$\frac{dP}{dt} = \frac{\rho(t) - \beta_{\text{eff}}}{\Lambda} P(t) + \sum_{k=1}^K \lambda_k C_k(t), \quad (1)$$

$$\frac{dC_k}{dt} = \frac{\beta_k}{\Lambda} P(t) - \lambda_k C_k(t), \quad k = 1, 2, \dots, K, \quad (2)$$

where P is the total power, C_k , β_k , and λ_k are the modified delayed neutron precursor concentration, delayed neutron fraction, and decay constant of the delayed neutron family k , respectively. β_{eff} is the effective delayed neutron fraction, Λ is the mean neutron generation time and ρ is the total reactivity of the system. β_{eff} , Λ , and ρ need to be calculated in advance in order to solve the PKE assuming the system initial conditions are known. The detailed definition of these parameters can be found elsewhere [20]. Typically, the total or net reactivity is calculated at each time step assuming the inserted reactivity ρ_{CR} (i.e., due to control rod movement) and the feedback reactivity ρ_{FB} as

$$\rho(t) = \rho_{CR}(t) + \rho_{FB}(t), \quad (3)$$

As explained in the previous section, the control rod worth and feedback coefficient are changing depending on the state of the system. So, using a fixed control rod worth and a constant feedback coefficient, as in typical PKE solutions will lead to miscalculating the reactivity. This situation can be overcome by calculating the reactivity via a steady-state solution and feeding it back to the PKE at each time point. Then eigenvalue calculations are performed, and the system total reactivity is calculated according to the following relation at each time step

$$\rho(t) = \frac{1}{k_{\text{eff,ss}}} - \frac{1}{k_{\text{eff}}(t)}. \quad (4)$$

where $k_{\text{eff,ss}}$ is the eigenvalue of the system at initial steady state conditions prior to the start of the transient, while $k_{\text{eff}}(t)$ is the eigenvalue of the system at time t adopting the latest changes in the system. In order to fulfill the above relation, steady-state calculations need to be performed at each time step, which can be very expensive computationally, especially for a problem of large size and considering a small-time step size. In this work, a new approach is introduced to eliminate the need for performing steady state eigenvalue calculations to obtain $k_{\text{eff}}(t)$ at each time step by leveraging machine learning capabilities to estimate the system reactivity using a regression model of precalculated data sets that covers a wide range of system changes. In this way, the reactivity of the system can be calculated knowing altered parameters and utilizing a surrogate model at each time step without the need for performing eigenvalue calculations.

Based on the above discussion, a predictive transient analysis methodology has been developed and applied to the TREAT transient experiments for validation. The developed transient model solves the PKE along with an adiabatic feedback model to calculate the reactor total power and the average fuel temperature. Then, the total reactivity was estimated using a surrogate model that performs polynomial regression of precalculated eigenvalue data using the Serpent model discussed in the previous section. Figure 9 shows a schematic diagram of the calculation flow of the developed predictive model.

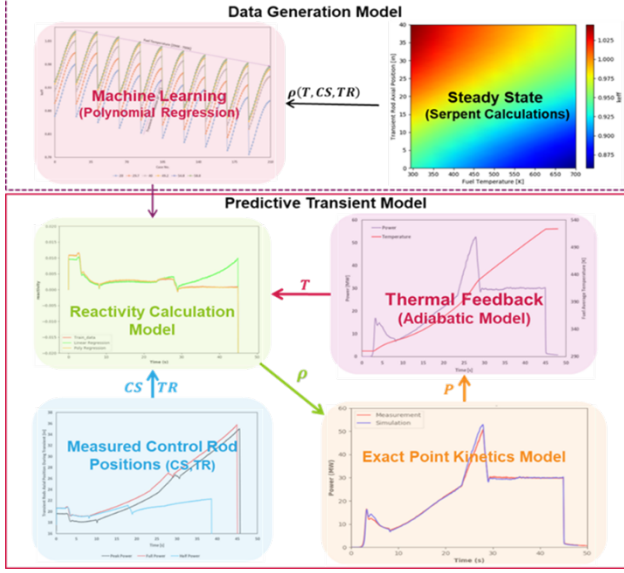


Fig. 9. Predictive transient model calculation workflow.

IV.A. Steady State Monte Carlo Model

The main reactivity insertion mechanisms of the TREAT reactor are control rod motion and the corresponding feedback reactivity due to increased fuel temperature. As discussed in the previous section, during the transient only the C/T rods are moved to insert the desired reactivity while other control rods are at fixed positions. However, the C/S rods are partially inserted, and their position affects the C/T rods worth as well as the temperature feedback coefficient. To be able to calculate the reactivity during the transient without performing eigenvalue calculations at each time step, a set of eigenvalue data were generated with the TREAT Serpent model considering average fuel temperature, C/S, and C/T axial positions. 1260 data points for reactivity calculations were generated at 10 fuel average temperatures (294, 300, 350, 400, 450, 500, 550, 600, 650 and 700K), 6 C/S rod axial positions (20, 29.7, 40, 49.2, 54.8 and 58.8”), and 21 C/T rod positions (0 – 40”). Figure 10 shows all the calculated eigenvalues at each point. Each data point was obtained via a Serpent calculation performed with 600 cycles of 10^5 particles after 100 inactive cycles.

IV.B. Surrogate Model

A surrogate model was developed using the stochastic tools module of the Moose framework with polynomial regression [21]. The generated data with Serpent was used to train the regression model and generate the coefficients of the polynomial terms. Then this model was used to predict the reactivity knowing the fuel average temperature, C/S, and C/T axial positions. As a verification test, the training of the model was fed back to the model to test if the model is able to reproduce the original data set. This is shown in Fig. 11. For comparison purposes, two regression models were considered: linear and 4th order polynomial. The polynomial regression model was able to reproduce the original set of data while the linear regression model was mis-predicting the reactivity

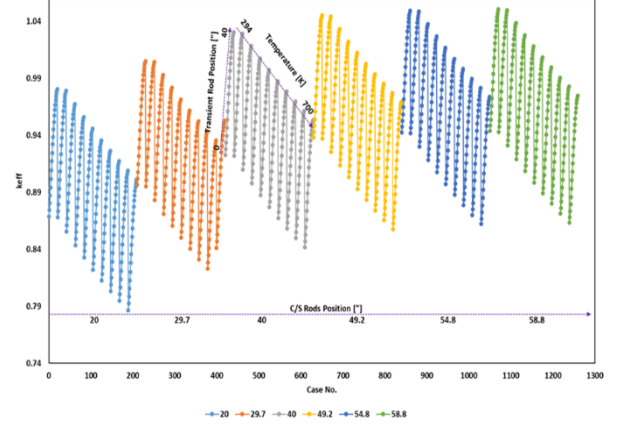


Fig. 10. Tabulated eigenvalue as function of fuel average temperature, C/S and Transient rods axial positions.

value for most of the points.

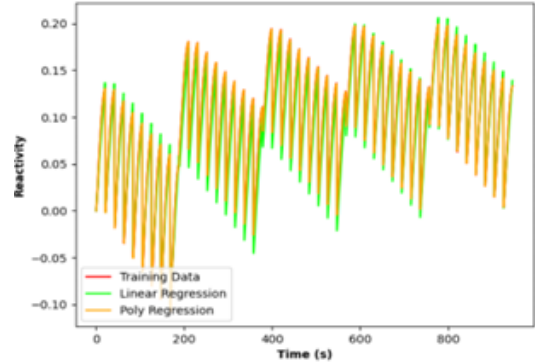


Fig. 11. Comparison of predicted reactivity of surrogate models and original training data set.

Also, these models were tested within the predictive PKE model for a transient case where the temperature and control rods positions were provided at each point and compared to the total reactivity reproduced from the power signal as provided in Fig. 12. It can be clearly seen that polynomial regression model was able to predict the reactivity accurately for the real transient, while a large deviation was observed using the linear regression model. In the remaining analysis, only the polynomial regression model was used in the predictive transient model.

IV.C. Adiabatic Thermal Feedback Model

The fuel average temperature T is calculated using an adiabatic feedback model [22] given by:

$$\rho C_p(T) \frac{dT(\mathbf{r}, t)}{dt} = q(\mathbf{r}, t), \quad (5)$$

where ρ is the fuel density, q is the power density, and C_p is the fuel heat capacity which is obtained from direct measurement that was performed at high and low temperatures [19]. The adiabatic approximation is valid for the TREAT reactor since there is no cooling mechanism is employed during the

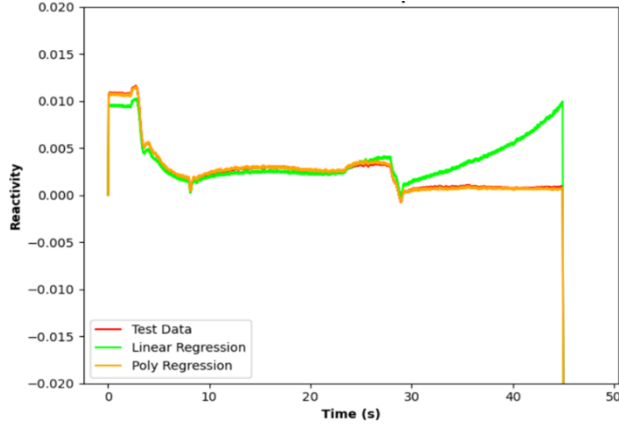


Fig. 12. Comparison of predicted reactivity of surrogate models during transient test.

transient, and the reactor is made from graphite which has a large heat capacity. Integrating Eq. 5 over the reactor volume the following relation for calculating the fuel average temperature T can be obtained knowing the fuel mass M and the total deposited energy E at time t as

$$T(t) = T_0 + \frac{1}{MC_p(T)} E(t). \quad (6)$$

IV.D. Point Kinetics Model

Once the total reactivity is estimated using the developed surrogate model and knowing the average fuel temperature and axial positions of the C/S and C/T control rods, the PKE can be solved at each time step and the reactor total power can be calculated. Using the neutronics code Griffin, a PKE model of the TREAT reactor was developed with an adiabatic feedback model and coupled to the surrogate model, as discussed in the previous subsections.

V. VALIDATION TESTS

The developed predictive transient model has been validated with available transient tests of the SIRIUS experiments performed at the TREAT facility. In these transient tests, the control rods are moved to introduce a positive reactivity to increase the power from a cold state to the MW range within a short time. This will lead to a significant increase in the temperature of the fuel sample. The length and shape of the power are determined by the total amount of energy that needs to be deposited in the fuel to achieve the desired temperature. The current experimental data are available for SIRIUS-1 and SIRIUS-3 experiments, and these transients were run for 40 to 80 s. Other experimental data will be available soon for SIRIUS-2 and SIRIUS-4, which can be used for further validation.

V.A. SIRIUS-1 Power Tests

The SIRIUS-1 experiment was performed at three different power levels compared to the full power (FP): half power (30.0 %FP), full power (100.0 %FP), and peak power (120.0

%FP) power. The measured control rod axial position of the C/T rods and measured power for all the experiments are shown in Fig. 13. Also, Table I provides the initial positions of the control rod sets at each power level. Each transient test can be divided into three regions: prompt reactivity insertion or first peak region (first 10 s of the transient), peak power region (middle of the transient where the peak power occurs), and feedback-controlled region (region after the peak power).

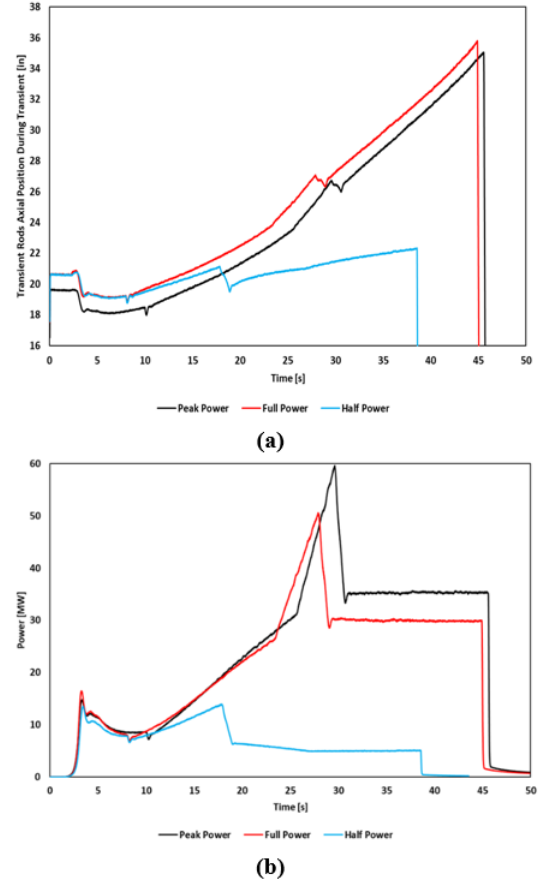


Fig. 13. Measured power and C/T rods axial positions during SIRIUS-1 Transient Experiments.

The first region of the transient is influenced by initial reactor power, temperature, kinetics parameters, and precise control rod position. The second region is driven by the reactivity worth of the C/T movement and mild feedback effect. In the last region of the transient, the power stabilizes at a certain level and remains at the same level until the end of the transient. In this region, a stronger feedback effect is introduced due to increased fuel temperature, and it is compensated by withdrawing the C/T rods at a level that compensates for the negative reactivity to maintain a constant power level.

Figure 14 shows a comparison of the measured and calculated reactor power using the predictive transient model of the three SIRIUS-1 power experiments. The calculated results are in very good agreement with measured power for all of the transient regions at each power case. A little deviation was noticed in all three tests after the first peak region, which can be related to poor measured initial power resulting from a

TABLE I. SIRIUS-1 control rods initial axial positions.

Experiment	Rod No.	Control Rod Position[in]		
		C/C	C/S	C/T
Half Power	1	58.50	49.20	17.53
	2	59.00	49.40	17.63
	3	58.50	49.20	17.59
	4	58.60	49.00	17.52
	Avg.	58.65	49.2	17.57
Full Power	1	58.40	48.10	17.42
	2	59.00	49.50	17.54
	3	58.50	49.50	17.60
	4	58.70	49.50	17.52
	Avg.	58.65	49.15	17.52
Peak Power	1	58.40	54.80	16.42
	2	59.00	54.70	16.51
	3	58.50	54.90	16.60
	4	58.70	54.80	16.57
	Avg.	58.65	54.80	16.53

very low neutron signal, and uncertainty of the exact control rod position as it moves a little faster in that region. Also, for the peak power experiment a non-negligible deviation of the calculated power from the measured values at the feedback region which is related to the simplified thermal feedback model, and experimental values of the heat capacity that is used in the model, which becomes more pronounced at higher temperatures.

V.A. SIRIUS-3 Full Power Test

Further testing and validation of the predictive transient model with the most recent available transient experimental data of TREAT facility, the SIRIUS-3 full power experiment was simulated, and the results are compared in Fig. 15. Similar to the previous tests, the predicted power is in very good agreement with measured values for the whole experiment duration except for the time between 5-10 s (after the first peak) which shows that the power is slightly overestimated and then underestimated. This might be explained by large uncertainty in the initial power and control rod position at that point of the transient. However, for the remaining period of the transient, the calculated power matches the measured value at the peak region and thermal feedback region.

VI. CONCLUSIONS

As an initial stepping stone of experiments modeling and simulation and to support transient analysis of the NASA-sponsored SIRIUS experiments in the TREAT reactor, a predictive transient model was developed with a simple point kinetics model along with an adiabatic feedback model to calculate the reactor power and fuel average temperature. The reactivity of the system was calculated using a surrogate model that leverages pre-calculated eigenvalues at different state points using the Serpent model of the TREAT facility.

The TREAT Serpent model was first validated against measured control rod worth and used to understand the behav-

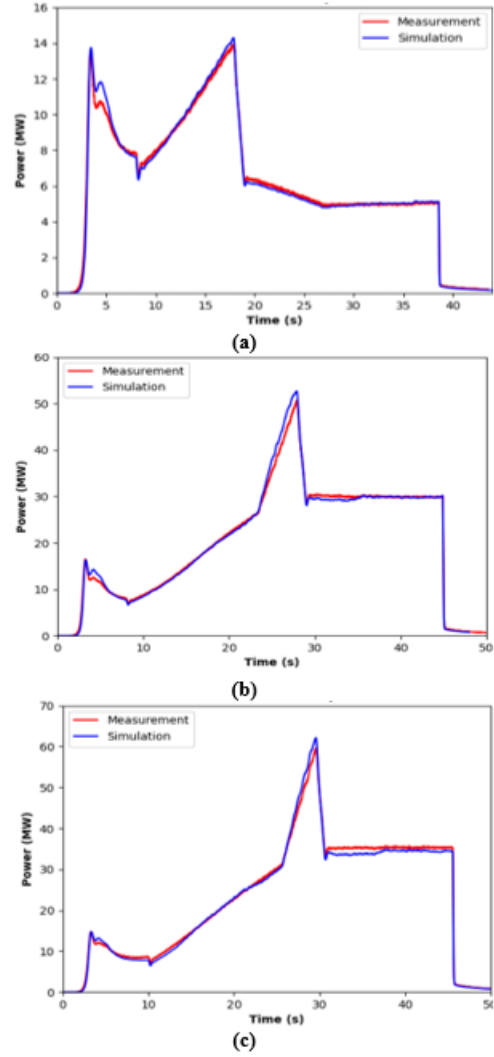


Fig. 14. Comparison of the predicted and measured powers for SIRIUS-1 experiments (a) at half power, (b) full power, and (c) peak power.

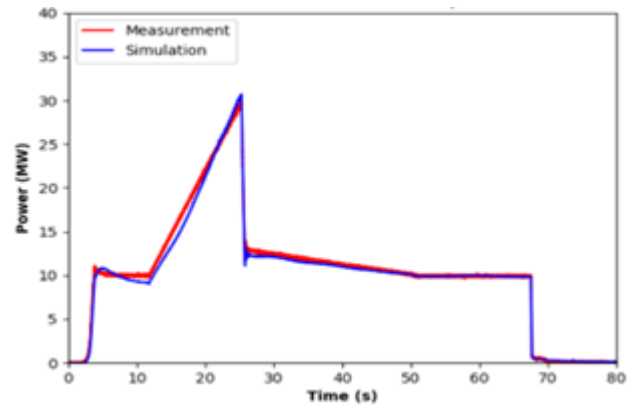


Fig. 15. Comparison of predicted and measured power for SIRIUS-3 full power experiment.

ior of the important reactor parameters such as integral rod worth, feedback coefficient, leakage, and spectral changes of the core at different reactor states. With knowledge of the fuel average temperature and control rod positions, the reactivity is estimated with a surrogate model and used in the PKE to obtain the reactor total power. Initial validation test results of the model against SIRIUS-1 and SIRIUS-3 experimental data show very good agreement with measured power at different power levels and considering various control rod movements.

This model will help the reactor engineering team in preparing and predicting the power and temperature of the experiment. Also, the model helps in reducing the computational time significantly compared to a dynamic 3-D model without losing accuracy level and allows to perform uncertainty quantification for the whole transient. The major drawback of the current model is that it cannot currently separate the reactivity components, instead, the total inserted reactivity is calculated. Also, to enhance the accuracy of the model, more data point needs to be collected and used in the surrogate model to obtain a better predictive reactivity model. Furthermore, a more sophisticated thermal feedback model needs to be considered to account for temperature distribution within the core. Future work will be focused on upgrading the model by allowing control rod axial position prediction and coupling the current predictive model with the thermal mechanics model to be able to predict the temperature of the tested fuel samples.

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