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Verification of the Time-dependent Transport Code TDKENO with the Monte Carlo Code KENO-VI

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ABSTRACT

The loss of coolant accident at the Daiichi plant has increased attention to the development of fuels for United States commercial reactors with enhanced accident tolerance. Testing of new fuels is scheduled at Idaho National Laboratory's Transient Reactor Test Facility (TREAT). Typically a number of pre-test calibrations are required before actual experimentation may begin. We hope to simulate TREAT experiments to minimize the number of calibrations needed. Systems such as TREAT pose several modeling challenges due to the non-uniform insertion of reactivity from transient rods and complex core geometries. To simulate complex geometries with ease, the code TDKENO has been modified to incorporate the Monte Carlo code KENO-VI in its calculation sequence. Previously, TDKENO relied on KENO V.a, which only supports simple geometry inputs. TDKENO provides advantages over typical codes by solving the three-dimensional time dependent transport equation with delayed neutrons partially via Monte Carlo calculations. Newly added capabilities in TDKENO are verified through comparison to computational benchmark and sample problems. Finally, TREAT temperature-limited transients are simulated with KENO V.a and KENO-VI inputs. Simulations with KENO-VI inputs resulted in improved agreement between calculated TDKENO values and experiment over KENO V.a inputs.

Key Words: **TDKENO, TREAT, Improved Quasi-Static (IQS) Method, Transient**

1. INTRODUCTION

Nuclear power has long been a reliable, safe, and carbon free method of producing tremendous amounts of electricity in the United States (U.S.). Continual improvement of fuel burnup, reliability, and safety during normal and transient operation of nuclear reactors is essential for the industry's success. Safety is always a priority in a plant, however the accident at the Fukushima Daiichi nuclear power plant raised questions regarding fuel performance of U.S. reactors during off normal conditions. The result is a renewed interest in enhancing the accident tolerance of fuels used in the U.S. commercial fleet. Congress formally outlined a schedule for the development of accident tolerant fuel (ATF), with proposed fuel being placed in a commercial reactor by 2022 [1].

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This time frame has prompted new methods to expedite experimentation. These new methods will rely on high fidelity simulation of experimental systems, primarily to reduce the series of pre-test experiments required to achieve the desired environment in the test-vehicle. One facility capable of performing the experiments is the Transient Reactor Test Facility (TREAT) at Idaho National Laboratory (INL). Since TREAT's decommissioning in 1994, there have been great advances in computing speed and memory that now makes high fidelity simulation of TREAT experiments feasible. Transient experiments carried out with TREAT are difficult to simulate with conventional codes due to the non-uniform perturbations produced within the core. Additionally, codes tailored to TREAT are based on high-enriched uranium systems and are not guaranteed to work on the low enriched fuel that will be tested. The fission yield from such experiments is time dependent and a function of many system parameters. These parameters include (but are not limited to) the fissionable material type, neutron interactions in the system (thermal, intermediate, fast), enrichment (or presence of resonance capture isotopes), the reactivity insertion rate and amount, and heat capacity and heat transfer features of the materials including any cooling mechanisms [2]. To understand these multi-physics systems requires accurate simulation of the neutronic behavior, geometry, and temperature distribution. At present, the most rigorous analytical methodology for understanding neutronic behavior involves solving the time-dependent governing equations for three-dimensional (3-D) geometries, commonly referred to as spatial kinetics [3].

We propose the use of the code TDKENO to model TREAT experiments. TDKENO solves the time dependent 3-D Boltzmann transport equation with the explicit representation of delayed neutrons to obtain the neutron flux. Directly integrating this equation is difficult and requires frequent recalculation to handle the time dependence. Instead we assume the flux may be factored into components to improve computation time while preserving accuracy. The neutron flux is factored into a rapidly varying amplitude equation and a slowly varying shape equation (an assumption that has generally shown to be true) [4]. The shape equation is solved with a modified version of the Monte Carlo code KENO (part of the SCALE package) [5,6]. Solving the shape equation via Monte Carlo is computationally intensive, therefore is only updated when needed. By solving the rapidly varying amplitude equation deterministically many times between shape calculations results in a highly accurate solution without the expense of direct integration.

The desire to model complex cores such as TREAT prompted the modification of TDKENO to support generalized geometry inputs. This is advantageous as the input may be created to exact system parameters. TDKENO was initially developed with KENO V.a: the geometrically simpler version of KENO. While quicker than Monte Carlo codes with generalized geometry, KENO V.a places practical limits on input designs as only combinations of cuboids, spheres, cylinders, etc. are possible. To illustrate this problem, two input strategies for modeling the chamfered corners of a TREAT fuel element are shown in Figure 1 for KENO V.a and KENO-VI .

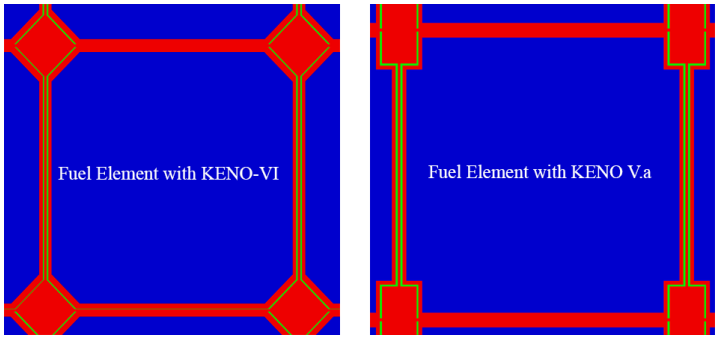


Figure 1. Chamfered corners of fuel elements in KENO V.a and KENO-VI. Fuel elements have one step and non-fuel elements have a stair like structure in KENO V.a. The KENO-VI structure mimics the chamfered corner for all elements and requires less regions.

As depicted in Figure 1, the corners are approximated with a stair-like combination of cuboids with KENO V.a. The goals of creating KENO-VI inputs is to better capture the geometry (e.g. corners may be created using planes) with fewer regions.
In order to achieve high fidelity modeling of TREAT experiments the following has been done:

- Modification of KENO-VI to solve the flux shape equation inside of TDKENO.
- Verification of these modifications through comparison of identical inputs from KENO V.a and KENO-VI.
- Simulation of TREAT transients from the M8CAL experiments (Transients #2855, #2856, and #2857) using KENO V.a and KENO-VI inputs further verify modifications. Additionally, the improved KENO-VI inputs show better agreement with experiment.

2. TDKENO: A HYBRID TIME-DEPENDENT TRANSPORT PROGRAM

Transient analysis of system such as TREAT cannot be analyzed with high degrees of accuracy using conventional nuclear engineering codes. These codes typically employ diffusion theory or point kinetics approaches. Diffusion theory fails in highly absorbing regions and point kinetics approaches that are insufficient to capture spatial reactivity effects. Therefore, transport theory is required to simulate voided and/or strongly voided regions, and asymmetric material movements accurately [3].

The code TDKENO is a large program containing several large subroutines that solves the time dependent, 3-D Boltzmann transport equation with the explicit representation of delayed neutrons (precursor equations). Numerical techniques with varying degrees of accuracy are required as analytical solutions for transport equations only exist for simple geometries. The methodology utilized within TDKENO is the improved quasi-static (IQS) method [3,7]. This method relies on factoring the neutron flux into a purely time dependent, rapidly varying amplitude equation and a slowly varying shape equation. Equation (1) describes the flux factorization, where $\psi(r, E, \Omega, t)$ is the angular flux at position (r), energy (E), angle (Ω) and time (t). $T(t)$ is the amplitude function, described by point kinetics equations and $\Phi(r, E, \Omega, t)$ is the flux shape function with weak time dependence. The flux factorization is made unique by imposing a normalization condition [3].

$$\psi(r, E, \Omega, t) = T(t) \cdot \Phi(r, E, \Omega, t) \tag{1}$$

The result of this factorization is two coupled equations that are solved on different time scales. Calculation of the flux shape is computationally expensive. It is only calculated when an update is required, like a large change in system behavior. Conversely, the amplitude function requires significantly less time and can solve the point kinetics equations deterministically over shorter time steps. The time derivative in the Boltzmann transport equation is replaced with a first order backwards difference approximation [4]. The result of this factorization is a computationally efficient solution that is able to extract neutronic information where typically employed methodologies are invalid.

TDKENO is considered a hybrid solution method; the amplitude equation is solved deterministically while the flux shape is calculated via Monte Carlo with KENO (from the SCALE package) [2,3]. KENO may refer to either KENO V.a (simple geometry) or KENO-VI (generalized geometry). Both are now available in TDKENO.

An additional component of TDKENO that makes it suitable for transient analysis is the incorporation of a feedback model. A feedback model is required to accurately determine the power, total yield, and point kinetics parameters, such as reactivity and effective delayed neutron fractions. Values such as reactivity and effective delayed neutron fractions are not measured directly [4]. Rather, the periods of delayed or prompt supercritical systems is used to infer the reactivity. In addition, time lag of delayed neutrons allows better-controlled transients. TDKENO incorporates feedback via quenching coefficients provided *a priori* [3,4]. The temperature distribution within core materials affects reactivity as well. To incorporate temperature–dependent cross sections, TDKENO would need to be coupled to a code that provides the temperature distribution as a function of energy created in the core. As this currently isn't implemented, an approximation is used instead. The feedback mechanism that calculates the reactivity as a function of total energy produced in the core is implemented and described in Equation (2):

$$\rho_{fb}(t) = \sum_{i=0}^{3} a_i Y^i(t) \tag{2}$$

where $\rho_{fb}(t)$ is the feedback reactivity, $Y(t)$ is the total yield in the core at time t in MJ, and a_i refers to the empirical coefficients for a third order polynomial.

The neutronic capabilities of TDKENO come from the ability to solve the time-dependent Boltzmann transport equation efficiently. Even utilizing a simple feedback method makes TDKENO an excellent code for transient analysis as few codes accurately determine the time dependence, neutronics, and geometry with such high fidelity.

3. INCORPORATION OF KENO-VI INTO TDKENO

TDKENO was first constructed with KENO V.a performing fixed source calculations and flux shapes. KENO V.a allows inputs to be constructed in a combinatorial manner with basic shapes such as spheres, cylinders, and cuboids [5]. It is further restricted as regions may not intersect or be rotated. The advantages are all regions are easily defined and determining neutron locations is less intensive compared with generalized geometries. KENO-VI is referred to as a generalized geometry

code that supports many constructs including planes, dodecahedrons, wedges, parallelepiped, etc. [6]. In addition, it allows regions to be rotated and to intersect. The drawback is the calculations take approximately four times as long as KENO V.a, primarily because neutron tracking requires the evaluation of many quadratic functions.

For this work, KENO-VI code (from SCALE 6.1) was modified and incorporated into TDKENO to calculate the flux shape. Modifying KENO-VI files for TDKENO required updating the build environment for TDKENO. CMAKE is currently used to handle the building of TDKENO, holding hundreds of files across many directories. As of now CMAKE scripts have been written so TDKENO can be built on Linux and Mac based computers. These modifications allow user to make use of either KENO V.a or KENO-VI inputs.

4. VALIDATION OF MODIFICATIONS TO TDKENO

To verify the modifications to TDKENO, a series of transients are simulated with both KENO V.a and KENO-VI inputs. It should be noted that TDKENO has been extensively benchmarked with KENO V.a in Reference [4]. As KENO V.a and KENO-VI only differ in the treatment of geometry, similar behavior is expected between the two. The problems are presented in order of increasing complexity, beginning with the 16A1 benchmark problem [8]. With much of the motivation for modifying TDKENO to better simulate TREAT, we first examine a single element input of TREAT then proceed to the full core.

4.1. 16A1 Benchmark

The 16A1 benchmark problem describes a seven region transport model (Figure 2) of a liquid metal fast breeder reactor. The configuration consists of three core regions (Zones 2, 4, and 6) containing core material and sodium, two control rod regions (Zones 3 and 5) containing control rod material and sodium, and two fuel blanket regions (Zones 1 and 7) containing blanket material and sodium [4]. This problem is one-dimensional; it simulates three dimensions by utilizing reflective boundary conditions in the y- and z-directions. This computational benchmark is a relatively simple transient and provides an excellent starting point for validating code modifications. Transient behavior is imitated with a perturbation caused by a 5% increase in density of the material in Zone 2 and a 5% decrease in density of the material in Zone 6, resulting in a delayed supercritical transient [4]. Input parameters are provided in Table 1.

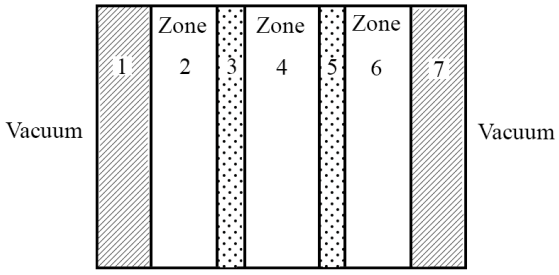


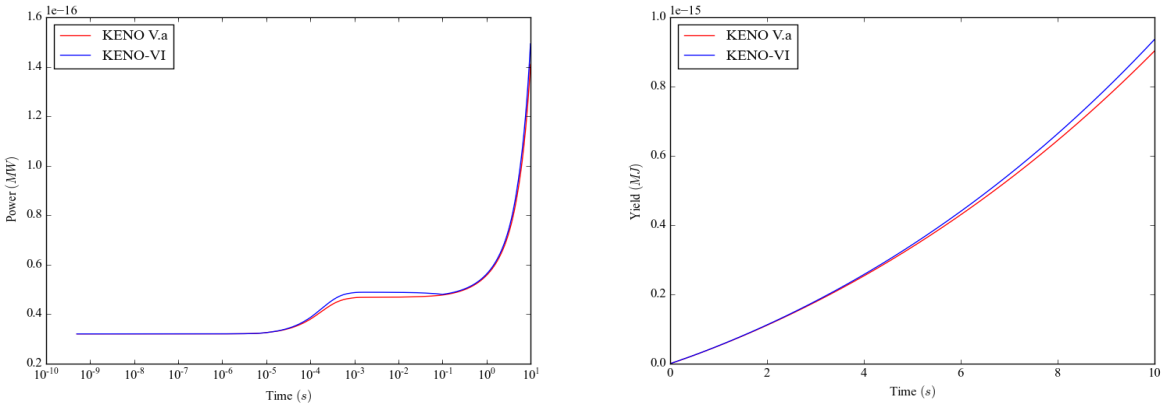
Figure 2. 16A1 geometry description.

For a preliminary comparison, the calculated power and yield using TDKENO with KENO V.a and

KENO-VI inputs are respectively plotted in Figures 3a and 3b. The calculated power and yield show excellent good agreement between the KENO V.a. and KENO-VI inputs. The large number of histories give us confidence that TDKENO is indeed working as intended with KENO-VI.

Table 1. Input parameters for the 16A-1 Benchmark input.

	KENO V.a	**KENO-VI**
Number of generations	1500	1500
Particles per generation	20000	20000
Number of regions	7	7
Number of materials	5	5
Flux shapes	5	5
Calculation time	200 min	820 min



(a) **(b)**

Figure 3. Power (a) and yield (b) are calculated with TDKENO using both KENO V.a and KENO-VI inputs. The time scale is logarithmic in (a) to distinguish features varying over the small time scale. Very good agreement is observed between KENO V.a and KENO-VI.

4.2 Description of TREAT Core

The TREAT facility enables study of reactor safety research and fuel behavior. It serves as a non-destructive testing ground for fuel development and assessment of accident severity. TREAT experiments are accomplished by depositing transient energy to targets within experiment rigs. Detailed descriptions of TREAT may be found in References [9,10].

The fuel for the experiments described in the following section is composed of highly enriched (93.1%) UO_2 dispersed homogenously within a graphite mixture with a 10,000:1 graphite-to-uranium ratio. The fuel elements are 10.05 cm squares with 1.58 cm chamfered corners for air coolant flow. The active fuel length is 122.23 cm and the total fuel element length is 247.65 cm [11]. The fuel is encased in a Zircaloy-3 can and capped with graphite reflectors on the top and bottom that are encased in a 6063-aluminum can.

Transient conditions in TREAT begin and end with control rod insertion and removal. Control elements are identical to the fuel elements except they contain a 4.445 cm outer radius Zircaloy-2 tube surrounded by a carbon steel tube packed with B_4C powder [11]. There are three types of control rods. Transient rods are the first and are maneuvered to initiate transient conditions [11]. To maintain reactivity of the core during transient operation users rely on compensation rods. Shutdown rods end transient operation (forced back to subcritical) and signify the end of the experiment.

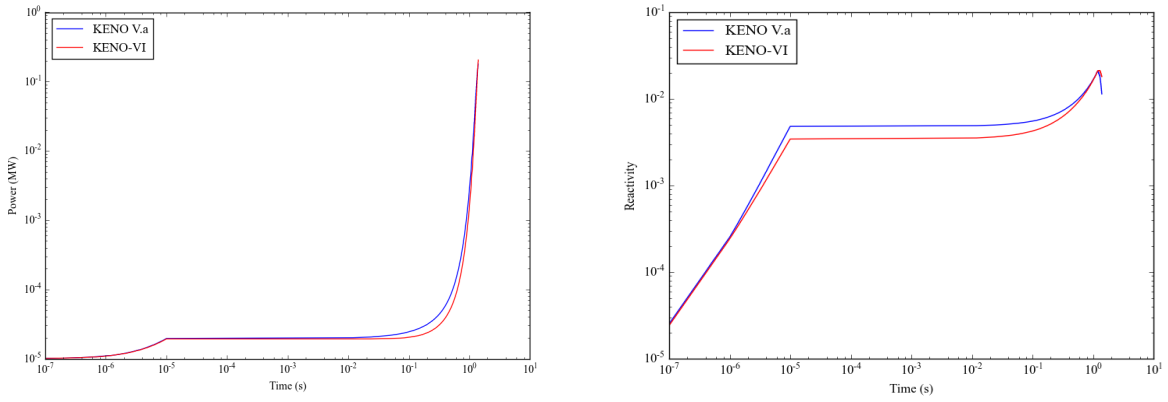
4.3 Arbitrarily Simplified Treat (Single Element)

As a precursor to simulating full TREAT experiments a simplified model was created. Chamfered corners are omitted, fuel elements are homogenized, and dimensions only approximate TREAT elements.

Table 2. Input parameters for the arbitrary simplified TREAT input. Parameters are given for both KENO V.a and KENO-VI inputs.

	KENO V.a	KENO-VI
Number of generations	1500	1500
Particles per generation	10000	10000
Number of regions	21	21
Number of materials	5	5
Flux shapes	5	5
Calculation time	500 min	1400 min

The simplified TREAT inputs transient behavior is simulated by rod withdrawal at time zero, followed by feedback at 1.2, 1.3 and 1.4 seconds with Doppler-broadened cross sections at 301K, 323K and 348K respectively. Cross sections are generated and provided for TDKENO to read in at these specified times. This is done instead of using the feedback model described in Section 2. Other input parameters are given in Table 2. The calculated system parameters are plotted for both KENO V.a and KENO VI to assess the validity of KENO-VI inputs. Power and reactivity, plotted as functions of time, are shown in Figure 4a and 4b, respectively. Inspecting these plots it is clear KENO V.a and KENO-VI agree well with one another.



(a) (b)

Figure 4. Calculated power (a) and reactivity (b) using KENO V.a and KENO-VI inputs.

4.4 Simulating TREAT Transients with TDKENO

The transient experiments selected to simulate with TDKENO are based on the M8 Calibrations Tests (M8CAL). They are some of the most recent experiments performed before the 1994 shutdown and have more complete data sets relative to other TREAT experiments. To assess TDKENOs ability to simulate TREAT transients we examine three temperature-limited transients referred to as #2855, #2856, and #2857. These transients define maximum reactivity of the core and establish limiting safety system settings and safety limits for the core loading [11].

Transient behavior is initiated by quickly withdrawing the bank of transient rods causing a spike in power. An example using fuel element cut-outs of the #2855 input in Figure 5 illustrates the two configurations.

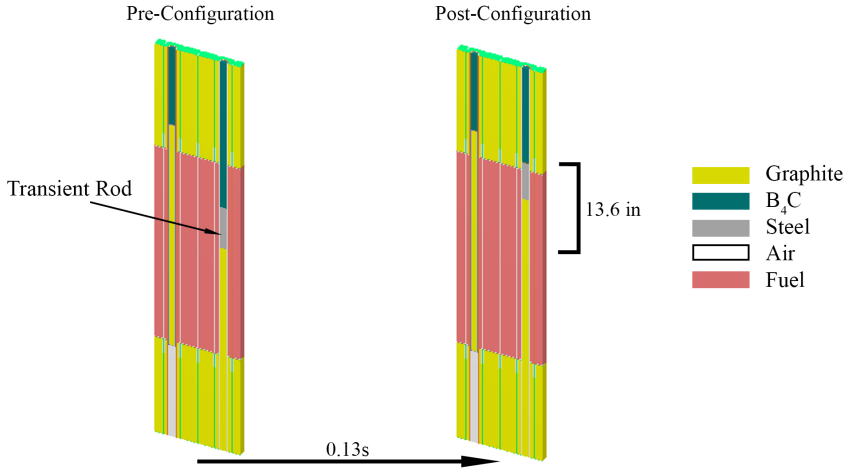


Figure 5. The pre and post rod configurations are illustrated here for transient #2855. The transient rods are pulled up over 0.13s a distance of 13.6 in. resulting in a power pulse.

Simulating each transient begins by creating several inputs corresponding to the pre- and post-configurations of the TREAT core. Additionally, an adjoint input (identical to pre-transient) is required to calculate the adjoint flux. The forward flux is recalculated by KENO at the specified time steps and recombined with the adjoint flux and amplitude portions each time to generate the total flux. Pre and post-transient inputs may be run as stationary cases with CSAS (Criticality Safety Analysis Sequence) to obtain effective multiplication values (k_{eff}). The difference between pre- and post-transient ($\Delta k/k$) provides an estimate of the reactivity insertion that may be compared with reported values from M8CAL.

For each transient several models were generated. One with KENO V.a inputs and another with KENO-VI inputs with no chamfered corner approximation and fewer regions.

4.4.1 Temperature-limited transient 2855

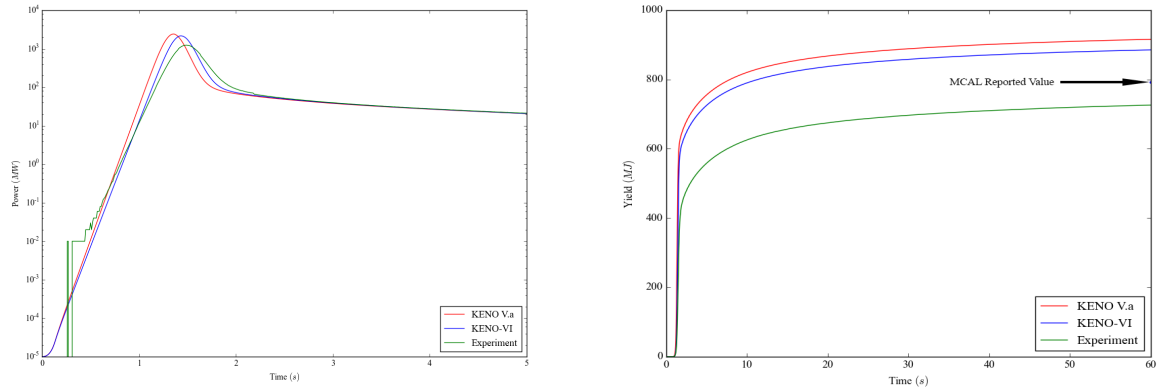
The core loading in each transient experiment remained constant and the control rod removal times and depth were varied. In the temperature-limited transient 2855, transient rods were removed at

time zero and travelled a total of 13.6 in. over 0.13 seconds [11]. The rapid removal results in a power spike, which relaxes due to the negative temperature reactivity feedback [12]. The reported reactivity insertion was 1.8% with no reported uncertainty.

Table 3. The reactivity calculations between experiment, KENO V.a inputs, and improved KENO-VI inputs are summarized. K_{eff} calculations were run with 2000 generations (first 500 skipped) and 20000 particles with CSAS using ENDF-VII cross-sections. The yield is calculated with TDKENO.

Case	Regions	k_{eff} Pre-Transient	k_{eff} Post-Transient	Reactivity Insertion	Yield (MJ)
Experiment	N/A	N/A	N/A	1.8%	792±10%
KENO V.a	11886 4332	1.01019 ± 0.00012	1.03007 ± 0.00012	1.967% ± 0.010%	916 885
KENO-VI		1.01311 ± 0.00014	1.03143 ± 0.00015	1.808% ± 0.012%	

The k_{eff} calculations were performed in multi group and utilized ENDF-VII cross-section libraries. TDKENO simulations with both inputs over estimate the reactivity insertion compared to the experiment. This over estimation is propagated into TDKENO and is observable when calculated parameters are plotted against experiment in Figures 6a and 6b. This is clearly visible in the KENO V.a where a much large power and yield values calculated compared to experiment is observed. The blocky structure of the experimental data is noted during the first half-second and is due to the uncertainty in the detector being on the order of the measured values. As expected, the KENO-VI input agrees better with experiment for reactivity insertion, power and yield. The yield differs from experiment by 11.7%, while KENO V.a differs by 15.7%. This is significant improvement and highlights the need for exact representation of the geometry. Due to time constraints, fewer histories were run with KENO-VI cases than KENO V.a. However, having fewer regions should allow adequate sampling of the system with fewer particles per generation.



(a) **(b)**

Figure 6. TDKENO calculated parameters. The KENO V.a inputs were run with 50000 particles and 5000 generations taking approximately 38900 minutes. Due to time constraints KENO-VI inputs were run with 5000 particles and 2000 generations taking approximately 1175 minutes.

Of all the transients analyzed, #2855 had the largest discrepancy between simulation and experiment. Similar analysis in Reference [10] reported higher than experiment values for peak power and yield.

There are a number of possible reasons for this disagreement. One may be slightly incorrect material definitions resulting in a pre-transient k_{eff} greater than 1. Another may be the reliance on a simple feedback model as opposed to coupling thermal feedback. Quantifying how far the calculations deviate from experiment is difficult due to apparent inconsistencies in the M8CAL document. For instance, the reported value in Table 3 of 792 ± 10% MJ disagreed with the yield of 726 MJ of the experimental plot.

Despite the inconsistencies in the M8CAL data, the agreement is sufficient and TDKENOs ability to accept generalized geometry inputs results in better simulation of transients. Additional histories will be run in the future in order to further validate these conclusions.

4.4.2 Temperature-limited transient 2856

The temperature-limited transient 2856 experiment was carried out by withdrawing the transient rods a distance of 18.60 in. over 0.16 seconds. The experiment was run for 60 seconds and a total of 1572 ± 10% MJ was deposited in the TREAT core [11]. It was also reported that the reactivity insertion is 3.01% with no given uncertainty [11]. TDKENO simulations were carried out and compared to experiment. Results are provided in Table 4. In this case the KENO-VI input performed worse than KENO V.a. We suspect the lack of histories may be responsible as only 1500 generations with 2000 particles per generation were run due to time constraints.

Table 4. The reactivity calculations between experiment, KENO V.a inputs, and improved KENO-VI inputs are compared.

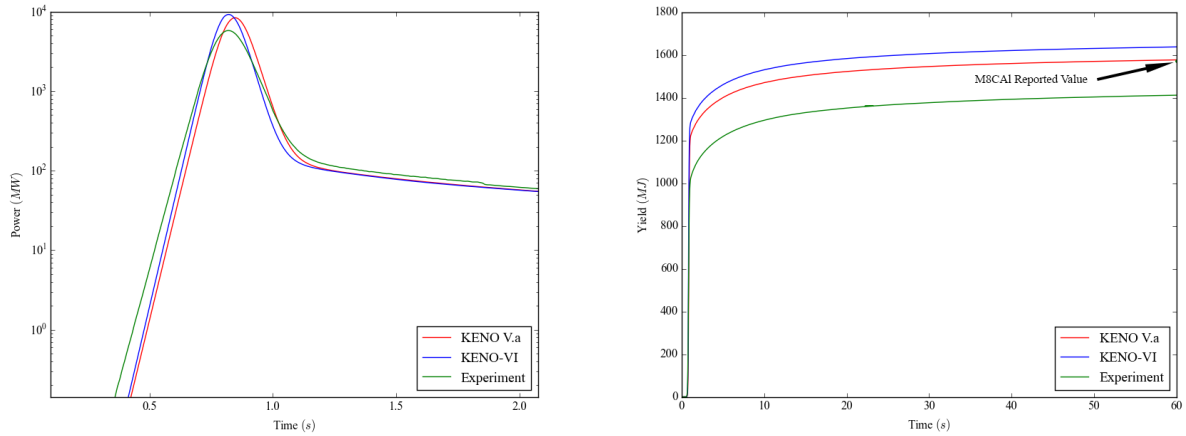
Case	Regions	k_{eff} Pre-Transient	k_{eff} Post-Transient	Reactivity Insertion	Yield (MJ)
Experiment	N/A	N/A	N/A	3.01%	1572±10%
KENO V.a	11902	1.01257 ± 0.00013	1.04333 ± 0.00012	3.04% ± 0.010%	1576
KENO-VI	4332	1.01303 ± 0.00015	1.04474 ± 0.00015	3.13% ± 0.014%	1637

Both calculations are larger than the reported reactivity insertion. Again, this is attributed to the larger than experimental values for peak power and yield in TDKENO. The results of TDKENO with both inputs are in Figures 7a and 7b. Figure 7a has a shorter time scale to highlight the pulse where the deviation between TDKENO and experiment is greatest.

Again there are inconsistencies in the M8CAL document between reported values and plotted data. For example, the yield after 60 seconds is 1400 MJ according to the experimental plot, while the M8CAL document specified a yield of 1572 MJ [11]. If the reported value is correct than

TDKENO is doing well to predict the yield. Issues with the slope to the peak remain most likely due to the lack of thermal feedback.

Overall, the results TDKENO produced with both versions of KENO are promising and with additional development will be able to predict the behavior of TREAT experiments with high degrees of accuracy.



(a) **(b)**

Figure 7. Comparison of experimentally reported and TDKENO calculated power (a) and yield (b) over the first 5s of transient 2856. The KENO V.a inputs were run with 50000 particles and 5000 generations taking approximately 38900 minutes. Due to time constraints KENO-VI inputs were run with 2500 particles and 1500 generations taking approximately 1175 minutes.

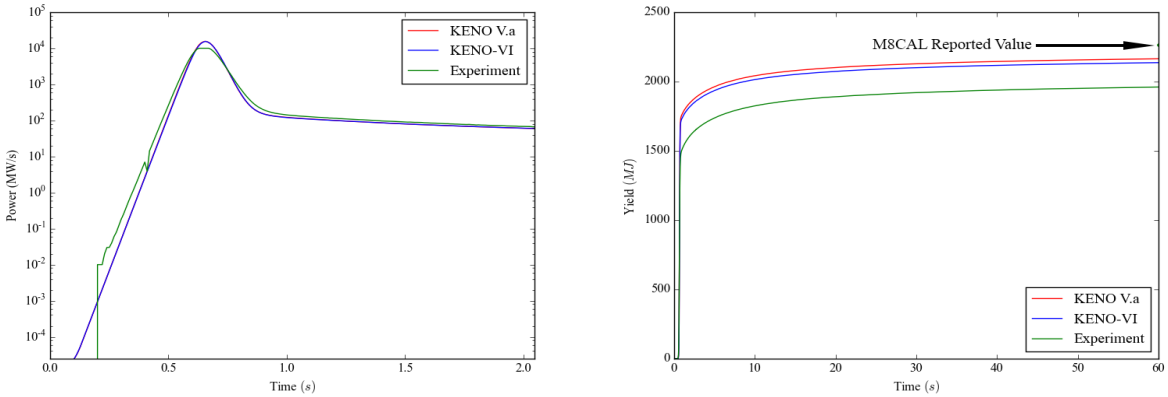
4.4.3 Temperature-limited transient 2857

The final experiment simulated with TDKENO is temperature-limited transient #2857. Here the transient rods travelled 21.5 in. over 0.18s [11]. Over the 60 second period, a total of 2265 ± 10% MJ was deposited in the TREAT core [11]. Reactivity insertion was reported as 3.84%.

Table 5. The reactivity calculations between experiment, KENO V.a inputs, and improved KENO-VI inputs are summarized. Each input is run with 2000 generations (first 500 skipped) and 20000 particles. All inputs are run with KENO using ENDF-VII cross sections.

Case	Regions	Pre-Transient	Post-Transient	Reactivity Insertion	Yield (MJ)
Experiment	N/A	N/A	N/A	3.84%	2265±10%
KENO V.a	11878	1.01416 ± 0.00013	1.05331 ± 0.00013	3.86% ± 0.011%	2164
KENO-VI	4332	1.01510 ± 0.00014	1.05443 ± 0.00014	3.87% ± 0.012%	2136

This experiment was simulated with TDKENO. The results of calculations and experiment are compared in Table 5. Both calculated reactivity insertion values and peak power are slightly over estimated when compared to the experiment. This is not as much of a concern for the peak power as we are more interested in the yield. Once again there is a discrepancy between the experimental data plot and what was reported in M8CAL as is shown in Figure 8b. Though both models of TREAT are calculating a yield value within the uncertainty given in the M8CAL experiment. Other papers, such as Reference [12], suggest using the value given in the M8CAL document, which give us confidence that TDKENO is doing quite well for this transient.



(a) **(b)**

Figure 8. Comparison of experimentally reported and TDKENO calculated power (a) and yield (b) over the first 5s of transient 2857. The KENO V.a inputs were run with 50000 particles and 5000 generations. Due to time constraints KENO-VI inputs were run with 2500 particles and 1500 generations.

5. CONCLUSION/FUTURE WORK

Through comparison to benchmark and sample problem the integration of KENO-VI into TDKENO appears successful. Using improved inputs made possible with KENO-VI we generally see greater agreement with experiment. The large uncertainties in the M8CAL document and inconsistencies in reported values will require additional comparison between TDKENO and TREAT experiments. To further improve these simulations, TDKENO may be coupled to a thermal hydraulics code. Running these simulations is time consuming. Additional work is underway to incorporate a parallel version of KENO-VI into TDKENO and to accelerate intensive tasks by offloading onto graphics cards. Currently, TDKENO is an excellent tool for transient analysis. Future improvements to the physics and computational time will make it an exceptional tool for calibrating TREAT experiments.

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