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## Enhanced geometric capabilities for the transient analysis code T-ReX and its application to simulating TREAT experiments



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#### ABSTRACT

Advances in computational architecture have prompted a resurgence in the simulation of reactor transients from first principles. Most codes are unable to simulate transient events with complex models, and require numerous approximations. The code T-ReX (Transient-Reactor eXperiment simulator), an extensive update to TDKENO, has been developed as a transient analysis tool with few geometric limitations, and minimal theoretical approximations. T-ReX achieves this by employing the Improved Quasi-Static (IQS) method to solve the timedependent Boltzmann transport equation with explicit representation of delayed neutrons. The primary change in T-ReX relative to TDKENO is the incorporation of a modified version of the Monte Carlo code KENO-VI to calculate the flux shape and model the geometry of a problem. Using KENO-VI to model systems allows exact representation of the geometry. The changes to T-ReX are verified by comparison of solutions to computational benchmark problems found with a previous version of TDKENO that made use of KENO V.a, and several other codes with time-dependent capabilities. In addition, a three-dimensional KENO-VI model of the Transient Reactor Test Facility (TREAT) core is used in simulations of several temperature-limited transient experiments from the M8 Calibration series. T-ReX produces results that agree with benchmark problems and are in better agreement with TREAT experimental data than TDKENO.

#### 1. Introduction

The typical approach for simulating reactor transients relies on theoretical constructs that discretize the solution space of the neutron transport equation, thereby requiring a mesh-based description of the model. Generating such meshes may be time consuming for large threedimensional problems and often makes several approximates to the geometry (e.g., curved surfaces). This motivates the usage of Constructive Solid Geometry (CSG) employed in Monte Carlo codes as the means to generate detailed reactor models. The code T-ReX (Transient-Reactor eXperiment simulator) is able to solve the time-dependent transport equation with the explicit representation of delayed neutrons with minimal approximations using the Improved Quasi-Static (IQS) method and making use of a Monte Carlo code to represent the geometry of system. A fundamental assumption in the IQS method is that the total angular flux may be factored into the product of two functions: the flux shape and flux amplitude [\(Henry, 1958](#page--1-0)). The amplitude is highly time-dependent following a reactivity change and is formulated as the solution to the point kinetics equations. Conversely, the flux-shape is obtained from the solution to a modified fixed source

neutron transport equation and in general, weakly dependent on time. It is important to note that IQS differs from the common Quasi-Static (QS) method, by explicitly representing the time-derivative of the flux shape with a backwards-difference approximation [\(Ott and Meneley,](#page--1-1) [1969\)](#page--1-1). Thus, in IQS the flux shape is coupled in time with the amplitude and may be found by solving the standard form of the transport equation, but with (1) a modification to the total cross section, and (2) an additional source term from the backward-difference approximation of the flux shape derivative [\(Ott and Meneley, 1969; Bentley, 1996\)](#page--1-1). The IQS method results in computational savings compared to direct integration, as the most computationally intensive portion of the calculation, the calculation of the flux shape, may be solved less frequently than the flux amplitude. Furthermore, the IQS method is enticing because it has fewer approximations than methods such as quasi-static, nodal, and finite difference methods ([James and Louis, 1976](#page--1-2)).

The main drawback of the IQS methodology implemented in TDKENO until recently is that only KENO V.a models could be analyzed. KENO V.a, while computationally efficient, is only able to analyze models constructed with combinations of basic shapes such as spheres, cylinders, and cuboids [\(Petrie and Landers, 1984](#page--1-3)). In addition,

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regions may not intersect or be rotated. KENO-VI, on the other hand, supports a wide array of geometries including planes, dodecahedrons, wedges, parallelepiped, etc [\(Hollenbach et al., 1995](#page--1-4)). Additionally, it allows regions to be rotated and to intersect. To represent systems exactly, KENO-VI has been modified to solve for the flux shape as the transport solver within T-ReX.

With significant modifications made to T-ReX, we verify the changes are correctly implemented by solving the TWIGL benchmark problems, described in [\(Hageman and Yasinsky, 1969\)](#page--1-5), with T-ReX using KENO V.a, and KENO-VI models. We then compare the results from T-ReX calculations to solutions from TDTORT ([Goluoglu and Dodds, 2001](#page--1-6)), CONQUEST [\(Gehin, 1992\)](#page--1-7), SPANDEX [\(Aviles, 1993\)](#page--1-8), QUANDRY ([Smith, 1979](#page--1-9)), and MAF ([Ban et al., 2012\)](#page--1-10).

In addition to verifying modifications to T-ReX, we investigate the particularly challenging problem of simulating experiments performed at the Transient Reactor Test Facility (TREAT) at Idaho National Laboratory (INL). TREAT is a reactor capable of safely simulating reactor transients in order to evaluate fuel performance under such conditions. It performed nearly three thousand transient experiments before being put in standby status in 1994 [\(Bess and DeHart, 2015\)](#page--1-11). In an effort to expand fuel testing capabilities including the testing of accident-tolerant fuel, TREAT is being returned to operation, with experiments beginning as early as 2018. Recent work in [\(Goluoglu et al.,](#page--1-12) [2014; Paluch et al., 2016; Mausol](#page--1-12)ff et al., 2016) using T-ReX has focused on simulating experiments performed at TREAT just before it was placed into standby status in 1994. The goal of such calculations is two part, one is to provide reference solutions for comparison to other codes, and the other is to one day help optimize the pre-test vehicle through simulation in order to minimize the number of costly pre-test calibration experiments required before useful experiments could take place. To further these efforts, the TREAT core is modeled exactly with KENO-VI, and simulated results are compared previous results with approximate KENO V.a models and to experimental data.

#### 2. Theory

Typical transient analyses techniques of reactor cores may have require approximations that may induce error in some situations. For instance, the often used point kinetics approach ignores variations in the flux shape as a function of time and therefore is unable to properly handle transients with spatial flux tilts [\(James and Louis, 1976\)](#page--1-2). Another example may be observed for methods which employ diffusion theory instead of transport, which have been shown to be invalid in void or strongly absorbing regions such as areas surrounding rod insertions [\(Rowlands and Eaton, 1980](#page--1-13)). The IQS method when built upon transport theory allows for the spatial variation in the flux over time with the ability to resolve the flux near highly absorbing regions, and outperforms standard Quasi-Static methods in thermal systems [\(Ott,](#page--1-14) [1966\)](#page--1-14). An essential part of the IQS (and QS) method is the observation that the flux may be factored into two functions, the amplitude and shape. ([Ott and Meneley, 1969\)](#page--1-1).

<span id="page-1-0"></span>
$$
\phi(\bar{r}, \bar{\Omega}, E, t) = A(t)\Psi(\bar{r}, \bar{\Omega}, E, t)
$$
\n(1)

In Equation [\(1\),](#page-1-0) A is the amplitude of the flux, and  $\Psi$  is the flux shape. The amplitude is assumed to be highly dependent on time, and as will be shown, is found from the solution to the point kinetics equations. The flux shape in general, varies on time scale much slower than the amplitude and thus does not require calculation as often. However, during events like control rod movement, the spatial distribution of neutrons changes rapidly, necessitating more frequent updates of the flux shape. One can think of the shape as providing the spatial distribution of neutrons at any one time and the amplitude as the magnitude of the flux at some time. In general, determining the flux shape requires calculation time on par with the total flux, computer time may be spared since the flux shape may be updated less frequently than the total flux as in direct methods for solving the time-dependent

transport equation. A brief overview for obtaining all the governing IQS equations is presented here, but can be found with greater detail in the literature [\(Waddell, 1993; Bentley, 1996; Goluoglu and Dodds, 2001\)](#page--1-15).

To derive the governing equations in the IQS methodology, we first consider the time-dependent transport equation with the explicit representation of delayed neutrons. It can be written as

$$
\frac{1}{\nu(E)}\frac{\partial \phi(\bar{r}, \bar{\Omega}, E, t)}{\partial t} + \nabla \phi \cdot \overline{\Omega} + \Sigma_t(\bar{r}, E, t)\phi(\bar{r}, \bar{\Omega}, E, t) =
$$
\n
$$
\iint \Sigma_s(\bar{r}; \bar{\Omega}', E' \to \bar{\Omega}, E; t)\phi(\bar{r}, \bar{\Omega}', E', t)d\Omega'dE' +
$$
\n
$$
\chi_p(E)(1 - \beta)\iint \nu\Sigma_f(\bar{r}, E', t)\phi(\bar{r}, \bar{\Omega}', E', t)d\Omega'dE' +
$$
\n
$$
\sum_j \lambda_j C_j(\bar{r}, t)\chi_j(E) + Q,
$$
\n(2)

with the following definitions,

- *υ* = neutron speed,
- $\phi$  = angular flux,
- $\bar{r}$  = position vector,
- $\overline{\Omega}$  = unit vector for particle direction,
- $E =$  energy,
- $\Sigma_t$  = total macroscopic cross section,
- $\Sigma_s$  = macroscopic scattering cross section,
- $\chi_p$  = normalized energy spectrum of prompt neutrons,
- $\beta$  = total delayed neutron fraction,
- $\nu$  = average number of neutrons per fission,
- $\Sigma_f$  = macroscopic fission cross section,
- $j$  = precursor group index,
- $\lambda_i$  = decay constant for delayed neutron precursor group *j*,
- $C_i$  = concentration of delayed neutron precursors for group *j*,
- $\chi$ <sup>*j*</sup> = normalized energy spectrum for precursor group *j*,

and the time-dependent precursor concentration equations are defined as:

$$
\frac{\partial}{\partial t}C_j(\mathbf{F},t) = \iint \nu \beta_j \phi(\mathbf{F}, \overline{\Omega}', E', t) d\Omega' dE' - \lambda_j C_j(\mathbf{F},t), j = 1...N ,
$$
 (3)

where  $N$  is the total number of delayed neutron groups. The prompt neutron spectrum is explicitly treated as well as the delayed spectrum.

Another important quantity used throughout the derivation and in the calculation of the point kinetics parameters is the adjoint neutron flux. The adjoint flux provides a weighting function for the relative neutron importance. The concept of neutron importance and relevant discussion may be found in a variety of reactor physics text books, e.g. ([Bell and Glasstone, 1970](#page--1-16)). A weighting function like the adjoint is useful, for instance, to prevent long lived neutrons may be overvalued compared to short lived neutrons. In [\(Gehin, 1992\)](#page--1-7), Gehin showed through comparison to other weighting functions the adjoint flux is the best choice in the IQS implementation. It is worth noting in this IQS formulation the adjoint is solved for the initial pre-transient system and used in all subsequent calculations. This gives the importance based on the initial neutron flux distribution of the problem, resulting in a weighting factor that is generally valid when the flux distribution does not change dramatically. However, one must keep in mind situations may arise in which the shape of the neutron flux does change significantly and requires recalculation of the weighting function ([Becker,](#page--1-17) [1968\)](#page--1-17).

$$
-\overline{\Omega}\nabla\phi^* + \sum_t \phi^* = \iint \sum_s (\overline{r}; \overline{\Omega}, E \to \overline{\Omega}', E') \phi^*(\overline{r}, \overline{\Omega}', E', t) d\Omega' dE'
$$
  
+ 
$$
\frac{1}{k_{eff}} \iint \chi(E') \nu \Sigma_f(\overline{r}, E) \phi^*(\overline{r}, \overline{\Omega}', E') d\Omega' dE'
$$
(4)

At this point we have defined the flux factorization, the time-dependent transport equation, the time-dependent precursor concentration equations, and the adjoint flux. Now we illustrate how the transport equation is modified to include the factorization that gives rise to the flux shape and amplitude equations. Before we can make use of the factorization we must impose a condition to ensure uniqueness. The factorization in Equation [\(1\)](#page-1-0) is made unique with the following definition [\(Henry, 1958\)](#page--1-0).

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