ANS NETS 2019 – Nuclear and Emerging Technologies for Space
Richland, WA, February 25–27, 2019, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2019)

MONTE CARLO-INFORMED DECAY HEAT MODEL FOR CERMET LEU-NTP SYSTEMS

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Two methodologies for performing decay heat analysis with Monte Carlo simulations were developed and implemented on a representative nuclear thermal rocket (NTR) design. This paper presents the underlying theory, discusses the methodology, and states the key results. This work investigated the importance of utilizing a time-dependent Q-value for fission in NTRs due to its short burn time. Two approaches for deriving the Q-value were taken: one based on deconvolving the fission rate from the power to yield the rate of fission energy deposition, and the other based on the convergence of the fission product decay power during a long burn. The fission product decay power method produces results closer to theoretical values, as it captures more of the underlying physics occurring during burnup such as fission product transmutation. The calculated Q-values were employed to derive decay power profiles which were compared to the Emrich[1] model. According to these new models, the Emrich model underestimates the amount of hydrogen required for decay heat cooling by as much as 23.3%.

I. Introduction

Nuclear Thermal Propulsion (NTP) systems can offer great benefits (e.g. reduced travel time, reduced launch cost) for deep space explorations. Unlike conventional rocket engines, nuclear rockets heat their propellant via a high-temperature fission reactor. As a result, the engine must be cooled even after shutdown due to the build-up and decay of fission products that continue produce heat. The removal of this decay heat is essential because the reactor still operates up to 7% of full power after shutdown due to the deposition of beta particles and gamma rays within the core. However, due to the short operating times of these engines, on the order of 12 minutes, the decay of the fission products is not in equilibrium with the fission product production, and as such, a steady-state value for the recoverable energy released by fission, denoted Q_f, cannot be used to accurately model decay heat. In order to derive an accurate model for the decay heat of an NTR, $Q_f(t)$ must be found via various Monte Carlo simulations and employed to calculate the power history. Unfortunately, Monte Carlo software codes like MCNP and Serpent have preprogrammed Q-values for fission for various fissile isotopes.

The current model for the decay heat produced by an NTR was derived by Emrich[1], who combined point kinetics and Todreas and Kazimi's[2] decay heat relationships. This model has flaws resulting from the use of the point kinetics equations whose derivation assumes that the flux shape remains constant during the transient and that reactivity is inserted in a stepwise fashion[1]. These assumptions are particularly invalid for NTR systems, as the shutdown mechanism is control drums on the periphery of the core. These drums cannot rotate infinitely quickly, and their rotation has an impact on the radial power profile of the system. Nevertheless, some assumptions must be made in this analysis as a first step toward developing a fully-accurate method of determining decay heat production in an NTP system. Because of the uncertainties about how quickly control drums rotate, the system is assumed to shut down according to the point kinetic equations via a negative ramp reactivity insertion of \$2 in 1.2 seconds. Similarly, the start-up transient is modeled as a 30 second transient with a 1.2 second linear reactivity insertion of \$0.6955. Serpent directly outputs the decay heat produced during each depletion step of a simulation, so this is used in place of Todreas and Kazimi's model to roughly estimate a new, Monte Carlo-informed, decay heat model for NTRs.

II. Methodology

The recoverable energy released during a fission event is classified in two categories: prompt energy and delayed energy. The following equations describe the contributions to $Q_f(t)$:

$$Q_f(t) = Q_p + Q_d(t) \tag{1}$$

$$Q_p = Q_{ff} + Q_{pn} + Q_{p\gamma} + Q_{n,\gamma} \tag{2}$$

$$Q_d(t) = Q_{dn}(t) + Q_{d\gamma}(t) + Q_{d\beta}(t) \tag{3}$$

where Q_p is the time-independent portion of the energy released by fission, typically released in the first millisecond after a fission event, and $Q_d(t)$ is the time-dependent portion of the energy released by fission, defined as time-delayed energy released greater than 1 millisecond after a fission event. Q_p is the sum of the energy released by the fission fragments (Q_{ff}), by the prompt neutrons (Q_{pn}), by the prompt gammas ($Q_{p\gamma}$), and by the gammas released in radiative capture reactions ($Q_{n,\gamma}$). $Q_d(t)$ is the sum of the energy released by delayed neutrons ($Q_{dn}(t)$), by delayed gammas released by the

decay of fission products ($Q_{d\gamma}(t)$), and by delayed betas released via the beta decay of fission products ($Q_{d\beta}(t)$). The goal of this study is to determine the contributions from each of these fission energy components to yield a design-specific $Q_f(t)$ which is applied to the core during a power history calculation, assuming the fission rate history is known from point kinetics.

II.A. Serpent Model

Serpent is the Monte Carlo software code of choice for this study, as decay heat from both fission products and actinides is a direct output of its simulations. Furthermore, Serpent's detector functions measure all prompt components of $Q_f(t)$ via heating tallies. In addition, Serpent's coupled neutron-photon transport capabilities have been improved in recent updates, allowing for higher-fidelity photon calculations.

While the focus of this paper is developing a methodology which can be applied to any reactor design in order to derive the time-dependent solution for the energy released by a fission event, it is important to briefly describe some key design parameters of the core used in this analysis. The representative core is composed of an LEU MoW-UN cermet fuel. The moderator is $ZrH_{1.8}$, and H_2 is used as the coolant/propellant. This design was derived through an optimization study to maximize engine performance. The basic elements of this concept are reminiscent of an inverted SNRE design.

Only two detectors in Serpent are required to derive the prompt component of the Q-value for fission. A macroscopic total heating cross section tally, essentially equivalent to an F8 tally in MCNP, is used to determine $Q_{ff} + Q_{pn}$. Using this tally, energy deposition is calculated based on the KERMA (Kinetic Energy Release in Materials) coefficients relating the neutron flux to the neutron heating rate. More specifically, calculating heating this way yields the local prompt neutron heating including the kinetic energy of fission fragments. The delayed heating and prompt gamma energy deposition are not accounted for with this tally. As a result, an analog photon heating tally, equivalent to an *F8 tally in MCNP, is employed in conjunction with Serpent's coupled neutron-gamma simulation mode. The analog photon heating tally scores the heat deposition due to neutron-induced reactions which primarily include both fission and radiative capture ($Q_{p\gamma} + Q_{n,\gamma}$).

It is important to remark that the coupled neutron-gamma simulations in Serpent do not include the delayed gammas emitted from the decay of fission products or from the decay of transmutation products. Two methods account for the delayed betas and gammas emitted in the decay of fission products and transmutation products. By using depletion steps, it is possible to determine the amount of decay heat released as a function of time along the operating period of the NTR. In addition, Serpent is capable of distinguishing between the decay heat from actinides (α-particles) and the decay heat from fission products (β-particles and γ-rays). This output parameter is used to derive the delayed Q-value.

The first method, which will be known as the pulse method, comes directly from a rigorous mathematical relation between the fission rate and power. It is important to note the separate time variables representing the time along the reactor's operational timeline, T, and the time after a fission event, t.

$$P(T) = \int_0^T R(T - t') * F(t')dt' \tag{4}$$

$$R(t) = \frac{d}{dt} Q_f(t) = \frac{d}{dt} Q_d(t) \tag{5}$$

$P(T)$ is the power of the reactor as a function of operating time, $F(T)$ is the fission rate as a function of operating time, and $R(t)$ is the rate at which recoverable energy is absorbed in the reactor due to a single fission event as a function of time after the fission event. Qualitatively, this type of relation is known as a convolution. If the fission rate history is known from solving the point kinetic equations, and the power is output by Serpent, then the fission rate is deconvolved from the power, yielding $R(t)$. However, to avoid complications, an even simpler method is adopted which involves the use of a Dirac delta function, $\delta(t)$. To avoid discussing the mathematics, the properties of the Dirac delta function are only briefly mentioned here. A delta function is a distribution which is zero everywhere except at a single point, at which the value is infinite. Conveniently, the Dirac delta function has the following sifting property:

$$\int_{-\infty}^{\infty} f(t)\delta(t - a)dt = f(a) \tag{6}$$

This sifting property is used to calculate $R(t)$ and, by extension, $Q_f(t)$. If the fission rate is in the form of a delta function, then $P(T) \propto R(T) \propto \frac{d}{dt} Q_d(t)$.

The second method, known as the long burn method, entails no rigorous derivation. For this approach, the NTR engine is run for a long time compared to the expected burn times at low power to avoid undesirable burnup effects. The time behavior of the decay heat is expected to mimic the time behavior of $Q_d(t)$. However, the decay power in Serpent is calculated with pre-determined default values for various isotopes based on the heating value of the respective isotope compared to U-235. Therefore, Serpent's calculated Q-value for the design is scaled based on the ratio of the decay power and fission power to yield $Q_d(t)$.

II.B. Emrich Model

Currently, the most accurate model for decay heat in an NTR was derived by Emrich[1]. The derivation combines point kinetics with Todreas and Kazimi's[2] relation for decay power as a function of time following reactor shutdown to yield the following expression:

$$P_{sd}(t) = P_{fp}\left\{\frac{\rho}{\rho-\beta}e^{\frac{\rho-\beta}{\Lambda}t} - \frac{\beta}{\rho-\beta}e^{\frac{-\rho\lambda}{\rho-\beta}t} + 0.066\left[t^{-0.2} - \left(t_{fp}+t\right)^{-0.2}\right]\right\} \quad (7)$$

where $P_{sd}(t)$ is the reactor power level t seconds after shutdown, P_{fp} is the reactor full power level, t_{fp} is the time in seconds during which the engine is at full power, ρ is the reactivity insertion causing the reactor to shut down, β is the delayed neutron fraction, Λ is the prompt neutron lifetime, and λ is the one-group neutron precursor decay constant. Note that this equation can be integrated over the shutdown period to yield the total energy released after the reactor operating period is over which can be used to solve for the propellant requirements for decay heat cooling. By performing decay heat analysis in a Monte Carlo code, this relation is improved, given its assumptions and simplifications.

III. Results

The results presented in this paper present a methodology to derive the value of Q_f in a reactor, specifically an NTR, that give reasonable results. While this methodology has some simplifications in the start-up and shutdown transients, the results improve upon Todreas and Kazimi's[2] decay heat relation for an NTR.

III.A. Prompt Contributions of Q-value

The prompt contributions of Q_f include the kinetic energy of the fission fragments, the kinetic energy of the prompt neutrons, the energy of the prompt gammas, and the energy of gammas produced in radiative capture reactions induced by prompt neutrons. The first two components, the energy from the fission fragments and prompt neutrons, are calculated using the dr -4 response function which measures the local prompt neutron heating component of the fission energy deposition. This tally gives the power deposited (or released, because this energy is deposited locally) via the previously-mentioned fission components. The Q-value is related to the steady-state power, P_f, via the following equation:

$$Q_f\Sigma_f\phi = P_f \quad (8)$$

in which $\Sigma_f\phi$ is the fission reaction rate. The Q-value is also defined by Eq. (9).

$$\sum_r Q_r = Q_f \quad (9)$$

where r represents the various fission energy components. In Serpent, a default Q-value is used for each fissile/fissionable isotope which includes all recoverable components of fission. The default value for U-235 is $202.27\ \mathrm{MeV/fission}$, and Serpent's calculation for the Q-value for the reference core is $202.379 \pm 4.25 \times 10^{-4}\ \mathrm{MeV/fission}$, denoted $Q_{f,Serpent}$. Therefore, if one measures the power deposition related to the fission energy component r, denoted as P_r, Q_r is calculated with Eq. (10).

$$\frac{Q_r}{Q_{f,Serpent}} = \frac{P_r}{P_f} \quad (10)$$

The dr -4 response function yields 427.015 ± 0.201 MW, representing all fission energy components except delayed neutrons, prompt gammas, radiative capture reactions, and delayed gamma/beta components. Plugging this result into Eq. (10) gives a value for $Q_{ff} + Q_{pn}$ of $172.838 \pm 0.0814\ \mathrm{MeV/fission}$.

A similar technique is employed for the prompt photon contributions. The dr -12 response function yields the analog photon heating component of fission due to prompt gammas and the binding energy released in capture reactions. The tally results in a value of 34.2387 ± 0.018 MW which, when used with Eq. (7), corresponds to a value for $Q_{p\gamma} + Q_{n,\gamma}$ of $13.8584 \pm 0.0073\ \mathrm{MeV/fission}$. Therefore, summing these two results yields the Monte Carlo-derived value for Q_p, the prompt fission energy component, of $186.696 \pm 0.0887\ \mathrm{MeV/fission}$. This particular value agrees well with two previously-derived prompt recoverable energy from fission values. Eades and Caffrey[3] calculated the prompt Q-value for a slightly different NTR to be $185.58\ \mathrm{MeV/fission}$, and Sterbentz[4] calculated the prompt Q-value for the Advanced Test Reactor (ATR) at Idaho National Laboratory to be $188.95\ \mathrm{MeV/fission}$. Both of these studies used MCNP for the simulations.

III.B. Delayed Contributions of Q-value

For the pulse method, a picosecond pulse with a fission rate of $10^{27}\ \mathrm{fiss/s}$ is used for a total of 10^{15} fissions and a fission rate, $F(T)$, described by the following equation:

$$F(T) = 10^{15}\delta(t) \quad (11)$$

Therefore,

$$P(T) = 10^{15}R(T) = 10^{15}\frac{d}{dt}Q_d(t) \quad (12)$$

because T and t are equivalent due to the instantaneous nature of the fission rate profile. $P(T)$ in Eq. (12) is the decay heat due to fission products. Scaling the decay power

profile to find $R(T)$ and numerically integrating to calculate $Q_d(t)$ yields a steady-state value of 9.905 ± 0.0887 MeV/fission. According to Sterbentz[4], the delayed gamma and beta components should be relatively close to 12.8 MeV/fission which indicates that the pulse method yields lower values than expected. On the other hand, the long burn method results in a delayed Q-value of $12.690 \pm 2.67 \times 10^{-5}$ MeV/fission which agrees well with the literature values. In Figures 1 and 2, the time behavior of these two cases are compared versus the analytical model presented in Todreas and Kazimi[2],

$$R_{analytic}(t) = 2.66t^{-1.2} \quad 10\ s \leq t \leq 100\ days \qquad (13)$$

with the prompt value for Q equal to 188.95 MeV/fission from the ATR report[4].

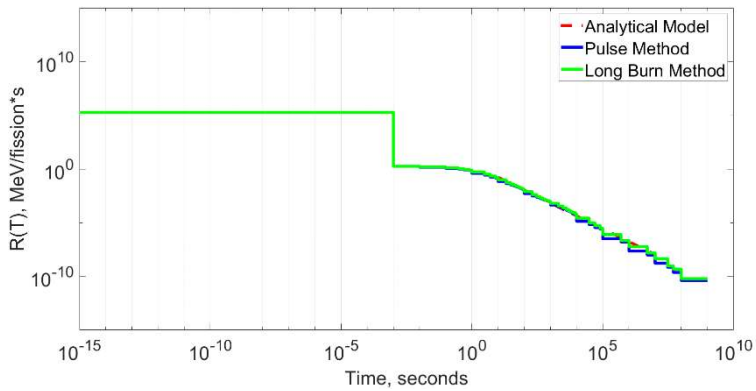

Figure 1. Rate of recoverable fission energy deposition as a function of time.

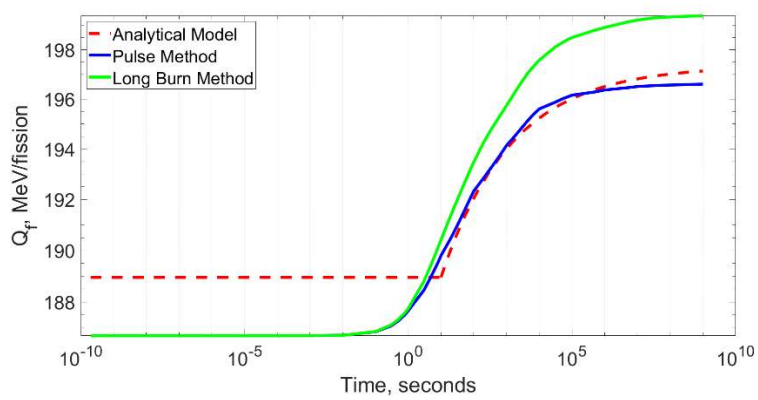

Figure 2. Recoverable fission energy deposition as a function of time.

It is hypothesized that the long burn method yields higher Q-values due to the sustained irradiation of the fission products inducing sdrgkjhdgjdshtransmutation reactions which release more energy compared to the pulse method in which no irradiation occurs after the first picosecond. A more accurate representation of the NTR is the long burn method, as many exothermic neutron capture reactions occur in the fission products which must be considered. Even though the philosophy underlying the pulse method is more substantiated with theory, the long burn method yields Q-values closer to previous work. This discrepancy must be evaluated further in future work.

III.C. Application of Results to NTR Burn

The two models are applied to a representative NTR burn, with a 30 second start-up transient followed by 12 minutes at full power and finally a $-\$2$ reactivity insertion for shutdown. The fission rate, pictured in Figure 3, during full power operation is assumed constant. The start-up and shutdown transients are assumed to occur due to linear reactivity insertions of $\$0.6955$ and $-\$2$, respectively, in 1.2 seconds. The value of the reactivity for the start-up transient is derived via a numerical point kinetics solver which assumes that P_0 is 1 MW, and the power at 30 seconds is ~520 MW.

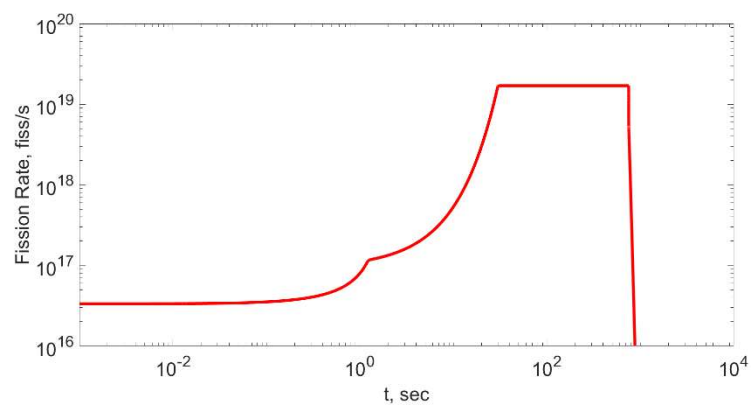

Fig. 3. Fission rate profile for typical NTR burn.

This fission rate profile is convolved with the rate of recoverable fission energy deposition profile in Figure 1 to yield the total power profile of the NTR during and after the operating period. This profile exhibits a stepped behavior in the tail of the power history. This is a manifestation of the same behavior in the $R(t)$ profile. Because the decay heat is measured over various time bins in Serpent, $R(t)$ is treated as constant over the time bin. Furthermore, once the fission rate has decayed to 0, the time behavior of the power is completely dependent on the time behavior of $R(t)$, resulting in the steps. However, due to a preference for smooth curves, the power tail is smoothed based on the midpoints of the steps with a moving average filter and fit to a best fit line as defined in Eq. (14).

$$\frac{P(t)}{P_0} = a\left[t^{-b} - \left(t_{fp} + t\right)^{-b}\right] \qquad (14)$$

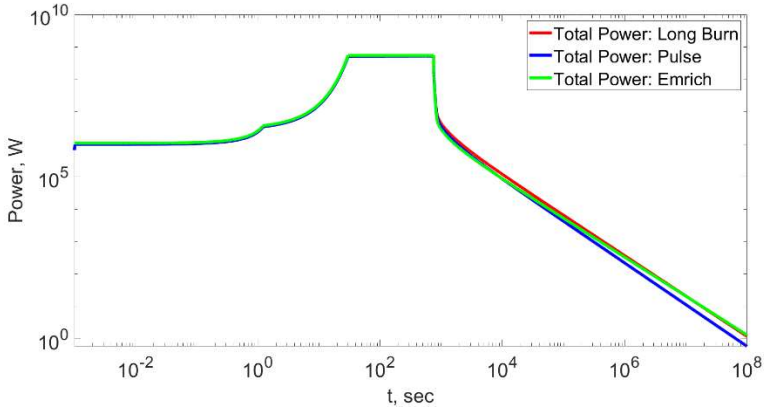

Fig. 4. Power profiles with the tail approximated by a best-fit equation for accurate comparison to Emrich model.

The equations derived from the two methods in place of Todreas and Kazimi's[2] relation are listed below:

$$\frac{P_{long}(t)}{P_0} = 0.1104\left[t^{-0.2436} - \left(t_{fp} + t\right)^{-0.2436}\right] \quad (15)$$

$$\frac{P_{pulse}(t)}{P_0} = 0.0993\left[t^{-0.2847} - \left(t_{fp} + t\right)^{-0.2847}\right] \quad (16)$$

The profiles demonstrate the expected behavior of a ~20 MW power increase over the 12 minute, full power portion of the burn, as the fission rate is constant, due to the increasing Q-value. Until approximately 150 minutes after shutdown, the Emrich model underestimates the decay power production for both models. After 150 minutes, the Emrich model overestimates the pulse method but continues to underestimate the long burn method until 142 days post shutdown. However, by this time, the decay power is on the order of Watts and actively cooling the engine is no longer necessary. With a radiative term of approximately 7 kW, the key parameter is the active cooling time predicted by each model. Figures 5 and 6 depict the decay power profiles during this time with the percent difference.

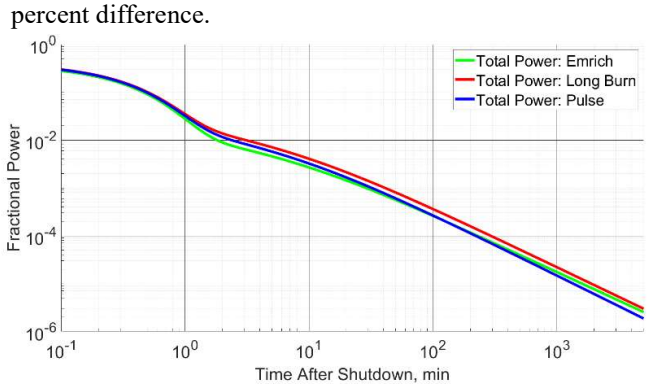

Fig. 5. Decay power profile during the period of reactor shutdown which requires active cooling.

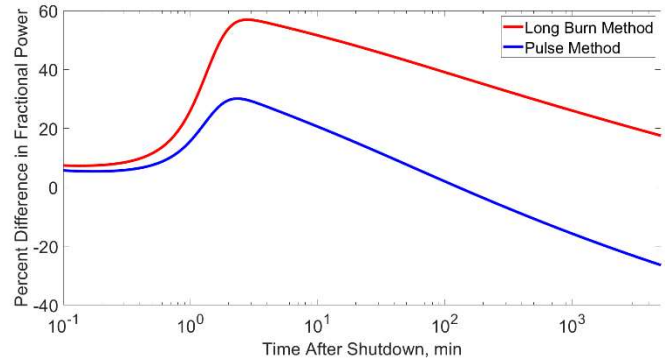

Fig. 6. Absolute percent difference between normalized decay power profiles and normalized Emrich model.

The Emrich model predicts that the core will reach 7 kW in 21.02 hours, the pulse method predicts 18.11 hours, and the long burn method predicts 25.14 hours. With the long burn method resulting in the most realistic Q-value due to the inclusion of fission product irradiation, its prediction is considered more accurate than the pulse method, meaning that the Emrich model underestimates the cooling requirements for decay heat removal by 23.3%.

IV. Conclusions

Even though this study focuses on presenting the basis of new methodology for decay heat analysis, the preliminary results demonstrate that the Emrich model should not be used to determine the amount of hydrogen required for decay heat removal. A more sophisticated approach, such as the one derived here, must be developed. Using a time-dependent Q-value is important not only for decay heat removal but also for controlling power during a burn. If a time dependent Q-value is not considered, then a change in fission rate may have unexpected consequences on the total power, potentially resulting in the violation of material constraints.

V. References

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