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Modeling ICF capsules and test problems involving thermonuclear plasmas requires modeling the charged particles produced by the thermonuclear reactions. The charged particles escaping from an ICF capsule are one of the main diagnostics of capsule performance. CALEICF *can locally deposit the charged particle energy into the electron and ion fields instantaneously or track them using a Monte Carlo algorithm. Test problems revealed that* CALEICF*'s charged particle package needed improvement. The package has been enhanced to include the thermal energy of the reacting particles and to model the created particles energy distribution.*

The thermal energy of the reacting particles is accounted for as described in Ballabio, et al. [Ballabio et al., 1998] and Warshaw [Warshaw, 2001] . This energy is removed from the background ion energy and distributed between the created particles. The particle energy distributions are modeled with an approximation used by Ballabio, et al. This distribution is a modified Gaussian (based on the square root of the energy) that has a functional form similar to the exact distribution (see Warshaw). The skewness of the distribution matches that of the exact distribution within 1-2%. The thermal energy and the parameters of the distribution can be calculated using $\langle \sigma v \rangle$ and its first two derivatives with respect to temperature.

The new model will be compared with the original one for several test problems and ICF calculations.

Introduction

This article describes changes made recently in the thermonuclear burn and Monte Carlo charged particle packages of CALEICF. The changes account for the change in the average energy and spectrum of the reaction products as the temperature of the plasma increases. The products of the thermonuclear reactions can either be locally deposited or tracked as Monte Carlo particles. The Monte Carlo package supports the five light charged particles produced by thermonuclear reactions, namely p, d, t, ^3He, and ^4He . Table 1 shows the reactions that are supported. Only the products of the $d + {}^3He \rightarrow p + n$, and the neutron from the $d + t$ reactions had their thermal shift and energy spread modeled since these were the diagnostic particles of interest from ICF capsules. All other particles were created with their zero temperature energy, *i.e.* with a delta function for their spectrum.

The Monte Carlo particles are tracked and as they slow down energy is deposited into the background plasma (the ions) until they thermalize. When the number of particles grows beyond the limit set by the user, particles are randomly selected and thermalized.

Neutrons are tracked only to determine their time of flight to a detector. They do not interact with the background plasma. Therefore their kinetic energy is immediately lost from the calculation.

Table 1: Thermonuclear Reactions in CALEICF

#	reactions			Q(MeV)
1	$d+d$	$\rightarrow$	$n+{}^3He$	3.26
2	$d+d$	$\rightarrow$	$p+t$	4.02
3	$t+t$	$\rightarrow$	$n+n+{}^4He$	11.32
4	$d+t$	$\rightarrow$	$n+{}^4He$	17.59
5	$d+{}^3He$	$\rightarrow$	$p+{}^4He$	18.35
6	$d+{}^6Li$	$\rightarrow$	$n+{}^7Be$	3.38
7	$d+{}^6Li$	$\rightarrow$	$p+{}^7Li$	5.03
8	$d+{}^6Li$	$\rightarrow$	${}^4He+{}^4He$	22.38
9	$d+{}^6Li$	$\rightarrow$	$t+p+{}^4He$	2.56

Reactions in flight can be edited but the products are not tracked. The assumption here is that the product of interest immediately escapes and does not interact with the medium. For some ICF capsules this is a good approximation.

Thermal Effects

Thermal effects on the average energy of reaction products has been added for all thermonuclear reactions. This change affects both the local deposition model and the Monte Carlo model. As the temperature of the plasma increases the average energy of the reaction products increases. If there is a single temperature that describes the plasma then this has no effect in the local depostion model for reactions that only involve charged particles since the thermal energy is removed from the plasma and immediately put back when the particles are thermalized. The exception is for reactions that produce a neutron since the neutrons immediately escape from the problem.

The correct amount of energy is removed from the background plasma due to the thermal energy of the reacting particles. When the plasma is described by two temperatures, T_e and T_{ion}, this energy is removed from the ions.

This summary of the calculation of this energy follows Warshaw [Warshaw, 2001]. Let the indices 1 and 2 refer to the reacting particles and the indices 3, 4, and, if necessary, 5 refer to the reaction products. For reactions with two products the outgoing particle energy at zero temperature is:

$$E_3(T=0) = \frac{m_4}{m_3+m_4}Q \tag{1}$$

When the effects of temperature are included we have to average over the Maxwellian distribution of the reacting particles. If we let E_R be the kinetic energy of the reacting particles in the centero fmass frame this results in:

$$\langle E_3\rangle = \left[\tfrac{3}{2}m_3kT + m_4\left(\langle E_R\rangle + Q\right)\right] / \left(m_3+m_4\right) \tag{2}$$

where the averaged quantities are averaged over the particles that actually react; $\langle E_R\rangle$ is the

average relative energy of the reactants in the center of mass frame. Thus it accounts for the Gamov peak resulting from the product of the cross section and the Maxwellian distribution of the particles. The equation for $\langle E_4 \rangle$ is derived from equation (2) by swapping the indices 3 and 4.

The energy update in CALEICF is handled in three steps. First the specific energy (energy per gram) is scaled to conserve energy due to any change in the zone mass. The mass will change due the difference in mass of the reactants and products and also because neutrons and Monte Carlo particles are not included in the zone mass since they are either ignored or they are tracked separately. Secondly, the thermal energy per reaction, $\frac{3}{2}kT + \langle E_R \rangle$, is removed from the ion energy. Finally, the energy of each product, say $\langle E_3 \rangle$, is added to the ions and electrons or put into Monte Carlo particles. For local deposition the particle energy is divided between ions and electrons by the simple formula $f_{ion} = T_e/(T_e + T_R)$ where T_R is a fitting constant that changes for each reaction and each product particle.

The thermal effects slow down the ion heating rate and can lower the peak ion temperature since the thermal energy is removed from the ion field and added to the energetic particles which then deposit it back into both the ions and electrons. Therefore there is a net energy transfer from the ions to the electrons.

The value of $\langle E_R \rangle$ can be calculated from the derivative of $\langle \sigma v \rangle$ [Ballabio et al., 1998, Warshaw, 2001]

$$\begin{aligned} \langle E_R \rangle &= \langle \sigma v E_R \rangle \,/\, \langle \sigma v \rangle \\ &= \tfrac{1}{\langle \sigma v \rangle} \sqrt{\tfrac{8}{\pi \mu}} \theta^{-3/2} \int_0^\infty E_R^2 \sigma(E_R) e^{-E_R/\theta} dE_R \;;\;\; \theta = kT \\ &= \theta^2 \tfrac{d}{d\theta} \ln \left(\theta^{3/2} \langle \sigma v \rangle \right) \end{aligned} \tag{3}$$

Looking ahead this can be generalized to any power of E_R [Brysk, 1973]:

$$\langle E_R^n \rangle = \theta^2 \left\langle E_R^{n-1} \right\rangle \frac{d}{d\theta} \ln \left(\theta^{3/2} \langle \sigma v \rangle \left\langle E_R^{n-1} \right\rangle \right) \tag{4}$$

Test Problem As a test problem consider an infinite media of equimolar DT gas starting at a temperature of 5 keV. The thermonuclear burn will proceed until the fuel is gone. The temperature time histories and peak values are sensitive diagnostics of the calculation. This calculation is sensitive to many things including the heat capacity of the equation of state, the electron-radiation coupling, the electron-ion coupling, and, for local deposition, the way the deposited energy is split between electrons and ions. Figure 1 shows how the thermal effects change the temperature history for a local deposition problem.

Particle Distributions

The plasma temperature also effects on the energy distribution of reaction products. As the plasma gets hotter the FWHM of the spectrum of the products increases. Warshaw [Warshaw, 2001] derives the outgoing particle distribution for two body reactions. It has

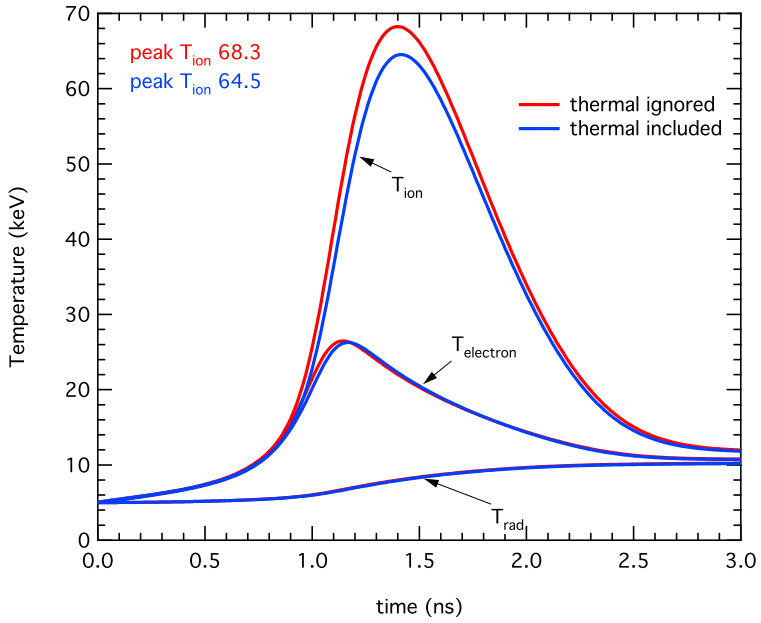

Figure 1: Comparison of accounting for thermal effects in local deposition with no thermal effects

two terms which before being integrated over E_R are proportional to

$$\exp\left(-a\left\{E_3^{1/2}-\left[b\left(E_R+Q\right)\right]^{1/2}\right\}^2\right)-\exp\left(-a\left\{E_3^{1/2}+\left[b\left(E_R+Q\right)\right]^{1/2}\right\}^2\right) \tag{5}$$

where

$$a=\frac{m_3+m_4}{m_3kT} \qquad b=\frac{m_4}{m_3+m_4} \tag{6}$$

The second term can be ignored when the thermal energy spread is small compared to the average energy and thus E_3 is nearly equal to $b(E_R+Q)$.

This lead Ballabio [Ballabio et al., 1998] to suggest a modified or skewed Gaussian particle distribution,

$$\begin{aligned} f(E) &= I_0\exp\left[-\frac{2E_0}{\sigma_0^2}\left(E^{1/2}-E_0^{1/2}\right)^2\right]\ ; \qquad 0<E<\infty \\ &= I_0\exp\left\{-2\left(\frac{E_0}{\sigma_0}\right)^2\left[\left(\frac{E}{E_0}\right)^{1/2}-1\right]^2\right\} \end{aligned} \tag{7}$$

$$I_0^{-1}=\sigma_0\left\{\sqrt{\tfrac{\pi}{2}}\left[1+\operatorname{erf}\left(\tfrac{\sqrt{2}}{k}\right)\right]+\tfrac{1}{2}ke^{-2k^{-2}}\right\}\ ; \quad k=\sigma_0/E_0$$

where E_0 is the peak of the distribution, not the average energy. Likewise σ_0 is not the second moment.

When $\sigma_0 \ll E_0$ or $k \ll 1$ the first and second moments are given by:

$$\begin{aligned}
\langle E\rangle &= E_0 I_0 \sigma_0 \left\{ \sqrt{\tfrac{\pi}{2}} \left(1+\tfrac{3}{4}k^2\right) \left[1+\operatorname{erf}\left(\tfrac{\sqrt{2}}{k}\right)\right] + \tfrac{1}{2}k\left(1+\tfrac{1}{2}k^2\right) e^{-2k^{-2}} \right\} \\
&\cong E_0 \left[1+\tfrac{3}{4}\left(\tfrac{\sigma_0}{E_0}\right)^2\right] \\
\sigma_{th}^2 &= \langle E^2\rangle - \langle E\rangle^2 \\
&= E_0^2 I_0 \sigma_0 \left\{ \sqrt{\tfrac{\pi}{2}} \left(1+\tfrac{5}{2}k^2+\tfrac{15}{16}k^4\right) \left[1+\operatorname{erf}\left(\tfrac{\sqrt{2}}{k}\right)\right] + \right. \\
&\qquad \left. \tfrac{1}{2}k\left(1+\tfrac{9}{2}k^2+k^4\right) e^{-2k^{-2}} \right\} - \langle E\rangle^2 \\
&\cong \sigma_0^2 \left[1+\tfrac{3}{8}\left(\tfrac{\sigma_0}{E_0}\right)^2\right]
\end{aligned} \tag{8}$$

The approximations ignore the terms proportional to $e^{-2k^{-2}}$.

Ballabio [Ballabio et al., 1998] gives formulae to calculate these moments for the two body reactions using a Maxwellian distribution for the reactants. For the two body reactions the moments of the product spectra are

$$\begin{aligned}
\langle E_3\rangle &= \left[\tfrac{3}{2}m_3\theta + m_4\left(\langle E_R\rangle + Q\right)\right]/(m_3+m_4) \\
\sigma_{th}^2 &= \left[2m_3m_4\theta\left(\langle E_R\rangle + Q\right) + \tfrac{3}{2}m_3^2\theta^2 + m_4^2\left(\langle E_R^2\rangle - \langle E_R\rangle^2\right)\right]/(m_3+m_4)^2.
\end{aligned} \tag{9}$$

The equation for σ_{th}^2 shows that care must be taken in numerically differentiating $\langle\sigma v\rangle$ so that $\left\langle \left(E_R - \langle E_R\rangle\right)^2\right\rangle = \langle E_R^2\rangle - \langle E_R\rangle^2 > 0$. Equations 8 are used to solve for E_0 and σ_0 of the modified distribution given values for $\langle E\rangle$ and σ_{th}^2 . For the approximate equations the solution is:

$$\begin{aligned}
E_0 &= \langle E\rangle \left[1-\tfrac{3}{2}\left(\tfrac{\sigma_{th}}{\langle E\rangle}\right)^2\right]^{1/2} \\
\sigma_0^2 &= \tfrac{4}{3}\langle E\rangle^2 \left\{ \left[1-\tfrac{3}{2}\left(\tfrac{\sigma_{th}}{\langle E\rangle}\right)^2\right]^{1/2} - \left[1-\tfrac{3}{2}\left(\tfrac{\sigma_{th}}{\langle E\rangle}\right)^2\right] \right\}.
\end{aligned} \tag{10}$$

This probability distribution function (PDF) works well unless the average energy drops so low that it is comparable to the temperature. For there to be any solution we must have $\sigma_{th} < \sqrt{2/3}\langle E\rangle$. I chose to limit $\sigma_{th} < 0.6\langle E_R\rangle$ or $\sigma_0 < 1.25E_0$. For these values the distribution and the neglected part are shown in Figure 2.

For smaller values of σ_0 the neglected part rapidly becomes smaller. One estimate of the error is the value of the PDF at $E = 0$ where the PDF should be zero.

$$f(0) = I_0 \exp\left[-2\left(E_0/\sigma_0\right)^2\right] \tag{11}$$

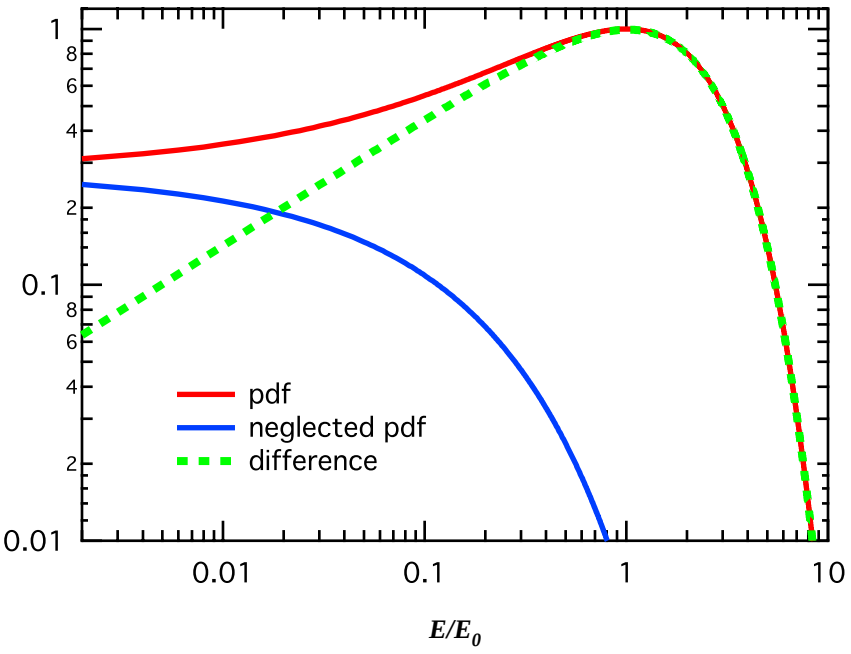

Figure 2: This shows the portion of the PDF that is neglected in the limiting case. The difference is the exact PDF that should be used.

Sampling

To sample from this distribution we need the cumulative distribution function. First we change variables:

$$\begin{aligned} f(y) &= \sqrt{2} I_0 E_0 k \left(1 + \tfrac{k}{\sqrt{2}} y\right) e^{-y^2} \quad ; \quad -\tfrac{\sqrt{2}}{k} < y < \infty \\ y &= \tfrac{\sqrt{2}}{k} \left[(E/E_0)^{1/2} - 1 \right] \quad ; \qquad k = \sigma_0 / E_0 \end{aligned} \tag{12}$$

Then the CDF is:

$$\begin{aligned} F(x) &= \sqrt{2} I_0 \sigma_0 \int_{-\frac{\sqrt{2}}{k}}^{x} \left(1 + \tfrac{k}{\sqrt{2}} y\right) e^{-y^2} dy \\ &= I_0 \sigma_0 \left\{ \sqrt{\tfrac{\pi}{2}} \left[\mathrm{erf}(x) + \mathrm{erf}\left(\tfrac{\sqrt{2}}{k}\right) \right] + \tfrac{k}{2} \left(e^{-2k^{-2}} - e^{-x^2} \right) \right\} \end{aligned} \tag{13}$$

For $y > 0$ ($E > E_0$) this CDF can be sampled as the sum of two distributions, a Gaussian and an exponential. (See *A Third Monte Carlo Sampler* entries C51, page 80 and C29, page 70 [Everett and Cashwell, 1983]) For $E < E_0$ the CDF is inverted numerically. The charged particle spectrum is shown in the upper two plots of Figure 3. It is compared with the exact spectrum as calculated by Warshaw.

Three Body Reactions

The two reactions, $d + {}^6Li \rightarrow p + t + \alpha$ and $t + t \rightarrow n + n + \alpha$ have a very different particle spectrum. The first reaction always breaks up immediately into the three particles. The second reaction can produce all three particles directly (70% branching ratio), produce a neutron and a ${}^5He$ ground state (20% branching ratio), or produce a neutron and a ${}^5He^*$ excited state (10% branching ratio). The ${}^5He$ or ${}^5He^*$ then breaks up into a neutron and an alpha.

For the direct three body breakup in the center of mass frame the distribution is

$$f(E) = \left[E\left(E_{max} - E\right)\right]^{1/2} \; ; \quad \text{where} \quad E_{max} = \left(1 - \frac{m}{M_{tot}}\right) Q \tag{14}$$

While it is incorrect in detail, to get a lab frame distribution I take the thermal energy of the reactant particles and add it to the Q. This distribution is easy to sample since it is just a semicircular region bounded by $E = 0$ and $E = E_{max}$.

$$E_{max} = \left(1 - \frac{m}{M_{tot}}\right)\left(\frac{3}{2}kT + \langle E_R \rangle + Q\right) \tag{15}$$

For the tritium reaction the direct break up into three particles is handled the same as the $d + {}^6Li$ reaction. The two stage break up is handled as a sequence of two body break ups. The energy of each ${}^5He$ state is assumed to be given by a Gaussian since no detailed information is available. The ground state, ${}^5He$, is 894.3 keV (FWHM 600 keV) above the ${}^4He + \alpha$ end state. The first excited state, ${}^5He^*$, is 4894.3 keV (FWHM 4000 keV) above the ${}^4He + \alpha$ end state.

For the two body sequences the energy, E_{lev} of the ${}^5He$ state is sampled from a Gaussian (limited so $0 < E_{lev} < Q$). This is sampled using an approximation to the inverse normal cumulative distribution function [Acklam, 2004].

Then a two body break up to $n + {}^5He$ with a Q of $Q^* = Q - E_{lev}$ is sampled for the ${}^5He$ energy. This gives us the energy, E_5, of the ${}^5He$ in the lab frame.

Finally, the ${}^5He$ break up to $n + {}^4He$ with a Q of $Q^* = E_{lev}$ is sampled ($-1 < \mu < 1$) to get a final energy for the alpha particle.

$$E_\alpha = \frac{m_n}{m_n + m_\alpha} E_{lev} + \frac{m_\alpha}{m_n + m_\alpha} E_5 + 2m_\alpha \left[\frac{m_n E_{lev} E_5}{m_\alpha m_5 (m_n + m_\alpha)}\right]^{1/2} \mu \tag{16}$$

The particle spectra that result for these three body breakup reactions are shown in the lower two plots of Figure 3. The $t + t \rightarrow n + n + {}^4He$ reaction is strongly influenced by the ${}^5He$ states.

Monte Carlo Results

In Figure 4 the local depostion results are compared with Monte Carlo for the infinite medium test problem on page 3. The time delay for the deposition of the energy in the Monte Carlo particles is evident. Otherwise there is not much change in the peak value of T_{ion}.

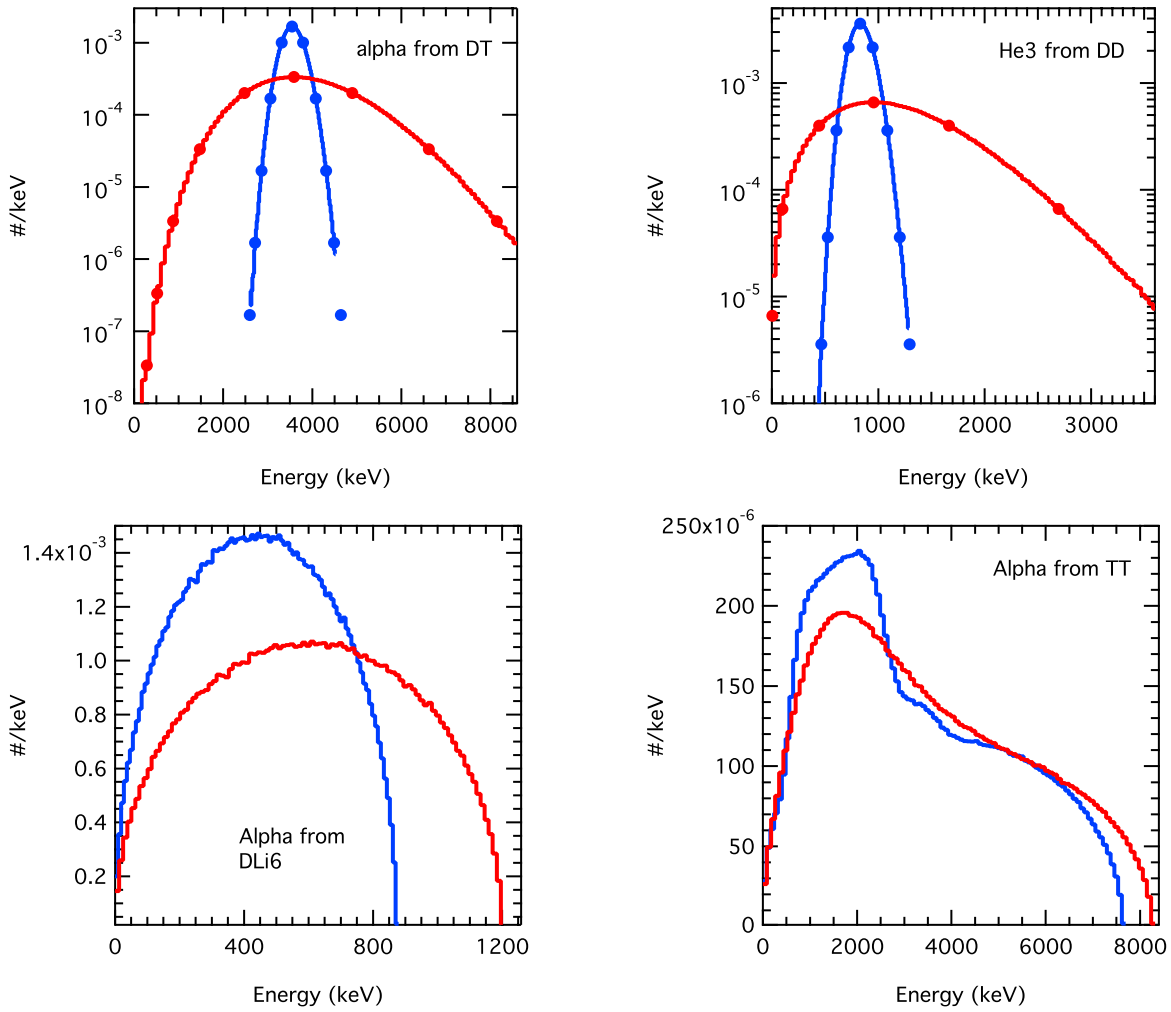

Figure 3: Several sampled particle distributions. The blue lines are for $T_{ion} = 10$ keV and the red lines are for $T_{ion} = 250$ keV. The two body results also have the exact PDF plotted as filled circles for comparison.

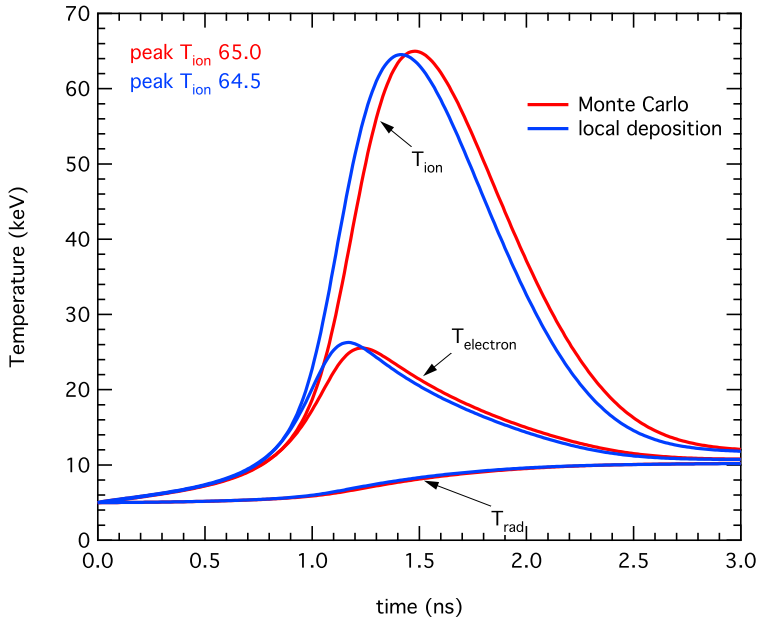

Figure 4: The time delay between the local deposition model and the Monte Carlo model is apparent in T_{ion}.

Future Work

- Use a method to sample the three body break up spectra that correctly includes the thermal effects.
- Study the error introduced by the approximate PDF as the temperature of the plasma rises. Compare with the exact PDF or an approximate PDF on that goes to zero as the energy goes to zero. For example,

$$f(E) = I_0 \left(\exp\left\{ -2 \left(\frac{E_0}{\sigma_0}\right)^2 \left[\left(\frac{E}{E_0}\right)^{1/2} - 1 \right]^2 \right\} - \exp\left\{ -2 \left(\frac{E_0}{\sigma_0}\right)^2 \left[\left(\frac{E}{E_0}\right)^{1/2} + 1 \right]^2 \right\} \right) \; ; \quad 0 < E < \infty \tag{17}$$

$$I_0 = 1/\left(\sqrt{2\pi}\sigma_0\right) \; ; \qquad k = \sigma_0/E_0$$

- Add better population control of the Monte Carlo particles.
- Add knock-on reactions and reactions in flight so that in addition to editing the number of reactions that take place the products can be tracked as well.

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