Alpha Particle Fusion Reaction Product Modeling in DRACO

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Abstract

Alpha particle fusion reaction product transport in DRACO is computed using either multi-group flux-limited diffusion theory or continuous energy Monte Carlo particle tracking. Both of these transport models incorporate the same basic slowing down model of Li and Petrasso. Detailed comparisons of particle transport and energy loss predicted by the two models will be presented. Results of 2D lagrangian fusion burn simulations will be compared for the two models. The Monte Carlo model can be used in either an adiabatic approximation on each time step or a time dependent model where in-flight particles are remembered for the next time step. Both models are implemented using parallel computing algorithms using the MPI parallel programming interface.

Outline

I. Charged Particle Stopping Power

II. Multi-group Diffusion Equation
   a. Flux limiter
   b. Energy deposition

III. Monte Carlo Particle Tracking
   a. Algorithm

IV. Comparison of Fusion Burn Simulation
   a. Heating rate by alpha particle source from origin
   b. Effect of two dimensional transport

V. Future Work

Stopping Power

Energy loss rate interacting with electrons (ions):

$$\nu_\varepsilon^{e/i} = \frac{2e_t^2 \ln \Lambda_b^2}{m_t v_t^3}\omega_{pf}^2 G(\mu)$$

ω_{pf} : the plasma frequency

$$G(\mu) = \underbrace{\mu - m_f \mu'/m_t}_{\mathrm{I}} + \underbrace{m_f(\mu+\mu')/(m_t \ln\Lambda_b)}_{\mathrm{II}}$$

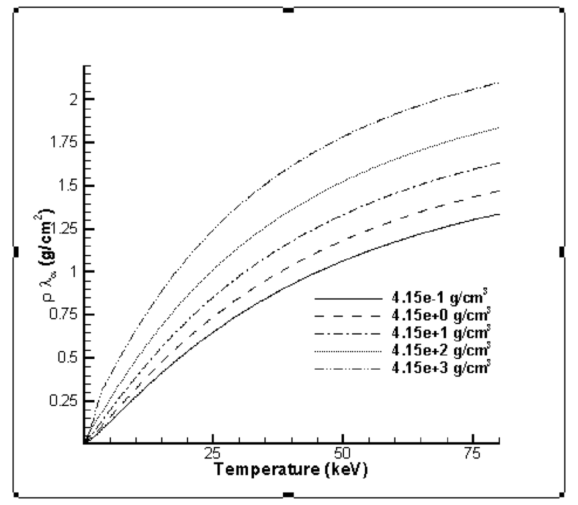
I - Classical Theory: Coulomb small-angle collision

II - Li and Petrasso modification: include large-angle scattering

Coulomb logarithm for electrons use random phase approximation with electron degeneracy effect

$$\ln\Lambda_{RPA} = 0.5[\ln(1+\Lambda_s^2(0.37+0.44\eta^2)-1]$$

Results of Stopping Power

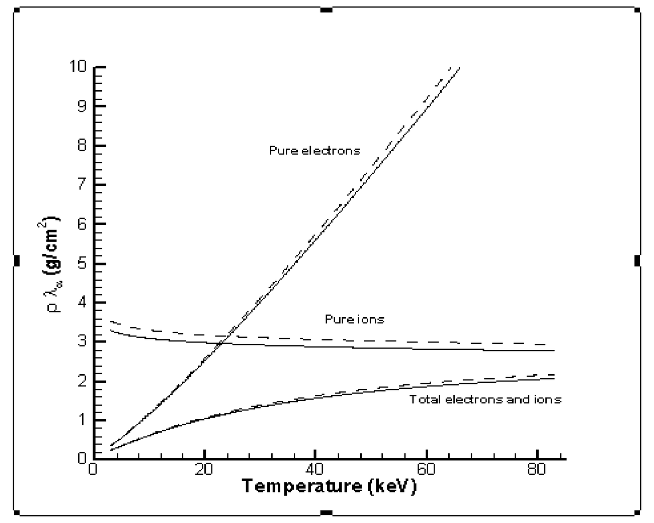


$$\rho\lambda_\alpha = \int_0^{E_0}\left(\frac{dE}{\rho dx}\right)^{-1} dE$$

Using this graph, we can estimate the alpha particle range.

$\rho\lambda_\alpha$ as a function of plasma temperature for several different densities.

Effect of Large-Angle Scattering is small



$\rho\lambda_\alpha$ for pure electron stopping, pure ion stopping and both electrons and ions The dashed lines represent the results without the large-scattering effect in the stopping power calculation.

Multi-group Charged Particle Diffusion Model

Multi-group Diffusion Equation:

$$\frac{\partial N_g}{\partial t} = \nabla \cdot D_g \nabla N_g - \frac{N_g}{\tau_g} + \frac{N_{g+1}}{\tau_{g+1}}$$

Alpha particle density in group g:

$$N_g = \int_{E_g}^{E_{g+1}} N_E(r,\theta,t)dE$$

Relaxation time from upper group g+1 to lower group g:

$$\tau_g = \frac{2}{3}\frac{1}{\nu_\varepsilon^e}\ln\frac{\nu_\varepsilon^e E_{g+1}^{3/2} + A_i}{\nu_\varepsilon^e E_g^{3/2} + A_i}$$

Flux Limiter and Energy Deposition

1. The sum flux limiter:

$$D_g = \frac{v_g}{3/\lambda_g + \bar{\mu}^{-1}|\nabla N_g|/N_g}$$

λ_g the particle mean free path with velocity $v_g = \sqrt{(E_g + E_{g+1})/m_t}$

$\bar{\mu}$ representing the deviation from the isotropic distribution

$$|\bar{\mu}^{-1}| = 1 + 3\exp(-\lambda_g N_g^{-1}|\nabla N_g|/2)$$

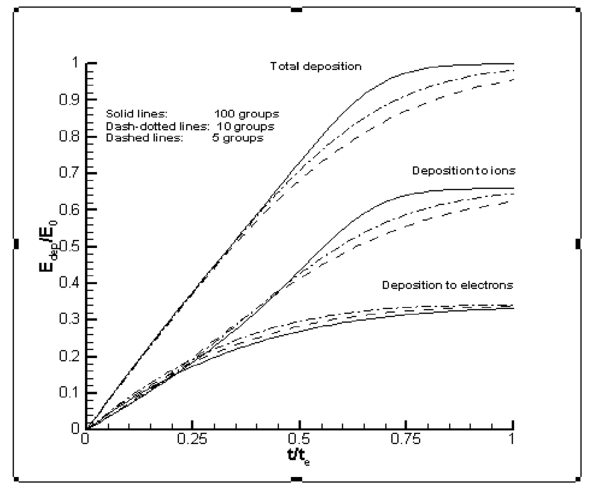
2. Levermore and Pomraning flux limiter:

$$D = \xi(\beta)\lambda \qquad \xi(\beta) = \left[\coth(\beta) - \frac{1}{\beta}\right]\frac{1}{\beta} \qquad \beta = \lambda\frac{|\nabla E|}{E}$$

Energy deposition rate by the mean value approximation:

$$\dot{E}_{dep}^i = A t_E \frac{N_g}{\tau_g}\frac{E_{g+1} - E_g}{E_g^{3/2} + A t_E} \qquad \dot{E}_{dep}^e = \frac{N_g}{\tau_g}(E_{g+1} - E_g) - \dot{E}_{dep}^i$$

Energy Deposition in Diffusion Model

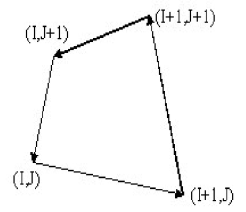


Energy deposition and its partition to electrons and ions for 3.5 Mev α particles in a 50 keV DT plasma

Monte Carlo Particle Tracking

Diffusion theory is valid for short mean-free-path transport.
For energetic alpha particles, the Monte Carlo technique provides more accurate results, however, requires more computing time and storage.

Geometry elements:

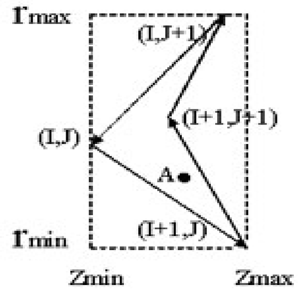


For the RZ two-dimensional geometry, it is actually a 3D problem. The position of generated particle is represented by a point (x,y,z) in a volume enclosed by four hyperbolas defined by the quadrilateral edges

Tracking Algorithm

The Monte Carlo particle transport algorithm has to fulfill the basic tasks:
(1) to generate particles randomly in the source cells,
(2) to determine the intersection with a quadrilateral and get the particle information updated.
(3) Other tasks, such as the treatment of boundary conditions and tally, are also required

❖ Rejection sampling method is used for the random particle generation

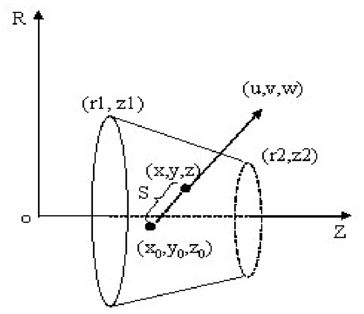


Tracking Algorithm (continued)

❖ Intersection with a quadrilateral

Careful procedures are required for all special cases in order to obtain the correct intersection.

It is the work horse for the Monte Carlo particle tracking.



Stopping power as in the diffusion model used for travel length, travel time and energy deposition calculations.

The distance to intersection is calculated from the equation:

$$S^2(1-w^2-k^2w^2) + S(2x_0u + 2y_0v - 2kw(r_1 + k(z_0 - z_1)) + r_0^2 - (r_1 + k(z_0 - z_1))^2 = 0$$

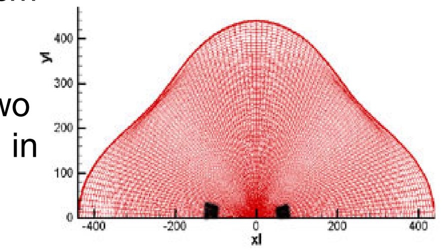
Comparison of Energy Deposition for Diffusion Model and Monte Carlo Tracking Model

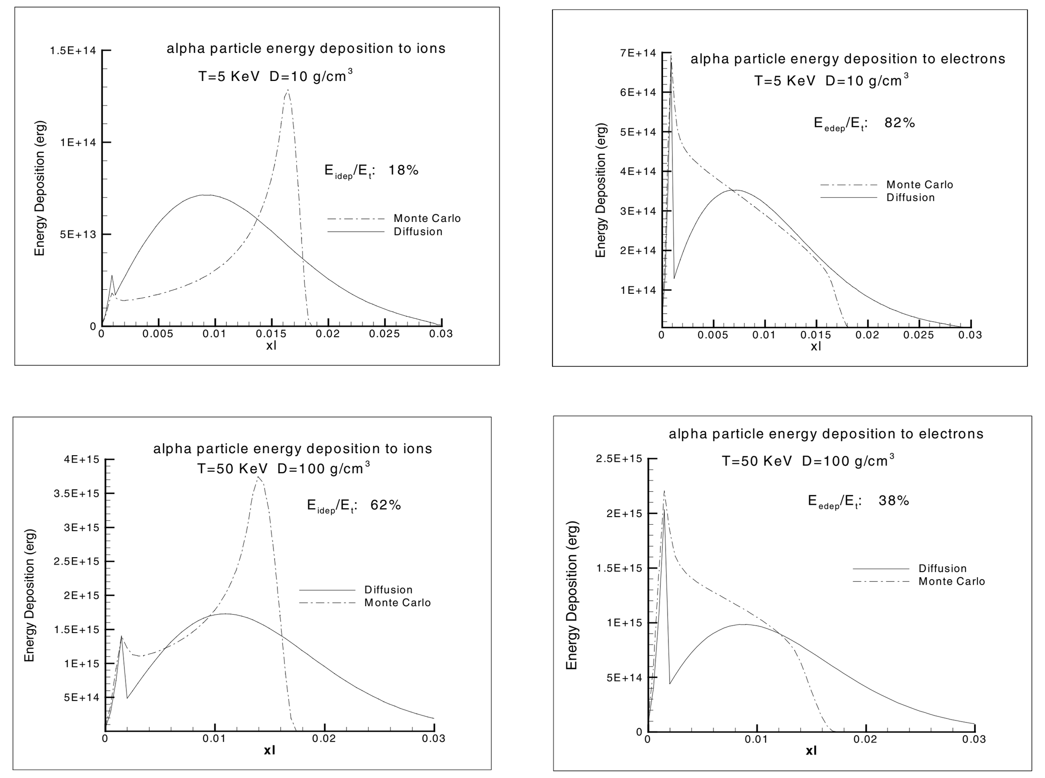
- Mesh size: 100 by 100
- The number of Monte Carlo particle is about one million
- Alpha source rate of 10^{30} at the origin of radius

$R_s < 4 \times 10^{-4}$ cm

Two cases:
1) DT plasma temperature at 5 keV and plasma density of 10 g/cm³
2) DT plasma temperature at 50 keV and plasma density of 100 g/cm³

- Alpha source rate of 10^{40} as two non-symmetric sources shown in mesh



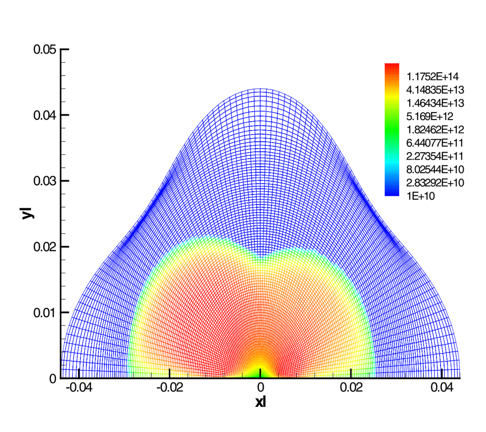


Comparison of Energy Deposition for Diffusion Model and Monte Carlo Tracking Model

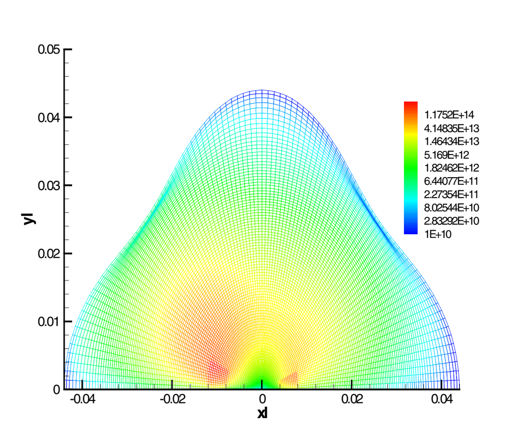
- Energy deposition to ions shows a "Bragg peak" for MC while there is only a gentle hump for the diffusion distribution.
- Both electron and ion energy deposition curves drop off rapidly at the tail.
- Transport of the alpha particles in the Monte Carlo method halts abruptly while the diffusion method smears the abrupt feature by spreading farther.

Spatial Energy Deposition to Electrons Under the Two Models

Two-dimensional effect using the Monte Carlo model and the diffusion Model (L mode = 4)



Monte Carlo model



Diffusion model

Future Work

- Statistical noise reduction for the Monte Carlo particle tracking method.
- Although the code is already implemented in the parallel MPI, systematic study of the speed up is necessary.
- Full burn simulations with hydrodynamics, thermal conduction and radiation transport especially for the break-even target configurations.
- Apply the Monte Carlo method to radiation transport (Implicit Monte Carlo) in DRACO.