Doppler Broadening of the Scattering Kernel

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References

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Time-Dependent Neutron Transport Equation

- The neutron transport equation is commonly expressed as

$$\begin{aligned}\frac{1}{v}\frac{\partial\Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} &= -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t)-\Sigma_t(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t)\\ &+\int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'\Sigma_s(\mathbf{r},E',\mathbf{\Omega}',t)f_s(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\ &+\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\chi(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\nu_f(E)\Sigma_f(\mathbf{r},E',\mathbf{\Omega}',t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\ &+Q(\mathbf{r},E,\mathbf{\Omega},t) \qquad \text{(D.1)}\end{aligned}$$

- However, Eq. (D.1) should be expressed by considering the material temperature, $T(\mathbf{r})$, as

$$\begin{aligned}\frac{1}{v}\frac{\partial\Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} &= -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t)-\Sigma_t(\mathbf{r},E,\mathbf{\Omega},t,T(\mathbf{r}))\Phi(\mathbf{r},E,\mathbf{\Omega},t)\\ &+\int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'\Sigma_s(\mathbf{r},E',\mathbf{\Omega}',t,T(\mathbf{r}))f_s(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t,T(\mathbf{r}))\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\ &+\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\chi(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t,T(\mathbf{r}))\nu_f(E)\Sigma_f(\mathbf{r},E',\mathbf{\Omega}',t,T(\mathbf{r}))\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\ &+Q(\mathbf{r},E,\mathbf{\Omega},t) \qquad \text{(D.2)}\end{aligned}$$

Time-Dependent Neutron Transport Equation (Contd.)

- The current cross section generation systems, for example, NJOY, applies an approximation that the scattering kernels are not dependent on the system temperature, which means that the following transport equation is solved in most of the neutronics analysis systems.

$$
\begin{aligned}
\frac{1}{v}\frac{\partial \Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} &= -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t) - \Sigma_t(\mathbf{r},E,\mathbf{\Omega},t,T(\mathbf{r}))\Phi(\mathbf{r},E,\mathbf{\Omega},t) \\
&+ \int_{E'} dE' \int_{4\pi} d\mathbf{\Omega}' \Sigma_s(\mathbf{r},E',\mathbf{\Omega}',t,T(\mathbf{r})) f_s(E' \to E, \mathbf{\Omega}' \to \mathbf{\Omega}, t, \cancel{T(\mathbf{r})})\Phi(\mathbf{r},E',\mathbf{\Omega}',t) \\
&+ \int_{4\pi} d\mathbf{\Omega}' \int_{E'} dE' \chi(\mathbf{r},E' \to E, \mathbf{\Omega}' \to \mathbf{\Omega}, t, \cancel{T(\mathbf{r})})\nu_f(E)\Sigma_f(\mathbf{r},E',\mathbf{\Omega}',t,T(\mathbf{r}))\Phi(\mathbf{r},E',\mathbf{\Omega}',t) \\
&+ Q(\mathbf{r},E,\mathbf{\Omega},t) \qquad \text{(D.3)}
\end{aligned}
$$

$\Uparrow$

$\boxed{\text{Asymptotic Model}}$

Three Treatments for Doppler Broadening

- MCNP (X-5 Monte Carlo Team, 2003) contains three methods for sampling the scattering kernel i.e. the probability of a neutron to change its initial energy and flight direction in new specific energy and spatial direction as a consequence of an interaction with a target nucleus. [8]
  - At sufficiently high neutron energies the thermal agitation of the target nuclide is ignored, implying zero velocity for the nuclide. The solution method in this case is known as the **asymptotic kernel**.
  - At thermal neutron energies, pre-prepared probability – **S(α,β)** – tables are available for several light nuclei. α and β stand here for the changes in neutron momentum and energy, respectively, after the scattering process. The tables usually consider internal changes in the molecule (crystal effect) or can principally be based on the ideal gas model.
  - The third category applies to cases which do not fit the previous two. It concerns mainly the epi thermal region where the motion of the target nucleus cannot be neglected but the crystal effects are of lesser importance. Here, the MCNP code adopts an entirely different philosophy, in MCNP manual bearing the heading ''**Sampling the Velocity of the Target Nucleus**'' (SVT).

[8] B. Becker, R. Dagan, G. Lohnert, "Proof and Implementation of the Stochastic Formula for Ideal Gas, Energy Dependent Scattering Kernel," Ann. Nucl. Energy, **36**, 470 (2009).

Scattering Models – (1) Asymptotic Model

- Asymptotic Slowing-Down Scattering Model (Asymptotic Model)
  - A collision nuclide and a reaction type are sampled by using Doppler-broadened cross sections.
  - However neutron energy and flight direction after the collision are determined using the two-body reaction kinematics **with the assumption of no thermal motion of a target nucleus**.

Thermal S(α,β) Table

- Data from thermal S(α,β) tables provide a complete representation of thermal neutron scattering by molecules and crystalline solids.
- Cross sections for elastic and inelastic scattering are found on the tables (typically for neutron energies below 4 eV).
- Moderator materials on the ENDF/B-III thermal data files are Be, BeO, C(graphite), C(polyethylene), C_6H_6, $D(D_2O)$, $H(H_2O)$, $Zr(ZrH_n)$, and $H(ZrH_n)$.

Doppler Broadening Theory

- The well known Doppler broadening equation can be written by

$$\sigma_\alpha^{eff}(v_n,T)=\frac{1}{v_n}\int_{V:v_r>0}\int_{-1}^{1}v_r\sigma_\alpha(v_r)M^T(V)dV\frac{d\mu_t}{2} \qquad \text{(D.4)}$$

where

$\sigma_\alpha^{eff}(v_n,T)$ = Doppler broadened cross section of reaction type α,

$\sigma_\alpha(v_r) = \sigma_\alpha(v_r,0)$ = zero-Kelvin cross section of reaction type α,

v_n = neutron speed,

v_r = relative speed of the neutron in the target-at-rest frame,

$M^T(V)$ = spectrum of the target velocity, V, given by a velocity distribution $p(\beta,V)$.

μ_t = cosine of the angle between the neutron and target velocity vectors

- The distribution $p(V)$ for the free gas model is given by a Maxwell distribution.

$$p(\beta,V)=\frac{4}{\sqrt{\pi}}\beta^3V^2e^{-\beta^2V^2};\ \beta=\sqrt{\frac{AM_n}{2kT}} \qquad \text{(D.5)}$$

M_n is the neutron mass.

Doppler Broadening of Double Differential XS

- Parallel to Eq. (D.4), the temperature dependent scattering cross section can be written as

$$\sigma_s^{eff}(E \to E', \Omega \to \mathbf{\Omega}', T)$$

$$= \frac{1}{v_n} \int_{V:v_r>0} \int_{-1}^{1} v_r \sigma_s (v_r \to E', \mathbf{\Omega}') M^T(V) dV \frac{d\mu_t}{2} \quad \text{.................. (D.6)}$$

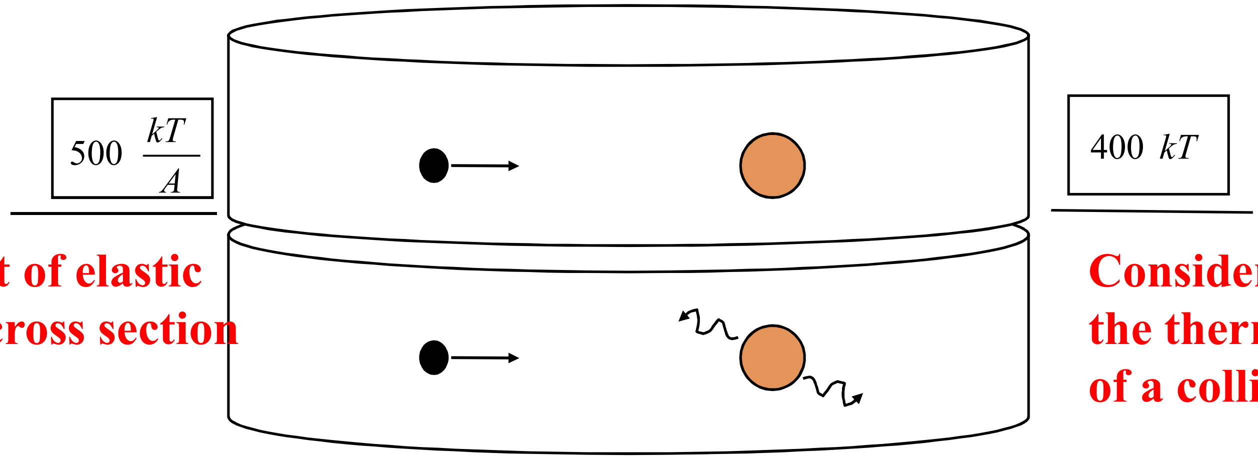
$$= \frac{1}{v_n} \int_{V:v_r>0} \int_{-1}^{1} v_r \sigma_s (v_r) f_s (v_r \to E', \mathbf{\Omega}') M^T(V) dV \frac{d\mu_t}{2}$$

- Ouisloumen and Sanchez [3] integrated in 1991 an energy dependent cross section into their evaluation of the effective, temperature dependent moments of the scattering kernel. They focused on an energy transfer change in the vicinity of ^{238}U scattering resonances compared to the **asymptotic kernel**. They showed that neutrons predominantly gain energy in a collision at some energies in the vicinity of resonances.

How to simulate Eq. (D.6) in the Monte Carlo simulations?

Conventional MC Simulation of Doppler Broadening

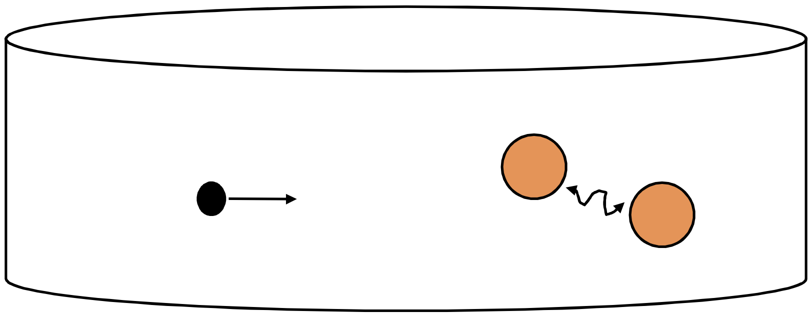
< Free Gas Thermal Treatment >



Adjustment of elastic scattering cross section

Consideration of the thermal movement of a collided atom

< Application of Thermal Scattering Library>



Conventional MC Simulation of Doppler Broadening (Contd.)

- Adjustment of the elastic scattering cross section

$$\sigma_{els}(T) = F\sigma_{els}(0)$$

$$F = \left(1 + \frac{1}{2a^2}\right) erf(a) + \frac{1}{a\sqrt{\pi}} e^{-a^2}, \quad a = \sqrt{\frac{AE}{kT}}$$

- Consideration the thermal movement of a collided atom

Sampling a velocity and direction of a collision nuclide: $\vec{V}$

↓

Calculation of neutron's rel. velocity: $\vec{v_r} = \vec{v_n} - \vec{V}$

↓

Sampling outgoing neutron's rel. velocity: $\vec{v_r'}$

↓

Calculation of outgoing neutron's velocity: $\vec{v_n'} = \vec{v_r'} + \vec{V}$

How to Sample V and μ_t?

- Eq. (D.6) implies that the probability distribution for a target velocity V and cosine μ_t is

$$\sigma_s^{eff} = \frac{1}{v_n} \int\int v_r \sigma_s p(\beta, V) dV \frac{d\mu_t}{2}$$

$$\Downarrow$$

$$\boxed{P^T(V, \mu_t) = \frac{\sigma_s(v_r) v_r p(\beta, V)}{2\sigma_s^{eff}(v_n) v_n} = \frac{\sigma_s(E_r) v_r p(\beta, V)}{2\sigma_s^{eff}(E) v_n}} \qquad \text{(D.7)}$$

- There are two approaches to sample V and μ_t based on Eq. (D.7):
  - Free-monatomic-gas Model with Constant Cross Section (Constant XS Model),
  - Free-monatomic-gas Model with Resonance Cross Section (Exact Model).

Scattering Models – (2) Constant XS Model

- Free-monatomic-gas Model with Constant Cross Section (Constant XS Model)
  - In the same way as in the asymptotic model, a collision nuclide and a reaction type are sampled by using Doppler-broadened cross sections.
  - In the constant cross section model, it is assumed that the variation of $\sigma_s(v_r)$ with target velocity can be ignored because (1) for light nuclei, $\sigma_s(v_r)$ is slowly varying with velocity, and (2) for heavy nuclei, where $\sigma_s(v_r)$ can vary rapidly, the moderating effect of scattering is small.[6]
  - Then the distribution function $P^T(V,\mu_t)$ can be approximated by

$$\boxed{\begin{aligned} v_r &\equiv \left|\mathbf{v}_n - \mathbf{V}\right| \\ &= \sqrt{v_n^2 + V^2 - 2v_n V\mu_t} \end{aligned}}$$

$$\begin{aligned} P^T_{CXS}(V,\mu_t) &= \frac{\cancel{\sigma_s(v_r)}v_r\, p(\beta,V)}{\cancel{2\sigma_s^{eff}(v_n)v_n}} \\ &\propto v_r\, p(\beta,V) \\ &\propto \sqrt{v_n^2 + V^2 - 2v_n V\mu_t}\, V^2 e^{-\beta^2 V^2} \\ &\propto \frac{\sqrt{v_n^2 + V^2 - 2v_n V\mu_t}}{v_n + V}\left(V^3 e^{-\beta^2 V^2} + v_n V^2 e^{-\beta^2 V^2}\right) \quad \text{(D.8)} \end{aligned}$$

$P_{CXS}(V,\mu_t)$

- If the scattering cross section at 0K is constant with neutron energy and its value is σ_{s0}, the Doppler-broadened scattering cross section can be written as [7]

$$\sigma_s^{eff}(v_n) = \sigma_{s0} g(\beta v_n); \quad \text{(D.9)}$$

$$g(\beta v_n) = \frac{1}{(\beta v_n)^2}\left\{\left((\beta v_n)^2 + \frac{1}{2}\right) erf(\beta v_n) + \frac{1}{\sqrt{\pi}}(\beta v_n)\exp(-(\beta v_n)^2)\right\} \quad \text{(D.10)}$$

erf is the error function.

- Then the $P_{CXS}(V,\mu_t)$ can be expressed by

$$P_{CXS}^T(V,\mu_t) = \frac{\cancel{\sigma_{s0}}\, v_r p(\beta,V)}{2\cancel{\sigma_{s0}}\, g(\beta) v_n} = \frac{v_r p(\beta,V)}{2g(\beta)v_n} \quad \text{(D.11)}$$

Scattering Models – (3) Exact Model: DBRC

- In the resonance energy regions, the variation of $\sigma_s(v_r)$ cannot be assumed to be negligible.
- Therefore V and μ_t should be sampled from the exact $P^T(V,\mu_t)$.

$$\boxed{P^T(V,\mu_t) = \frac{\sigma_s(v_r)v_r p(\beta,V)}{2\sigma_s^{eff}(v_n)v_n}}$$

- In 1996, a stochastic method was proposed by Rothenstein [2] to account for the energy dependent cross section in a scattering process of the Monte Carlo method.

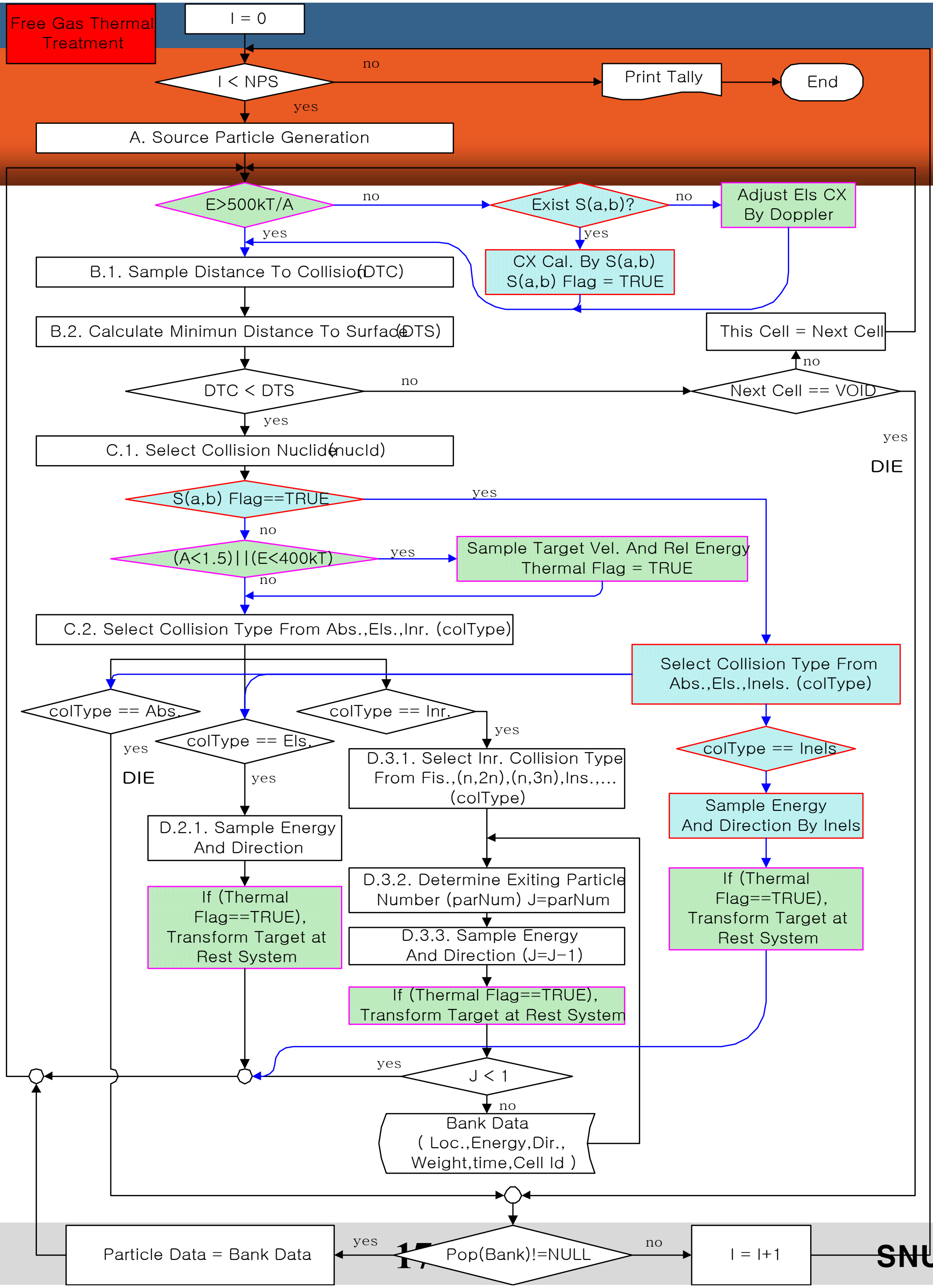
  This method, namely the Doppler Broadening Rejection Correction (DBRC) method, **adds the rejection probability $\sigma_s(v_r)$** to the sampling procedure of the constant cross section model.

Scattering Models – (3) Exact Model: Weight Corr.

- D.J. Lee et al. [3] developed a weight correction method for the exact scattering model.
- In this method, the thermal motion of the target nucleus, **V**, is sampled from Eq. (D.8) and the neutron weight is corrected using a factor *f*:

$$f = \frac{P^T(V,\mu_t)}{P^T_{CXS}(V,\mu_t)} = \frac{\dfrac{\sigma_s(v_r)\cancel{v_r}\,\cancel{p(\beta,V)}}{\cancel{2}\sigma_s^{eff}(v_n)\cancel{v_n}}}{\dfrac{\cancel{v_r}\,\cancel{p(\beta,V)}}{\cancel{2}g(\beta)\cancel{v_n}}} = \frac{\sigma_s(v_r)}{\sigma_s^{eff}(v_n)}g(\beta) \qquad \text{(D.12)}$$

Flowchart



Free Gas Thermal Treatment
I = 0
I < NPS
no
yes
Print Tally
End
A. Source Particle Generation
E>500kT/A
no
Exist S(a,b)?
no
Adjust Els CX By Doppler
yes
yes
CX Cal. By S(a,b) S(a,b) Flag = TRUE
B.1. Sample Distance To Collision(DTC)
B.2. Calculate Minimun Distance To Surface(DTS)
This Cell = Next Cell
no
DTC < DTS
no
Next Cell == VOID
yes
yes
DIE
C.1. Select Collision Nuclide(nucId)
S(a,b) Flag==TRUE
yes
no
(A<1.5)||(E<400kT)
yes
Sample Target Vel. And Rel Energy Thermal Flag = TRUE
no
C.2. Select Collision Type From Abs.,Els.,Inr. (colType)
Select Collision Type From Abs.,Els.,Inels. (colType)
colType == Abs
colType == Inr.
colType == Els.
yes
yes
DIE
yes
colType == Inels
D.3.1. Select Inr. Collision Type From Fis.,(n,2n),(n,3n),Ins.,... (colType)
Sample Energy And Direction By Inels
D.2.1. Sample Energy And Direction
D.3.2. Determine Exiting Particle Number (parNum) J=parNum
If (Thermal Flag==TRUE), Transform Target at Rest System
D.3.3. Sample Energy And Direction (J=J−1)
If (Thermal Flag==TRUE), Transform Target at Rest System
If (Thermal Flag==TRUE), Transform Target at Rest System
yes
J < 1
no
Bank Data (Loc.,Energy,Dir., Weight,time,Cell Id)
Particle Data = Bank Data
yes
Pop(Bank)!=NULL
no
I = I+1

McCARD Numerical Results for a Pin Cell Prob.

- Two independent runs were conducted varying the fuel temperature with and without DBRC for ^{238}U, repectively.

900K				800K			
w/o DBRC		with DBRC		w/o DBRC		with DBRC	
keff	SD	keff	SD	keff	SD	keff	SD
1.35250	0.00019	1.35003	0.00027	1.35612	0.00020	1.35414	0.00019

- From the above table, the fuel temperature reactivity coefficients are estimated as

< Fuel Temperature Reactivity Coeff. (mk) >

w/o DBRC		with DBRC	
$\Delta\rho$	SD	$\Delta\rho$	SD
-0.01974	-0.00150	-0.02248	0.00181