R. Dagan, B. Becker and Y. Danon

A complementary Doppler Broadening formalism and its impact on nuclear reactor simulation

The Boltzmann Transport equation is the governing formalism upon which simulations of nuclear reactors are performed, in particular when strong absorption or anisotropic scattering are significant. On the left (loss) hand side of the balance equation one finds the absorption and the scattering cross section $\Sigma_a(E')$, $\Sigma_s(E')$ respectively. Those cross sections are energy and temperature dependent i.e. Doppler Broadened. The scattering cross section appears explicitly again on the right (production) hand side of the equation in its differential form $\int\int_0^\infty \Sigma(E \to E';\Omega \to \Omega')\mathrm{d}E\,\mathrm{d}\Omega$. However, this term is commonly evaluated at 0 K and it does not account for the existing resonances which are the underlying characteristic for Doppler Broadening. Evidently one gets an inherent inconsistency between the integral and differential scattering cross section within the transport solver codes. In this study this missing Doppler Broadened formalism for the differential scattering cross section is introduced in its stochastic and deterministic form. The impact on core criticality is shown to be up to 600 pcm and the change in the nuclides' inventory significant, in particular the ^{239}PU content can be changed by several percents.

Ein komplementärer Dopplerverbreiterungsformalismus und dessen Wirkung auf Kernreaktorsimulationen. *Die grundlegende Gleichung der Neutronenphysik ist die Boltzmann-Transportgleichung. Falls in einer Kernreaktorsimulation starke Absorption oder anisotrope Streuung beschrieben werden soll, wird auf eine Näherung dieser Gleichung zurückgegriffen. Der Absoptions- und der Streuwirkungsquerschnitt treten implizit auf der linken Seite der Gleichung als integrale Verlustterme auf. Sie sind energie- und temperaturabhängig, d. h. Doppler verbreitert. Der Streuwirkungsquerschnitt tritt explizit in seiner differenziellen Form auf der rechten Seite der Boltzmanngleichung als Produktionsterm auf. Hier jedoch findet die Dopplerverbreiterung in der Regel nicht statt, d. h. die Temperaturabhängigkeit sowie die Existenz der Resonanzen bleiben unberücksichtigt. In dieser Studie wird der Doppler verbreiterte Streukern vorgestellt, sowie nach seiner Implementierung in einem stochastischen Transportcode dessen Einfluss auf Kenngrößen der Reaktorphysik diskutiert. Es wird gezeigt, dass sich dieses Verfahren mit bis zu 600 pcm in der Kritikalität im Vergleich zum Standardverfahren auswirkt. Darüber hinaus ändert sich das Nuklidinventar deutlich, insbesondere die erbrütete Menge ^{239}Pu.*

1 Introduction

For the calculation of neutron reaction rates and the power of a reactor the flux distribution must be determined in great detail throughout the reactor. All cross sections must be known in every region. If this is the case one can use diverse core solvers based on diffusion or transport theory. The latter formalism is used also for stochastic solution processes, e.g. the so called Monte Carlo method.

The transport approach gives the flux in greater detail than the diffusion one does. If one defines a vector flux $f(\vec{\Omega}')$which can evaluate the number of neutrons crossing a unit area perpendicular to a specific direction $\vec{\Omega}'$ per second then the number of directions is constraint by the solution method. The deficiency of the diffusion equation is that the flux Φ refers to neutrons moving in any direction; consequently anisotropy is excluded, which might lead to erroneous results. In a deterministic approach both methods are restricted to a limited number of energy groups at which the neutron flux is defined.

In a Monte Carlo method one improves the transport solution procedure by dealing with continuous energy spectrum as well as with increasing the number of neutron's allowable flight directions.

The above mentioned transport methods depends strongly on the Slowing Down treatment:

$$\frac{1}{v}\frac{\partial f(E',r,\Omega',t)}{\partial t} + \Omega' \bullet \nabla f(E',r,\Omega',t) + [\Sigma_s(E') + \Sigma_a(E')]f(E',r,\Omega',t) =$$

$$= \int_\Omega \int_0^\infty \Sigma(E \to E', \Omega \to \Omega')f(E,r,\Omega,t)\,\mathrm{d}\Omega\,\mathrm{d}E + S(E',r,\Omega',t) \qquad (1)$$

The first term on the right hand side is a summation of all neutrons at energy E' and direction Ω', which changed their initial energy E and their flight direction Ω, after an interaction with a target nuclei. The solution of those integrals is based upon two body kinetics model, which underlies most of the slowing down calculation methods.

On the other hand, the probability that a scattering interaction will indeed occur is exhibited through the integral scattering cross section on the left (losses) hand side of the transport equation. The probability of the scattering as well as the absorption process is temperature and energy dependent, namely Doppler Broadened.

The first term on the right hand side of Eq. (1) is the differential scattering cross section. Thereafter it must be Doppler Broadened as the integral scattering cross section.

The Doppler Broadened differential cross section which was missing in the conventional two body kinetics model is presented in this study. We present an analytical as well as a stochastically solution which is in full compliance with the Doppler Broadened scattering cross section. The inclusion of this phenomenon in core simulation exhibits considerable large deviation from the standard reference two body kinetic

method based solution. In addition it is shown that the definition of the resonance parameters themselves is sensitive to the Doppler Broadened scattering treatment. The recent effort in nuclear reactor simulations to evaluate local parameters like flux or power of a single fuel pin is also shown to be strongly dependent on this new developed Doppler Broadened complementary method.

2 The Doppler Broadened (DB) scattering kernel

The common way to describe a scattering interaction makes use of a two body kinematics model (e.g. *Bell* and *Glasstone* [1], *Emendörfer* and *Höcker* [2]) assuming that the target nucleus is at rest (0 K). The kinetic equations which define the energy E′ and the spatial direction of the scattered neutron after the collision are presented as a function of the incident neutron energy E. The probabilities of scattering are constant within the energy range $\alpha^* E < ; E' < E;\ \alpha^* = [(A-1)/(A+1)]^2$. A is the mass number of the target nucleus. This approach is known as the asymptotic method.

2.1 Introduction of a new scattering kernel treatment

The inclusion of the thermal agitation of the target nuclei and their resonant structure is reminiscent of the fundamental equation used by *Weisbin* and *Cullen* [3]. However it is used here for Doppler Broadening cross section in its differential form:

$$\sigma_s^T(E \to E', \vec{\Omega} \to \vec{\Omega}') = \frac{1}{v}\int \mathrm{d}\vec{V}\, M^T(V)\, P(\vec{v}, \vec{V} \to E', \vec{\Omega}')\{\mathrm{v}_r \sigma_s(E_r)\} \quad (2)$$

$M^T(V)$ is the Maxwellian spectrum and the cross-section is that for the target nucleus at rest i.e. 0 K.

In contrary to the Doppler Broadening of the integral cross section the above differential expression includes the probability density, that the interaction between the particles of velocities $\vec{v}$ and $\vec{V}$ leads to the neutron parameters E' and $\vec{\Omega}'$ after the collision, in addition to the scattering rate at 0 K, in the thermal averaging integral over the spectrum of the velocities of the target nuclei.

The solution of Eq. (2) was introduced by *Rothenstein* and *Dagan* [4]. Later on an equivalent solution adaptable to the NJOY [5] data processing code, was developed by *Rothenstein* [6] (Eq. (3)). It includes explicitly the energy dependent cross section $(\sigma_s^{\mathrm{tab}})$and the temperature T. The tab sign of the cross section indicates that it is a tabulated function, such as on a PENDF file, with specified (usually linear) interpolation laws between the successive entries. The data must be at 0 K, as indicated by the second argument of Eq. (3). In addition, one must further take into account that σ_s^{tab} is the bound atom scattering cross section and includes the factor $((A+1)/A)^2$ in its definition.

The integration over the variables ξ and τ replaces the integration over the velocity variables t and x where:

$$t = \frac{\tau+\xi}{2} = u\sqrt{(A+1)}\ ; \quad x = \frac{-\tau+\xi}{2} = c\sqrt{(A+1)}$$

In addition,

$$\varepsilon = v\sqrt{(A+1)}\ ; \quad \varepsilon' = v'\sqrt{(A+1)}$$

where v and v' are the velocities of the neutron before and after the interaction, respectively. The velocity of the centre-of-mass is c and the velocity of the neutron in the centre-of-mass frame is u.

$$\sigma_s^T\left(E \to E', \vec{\Omega} \to \vec{\Omega}'\right) = \frac{1}{4\pi E}\sqrt{\frac{A+1}{A\pi}}\int_{\varepsilon_{\max}}^{\infty} \mathrm{d}\xi \int_{\tau_0(\xi)}^{\tau_1(\xi)} \mathrm{d}\tau \left(\frac{\xi+\tau}{2}\right)$$

$$\times \left(\sigma_s^{\mathrm{tab}}\left[\left(\frac{A+1}{A^2}\right)\frac{(\xi+\tau)^2}{4}k_B T, 0\right]\right) \times \exp\left(\nu^2 - \left[\frac{(\xi+\tau)^2}{4A} + \frac{(\xi-\tau)^2}{4}\right]\right)$$

$$\times \left(\frac{\varepsilon_{\max}\,\varepsilon_{\min}(\xi-\tau)^2}{B_0 \sin\hat{\varphi}}\right) \quad (3)$$

The introduction of Eq. (3) into the NJOY code allowed for the generation of the probability tables known as the $S(\alpha,\beta)$ tables for heavy nuclide with pronounced resonances. Strictly speaking this methodology, usually kept for the chemical binding dependent scattering procedure of light nuclides, was extended to all nuclides [7] in particular to those where the resonances are well pronounced.

The above method calls for a huge storage due to vast amount of scattering data required for accurate representation of scattering angles and energies probabilities of emitted neutron after an interaction.

An alternative stochastically approach which was embedded into Monte Carlo codes was developed by *Becker* et al. [8]. This approach (DBRC – Doppler Broadened Rejection Correction) is based on the use of a complementary rejection technique [8]. Expression (4) describes this stochastic probability choice of the target velocity V and the angle of interaction μ.

$$P(V,\mu) \to \quad \text{a)} \quad \left\{\frac{(2\beta^4)V^3 e^{-\beta^2 V^2} + (\beta v\sqrt{\pi}/2)(4\beta^3/\sqrt{\pi})\,V^2 e^{-\beta^2 V^2}}{1+\beta v\sqrt{\pi}/2}\right\}$$

$$\text{b)} \quad \left\{\frac{v_r}{v+V}\right\} \qquad \text{c)} \quad \left\{\frac{\sigma_s(v_r,0)}{\sigma_s^{\max}(v_\xi,0)}\right\} \quad (4)$$

where:

$$\beta = \left(\frac{Am}{2k_B T}\right)^{1/2}$$

v is the neutron speed, V speed of the target and neutron speed v_r is relative velocity to the target at rest.

The last two factors in curly parenthesis in Eq. (4) represents two constraints on the chosen value of V and μ in step a. The ratio $v_r/(v+V)$ cannot exceed unity and a rejection technique is applied in MCNP. If a random number between 0 and 1 is less than $v_r/(v+V)$, the choice of the speed V and μ (which defines v_r) is accepted. The choice of the target velocity V in step a) in (4) is performed by sampling a specific velocity for the target nucleus out of a Maxwell Boltzmann distribution [8]. The last term c) expressed by the ratio of two cross sections is always below unity and it is the missing term added. It is exactly this term, which we defined above as DBRC, that introduces correctly the Doppler broadening of the scattering kernel. Again the representation of this term is via a rejection technique, namely if random number between 0 and 1 is less then the quotient of term c) in (4) the sampled values V and μ are rejected and step a) is repeated.

The confirmation of the additional rejection technique was given by comparison to the former mentioned method using $S(\alpha,\beta)$ probability tables for heavy nuclides with pronounced resonances. The advantage of the latter treatment is its flexibility and efficient introduction of the Doppler Broadened differential cross section. The importance of this new model for core calculations is presented in the next section.

3 Impact of the Doppler Broadened (DB) scattering kernel on reactor calculation

In order to assess the impact of the Doppler Broadened kernel on reactor simulation two types of calculation were performed. The reference case was performed with the standard method in Monte Carlo codes. Then in the second run the Doppler broadened scattering kernel was introduced within the MCNP code [9].

A typical PWR cell defined by *Rowlands* [10] was tested first. The pin geometry and material composition are listed in Tables 1 and 2 respectively. The enrichment of the fuel was about 3.1 % of ^{235}U. The temperature of the fuel is 1 200 K.

An MCNP input was prepared accordingly and the reference standard simulation was compared to the case where the DB scattering kernel was introduced for ^{238}U. Fig. 1 shows the differences in the criticality values in view of the introduction of the new kernel as a function of the burn up. It is seen that for fresh fuel the introduction of the DB kernel leads to reduction of about 440 pcm in criticality. With increasing of burn up the difference becomes smaller and at a certain point the criticality of the DB dependent kernel simulation is higher. The reason for the increasing criticality in the latter case is the surplus neutrons that are absorbed within the ^{238}U resonances from which eventually ^{239}Pu is generated. Consequently, the breeding of the fuel pin is increased and with it the criticality. The change in the ^{239}Pu inventory during the burn up cycle is shown in Fig. 2. It is seen that the relative increase in comparison with the reference case reaches about 2 % for ^{239}Pu and about 5 % for the ^{235}U.

The increased interest in accurate pin by pin calculation and the impact of the new kernel on local effects lead to the next analysis. In this case a whole subassembly was tested where the fuel pins were divided into groups according to their location within the subassembly as shown in Fig. 3. The specification of the subassembly was taken from the GRS benchmark The GRS S/A [11] is an 18 by 18 matrix with 4 % w/o ^{235}U enrichment including 24 water holes. This arrangement equates the commonly used pressurized water cooled reactors. As in the fuel pin analysis a reference calculation was followed by a simulation where the DB kernel was introduced. The different of the ^{239}Pu between the two calculations is presented in Fig. 4. In all three tested pin bundles the changes reach relatively early 0.8 %. It is slightly lower then the results shown for the pin case as the temperature chosen for this benchmark

Table 1. Geometrical dimensions of the pin cell

pin cell benchmark	PWR UOX
fuel radius	0.4 cm
cladding outer radius	0.45 cm
equivalent cell radius	0.67703 cm

Table 2. Particle densities of the PWR unit cell benchmark

isotope	zone	density atoms/b-cm
U_{235}	fuel	0.00070803
U_{238}	fuel	0.022604
O_{16}	fuel	0.046624
Zr	clad	0.043241
H	moderator	0.066988
O	moderator	0.033414

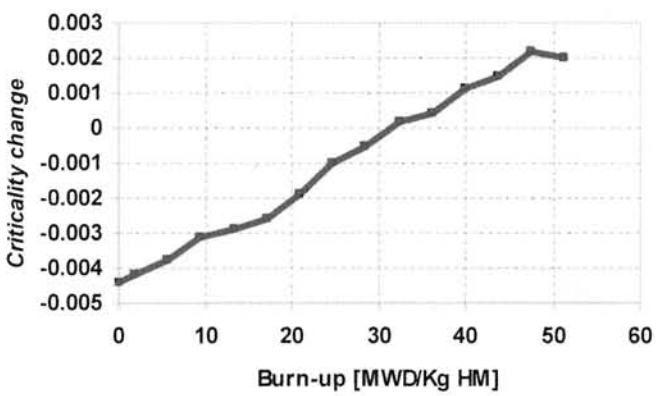

Fig. 1. Differences in criticality as a function of burn up due to the introduction of the new scattering kernel. Temperature of the fuel is 1 200 K

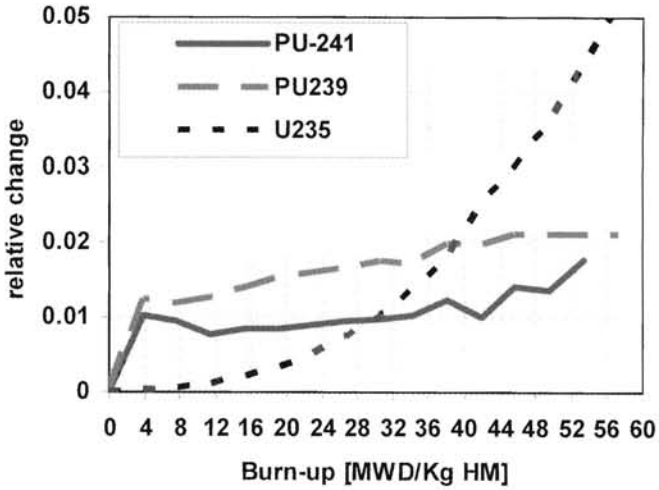

Fig. 2. Relative change during burn up cycle at 1 200 K in view of the Doppler Broadened kernel introduction

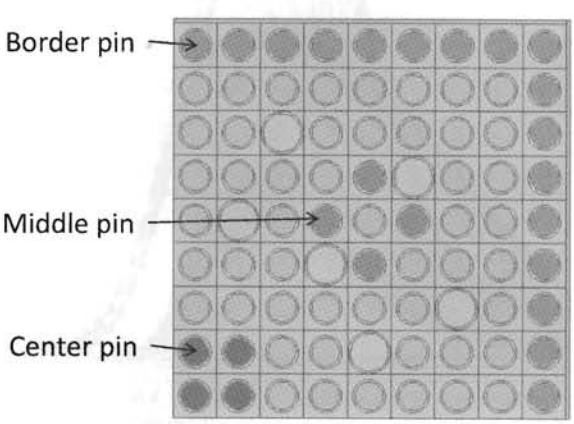

Fig. 3. One quarter of a subassembly with three different fuel pin burn up bundles

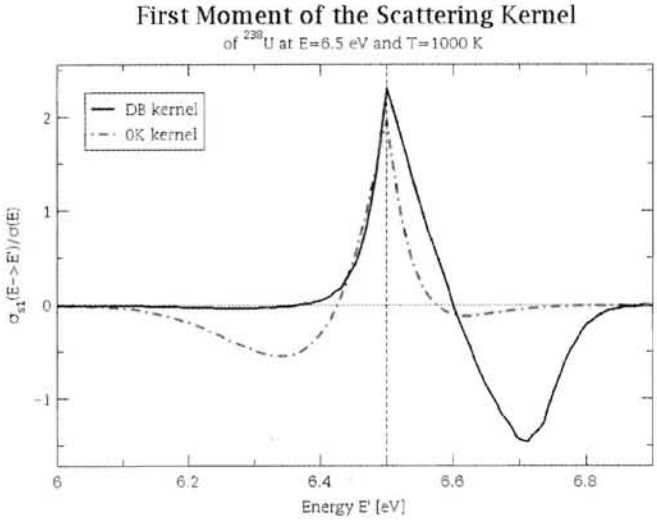

Fig. 6. Differences of first moment calculation for a neutron with incident energy of 6.5 eV at 1000 K due to the insertion of the DB kernel

4.2 Multiple scattering effects by determination of resonance parameters

The preparation and validation of resonances' parameters are based on simulations of dedicated experiments with unique tools which adjust the parameters in a manner that allows for best fit of the specific reaction type measurement. Well known are the codes REFIT [13] and SAMMY [14]. Both of them necessitate in their solver technique a so called "multiple scattering treatment" for the description of a neutron that passes through a sample and eventually might undergo different types of reactions and in particular, several scattering events. Consequently the correct treatment of each of those scattering interactions with the sample nucleus is part of the resonance parameters fitting. It has already been shown that inclusion of the DB kernel enabled a significantly improved fitting [15] in several cases.

5 Conclusions and outlook

A new Doppler Broadened Scattering kernel was introduced. It is in accordance with its integral part namely, the scattering cross section itself. Two solution methods were developed and validated against each other. The analytical one is based on the generation of scattering probability tables, known as the $S(\alpha,\beta)$ tables. Their use was extended to deal not only with the chemical binding effects for light nuclides but also with heavy nuclides with pronounced resonances. The second developed method is pure stochastic. It is based upon the so called DBRC approach which introduces the Doppler broadening of the resonances by means of an additional rejection technique. The impact of the new kernel is important for evaluation of different core characteristic such as criticality, fuel inventory and also concerning safety parameters such as the Doppler Effect value which is increased by about 10–17 % depending on the fuel temperature [7].

The successes to prove the DB kernel phenomenon experimentally was augmented by further investigations in related topics. In particular it is evident that the Legendre moments must be corrected in view of the new DB scattering kernel. In addition other processes which rely upon the correct scattering treatment like multiple scattering by resonance parameter fitting or other scattering processes in medical therapies etc. should be reevaluated to account for the noticeable impact of the DB scattering kernel.

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The authors of this contribution

PD Dr. habil. *Ron Dagan*
Forschungszentrum Karlsruhe Gmbh
Institut für Neutronenphysik und Reaktortechnik
Hermann von Helmholtz Platz 1,
76344 Eggenstein-Leopoldshafen, Germany
E-mail: dagan@inr.fzk.de

Dr. *Bjorn Becker*
E-mail: beckeb3@rpi.edu

Prof. Dr. *Yaron Danon*
E-mail: danony@rpi.edu

Rensselaer Polytechnic Institute
Department of Mechanical, Aerospace, and Nuclear Engineering
NES Bldg. 110, 8th Street, Troy, New York 12180, USA

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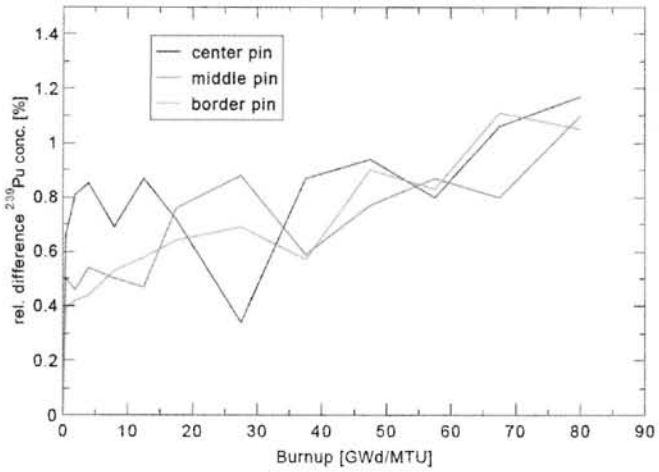

Fig. 4. Differences in Pu^{239} concentration in view of the Doppler broadened scattering kernel at 800 K

was only 800 K in comparison to the 1200 K for the pin cell case above. This result emphasizes, already at 800 K, the uncertainty of local estimation of pin power, flux, or fuel inventory, where the fluctuations, in the peak to average power, are about 2–3 %.

4 Further impacts of the Doppler Broadened (DB) scattering kernel

In the former section the explicit impact of the DB scattering kernel was presented. In this section two other relevant issues are shortly discussed, which indirectly influence any core calculation. They refer to two different domains in neutron physics. The first one is the deterministic representation of the angular distribution and the second the determination of the resonance parameters upon which the temperature dependent cross sections are defined.

4.1 The Legendre moments for heavy nuclides

The angular distribution experiments performed in RPI [12] showed very clearly that the estimated angular distribution in current MC codes is for some cases 80 % deviated. Consequently, an extensive study was performed to analyze the whole angular space. In Fig. 5 the impact of the DB kernel is shown for all scattering angles. For each angle two types of simulations were done. They are based on the experiment done in RPI [12] but with variety of angles. Two simulated angles in the range of 140° and a forward angle at about 39° were confirmed also experimentally, which gave the ground to simulate all other angles. Whilst all forward angles deviate only slightly from the reference case, all backwards angles show huge discrepancies when the DB scattering kernel is introduced into the MC simulation tool.

Consequently it is evident that for deterministic calculation the current Legendre moments, which are based on zero degree Kelvin lead to erroneous results. The zero moment itself which represent the energy transfer after the interaction between the neutron and the target nuclei must be evidently also amended to include the existence of the ambient temperature and the vicinity to the resonances of the specific nuclei at stake. Fig. 6 demonstrates the deviation of the DB kernel from its reference case. It elaborates that for heavy isotopes the current inclusion of the 0 K based higher moments in deterministic codes is questionable as far as its physical meaning is concerned.

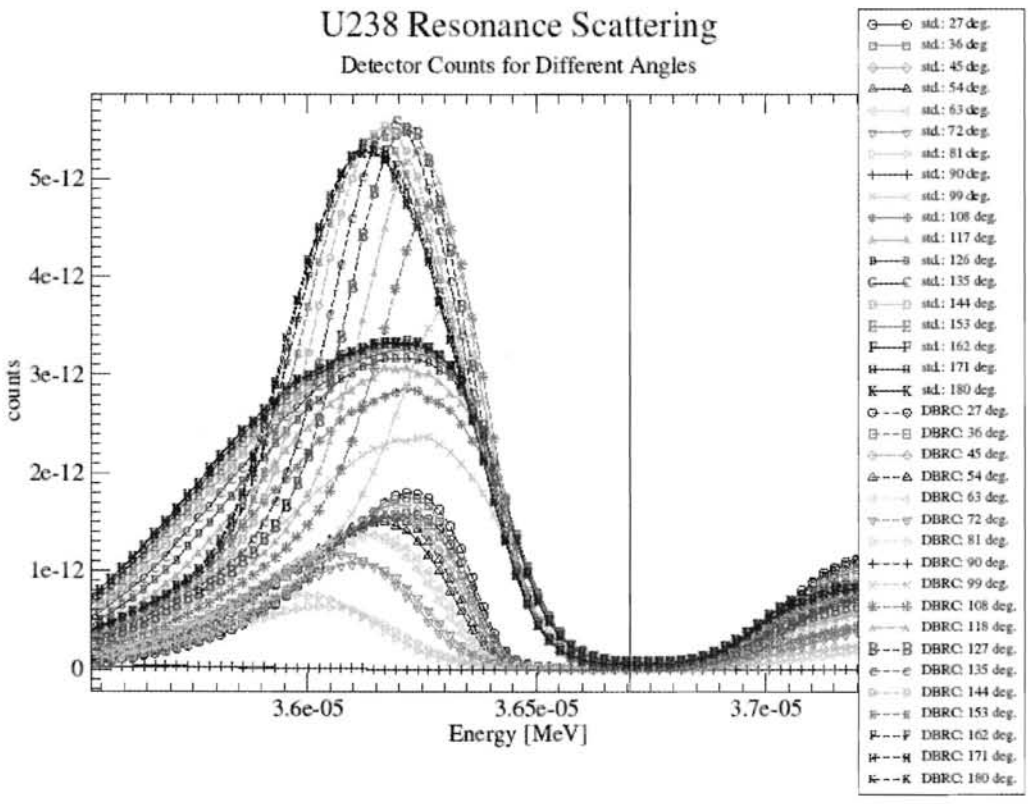

Fig. 5. Changes of the simulated counts of a detector at different angles of scattering from a target nucleus ^{238}U at 300 K. (Based on the experiment performed at RPI [12])