Delayed Neutron Fraction Calculation in PFBR using MCNP

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Abstract - Various Monte Carlo techniques for determination of effective delayed neutron fraction ($\beta_{eff}$) has been explained in this paper. Calculations are presented for the PFBR fresh core using MCNP for a 3D model of the reactor implementing prompt Monte Carlo method. The results were compared with a deterministic calculation implementing 1st order perturbation theory in a 2D geometry. The result from the deterministic calculation is in good agreement with the Monte Carlo calculation.

I. INTRODUCTION

The influence of the delayed neutrons on the reactor dynamics can be understood through their impact on the reactor power change rate, in spite of that they constitute only a very small fraction of the total number of neutrons generated from fission, they play a dominant role in the fission chain reaction control and accurate determination of the $\beta_{eff}$ value is an important requirement in the field of reactor physics.

In the past, $\beta_{eff}$ used to be traditionally calculated by taking the ratio of the adjoint and spectrum-weighted delayed neutron production rate to the adjoint- and spectrum-weighted total neutron production rate. An alternative method has also been used in which $\beta_{eff}$ is calculated from simple $k$-eigenvalue solutions [1].

This report briefly summarizes techniques for determination of $\beta_{eff}$ using various Monte Carlo methods. Earlier for PFBR $\beta_{eff}$ was estimated using 2D diffusion code NEWPERT. Since recently produced cross-section file ENDF/VII.1 and monte carlo code MCNP is available study was planned to compare the $\beta_{eff}$ estimated by a different method and cross-section to access the accuracy in the calculation. In this work $\beta_{eff}$ was estimated using a completely different methodology based on Monte Carlo which considers 3-dimensional reactor geometry modeled in MCNP4c code.

II. NOMINAL CORE CONFIGURATION OF PFBR

The second stage of Indian nuclear power programme involves establishing Fast Breeder Reactors for power generation. The Prototype Fast Breeder Reactor is being developed to demonstrate the techno-economic viability of Fast Breeder Reactor technology. The PFBR is a 500 MWe, sodium cooled, pool type, mixed oxide (MOX) fuelled reactor. The core layout is shown in Fig. 1. A conventional mixed oxide (PuO$_2$-UO$_2$) homogeneous two zone core has been chosen for the reactor. The radial and axial blankets are of depleted UO$_2$. It can be seen that the active core consists of 85 FSA of low Pu enrichment (20.7% PuO$_2$ in UO$_2$) in the central region followed by 96 FSA of higher Pu enrichment (27.7 % PuO$_2$ in UO$_2$). The active core contains 12 AR in two rings of six each for reactivity management and shutdown. Of the twelve AR, nine are designated as the Control and Safety Rods (CSR) and the other three as the Diverse Safety rods (DSR). The FSA are surrounded by 120 radial blankets and 138 steel reflector SAs. Each FSA contains 217 helium bonded fuel pins. Each pin has a 1000 mm column of fuel, 300 mm each of upper and lower axial blanket columns and an upper (230 mm) and lower (750 mm) fission gas plenum. The core layout and core parameters are shown in Fig. 1 and Table-I respectively.[2]

Table I. Core Parameters

<table>
<thead>
<tr>
<th>Reactor power</th>
<th>1250MWt/500 MWe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>PuO$_2$-UO$_2$</td>
</tr>
<tr>
<td>Coolant</td>
<td>Sodium</td>
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</table>
III. $\beta_{\text{eff}}$ ESTIMATION METHODS

In general, for the total neutron production rate by fission for a reactor near criticality, and without external source, one writes [4]

$$P = \int \psi(E) \Sigma_f (r, E) \phi(r, E, \Omega) dE \, dr \, d\Omega \quad \ldots(1)$$

where $E, \Omega$, and $r$ are the energy, solid angle, and position of the neutrons, $\phi$ is the neutron flux, $\Sigma_f$ is the macroscopic fission cross section of the material at position $r$, $\nu$ is the average neutron multiplicity per fission. For the production $P_d$ of delayed neutrons, one replaces the factor $\psi(E)$ by $\nu_d(E)$, the average delayed neutron multiplicity per fission. For the sake of simplicity, it is not distinguished between the several delayed neutron time groups all of which have their own energy spectrum. The ratio $P_d = P$ is then the fundamental delayed neutron fraction $\beta_0 = P_d / P$. So far, this is fairly straightforward. The problems start when trying to assess how effective this fraction is in terms of reactor dynamics. The effect that neutrons have on reactor behavior is through their ability to generate power, i.e., to induce the next fission. It follows that we should compute the number of fissions that are induced by delayed neutrons, as well as by all neutrons.

In transport theory one calculates the effectiveness in generating fission by multiplying by the energy spectrum of the generated neutrons, $\chi(E')$, and by the adjoint function $\psi(r, \Omega', E')$, often referred to as 'adjoint flux.' The adjoint function is defined as a fundamental mode eigenfunction of the equation adjoint to the time independent transport equation. Here $r, E'$ and $\Omega'$ are the position, energy, and solid angle of neutrons generated by the fissions that were induced by the incident neutrons characterized by $r, E, \Omega$. Position $r$ is obviously the same for both. Factor $\chi(E')$ is needed because the energy the neutrons start with has an impact on their effectiveness in inducing fission. The adjoint function $\psi(r, \Omega', E')$ is used because it is important to account for the significance of a neutron with properties $r, E', \Omega'$ for producing fission and is proportional to the asymptotic power level resulting from the introduction of a neutron in a critical system at zero power [1], leading to the so-called spectrum and adjoint weighted neutron production

$$P_{\text{eff}} = \int \psi(r, \Omega', E') \chi(E') \nu(E) \Sigma_f (r, E) \phi(r, E, \Omega) dE \, d\Omega \, dE' \, d\Omega' \, dr \quad \ldots(2)$$

One can calculate the same quantity for delayed neutrons only $P_{d,\text{eff}}$ by replacing $\chi(E')$ by $\chi_{\text{df}}(E')$ and $\nu(E)$ by $\nu_d(E)$. One arrives at the Keepin definition taking the ratio $\beta_{\text{eff}} = P_{d,\text{eff}} / P_{\text{eff}}$

$$\beta_{\text{eff}} = \frac{\int \psi \chi_{\text{df}} \nu_d \phi \, dE \, d\Omega \, dE' d\Omega'dr}{\int \psi \chi \nu \phi \, dE \, d\Omega \, dE'd\Omega'dr} \quad \ldots(3)$$

where $'m'$ means the $m$th isotope and $'i'$ is the $i$th delayed neutron group, other symbols are mentioned earlier. It is instructive to interpret $P$ as the neutron source (the number of neutrons produced per unit of time), and $P_{d,\text{eff}}$ as the number of fissions produced by this source per unit of time. In Monte Carlo calculations the physical processes are simulated as realistically as possible. Consider the introduction of a neutron with properties $r, E', \Omega'$ in a critical system with zero power. This neutron will produce other neutrons by inducing fission and these neutrons will in turn cause fission and thereby lead to further neutrons, etc. The number of fissions produced in this way will approach a limit which is given by the iterated fission probability that which is proportional to the adjoint function. Using the number of fissions counted and the knowledge of whether the neutron was prompt or delayed at its start, one can easily calculate $\beta_{\text{eff}}$ [11]. Iterated Fission Probability (IFP) method has been implemented in the codes like MCNPX, TRIPOLI, SERPENT etc.

(1) Prompt Method:

Denoting the integral in (2) as $<\chi\nu>$ making use of that the integrals are linear and introducing $v_{\nu} = \nu - \nu_d$, one can rewrite the expression for $\beta_{\text{eff}}$ as follows:

$$\beta_{\text{eff}} = \frac{<\chi_d \nu_d>}{<\chi\nu>} = 1 - \frac{<\chi\nu - \chi_d \nu_d>}{<\chi\nu>} \approx 1 - \frac{<\chi_p \nu_p>}{<\chi\nu>} \quad \ldots(4)$$

The approximation in the last step is based on the following arguments. The term $<\chi_d-\chi_p> \nu_d$ is two orders of magnitude smaller than $\chi_p \nu_p$ because $\nu_d$ is two orders of magnitude smaller than $\nu_p$. For the same reason, the shape of $\chi$ is almost equal to that of $\chi_p$. At this point a crucial step is taken. Often it is simply stated that,
\[
\frac{\langle \chi_p \nu_p \rangle}{\langle \chi_v \rangle} = \frac{k_p}{k} \rightarrow \beta_{\text{eff}} \approx 1 - \frac{k_p}{k} \quad \cdots (5)
\]

In fact, this is an approximation. It is true that the \( k \) -eigenvalue is the ratio of production \( P \) and loss \( L \), and that this also holds for the ratio of \( P_{d,\text{eff}} \) and \( L_{d,\text{eff}} \).

The total effective delayed neutron fraction is therefore,

\[
\beta_{\text{eff}} = \frac{k - k_p}{k} = \sum_i \beta_{\text{eff},i} \quad \cdots (6)
\]

where \( k \) is the eigenvalue for all neutrons and \( k_p \) is the eigenvalue for prompt neutrons only.

(2) Spriggs Method:

The delayed neutron fraction is traditionally counted \[1\] from,

\[
\beta_{\text{eff}} = \frac{\sum_i \int \int \int x_m \psi x_{d1} v_{d1}^m \sum_f \phi \ d\Omega \ dE \ d\Omega \ dE \text{ dr}}{\sum_m \psi X_m v_c^m \sum_f \phi \ d\Omega \ dE \ d\Omega \ dE \text{ dr}} \quad \cdots (7)
\]

Alternatively \[6\],

\[
\beta_{\text{eff}} = \frac{\langle \chi_d \nu_d \rangle}{\langle \chi_v \rangle} = 1 - \frac{\langle \chi_d \nu_d \rangle}{\langle \chi_v \rangle} = \beta_0' \frac{\langle \chi_d \nu_d \rangle}{\langle \chi_v \rangle} \quad \cdots (8)
\]

where we have introduced, after Spriggs et al., yet another delayed neutron fraction \( \beta_0' \). For the present purposes we restrict ourselves to the approximation that \( \beta_0' = \beta_0 \) because we still need to perform adjoint weighting to calculate \( \beta_0' \). By approximating \( \beta_0' = \beta_0 \) we can simplify the calculation to something that can easily be implemented in a Monte Carlo code. As remarked by Spriggs et al., this approximation works well for homogeneous cases. Also with the introduction of a ratio of \( k \) values,

\[
\frac{\langle \chi_d \nu_d \rangle}{\langle \chi_v \rangle} = \frac{k_d}{k} \rightarrow \beta_{\text{eff}} = \beta_0' \frac{k_d}{k} \quad \cdots (9)
\]

As in the case of the 'prompt' method, this is also an approximation. Here the problem lies in the definition of \( k_d \).

Since this parameter is supposed to be calculated by means of a transport theory code, it should be defined as the eigenvalue pertaining to a reactor with \( \chi = \chi_d \) and \( \nu = \nu_d \). Again, the shapes of \( \phi \) and \( \psi \) will not be the same as for the original system with \( \chi \) and \( \nu \), for which the eigenvalue is \( k \).

This subtlety is explained by Spriggs et al. for their method of calculating \( \beta_{\text{eff}} \).

(3) The HOLLAND MC Method

This method was proposed by van der Mark and K. Meulekamp from Petten NRG, Holland \[4\]. Therefore, the neutron production and the spectrum weighting, which can be provided by counting the number of fissions generated per history. One can then calculate the average number of fissions generated by all neutrons. This is \( \beta_{\text{eff}} \) as defined in equation (3), where \( \beta_{\text{eff}} = P_{d,\text{eff}}/P_{\text{eff}} \) \[4\].

On the other hand, when we apply the generation definition of history to \( \beta_{\text{eff}} \) calculation, an approximation is introduced because history now only runs until the next fission. Therefore our counting of the number of induced fissions also counts only until the next fission, i.e., we are not calculating the iterated fission probability but the next fission probability. This is no longer exactly proportional to the adjoint function, nevertheless, it is a useful approximation.

For the calculation of \( \beta_{\text{eff}} \) it is not required to know the adjoint function very precisely. The value for \( \beta_{\text{eff}} \) is largely determined by the value of \( \beta_0 \), the fraction of delayed neutrons produced. For most critical systems, the value for \( \beta_{\text{eff}} \) differs < 20% from \( \beta_0 \). Since the effectiveness of neutrons, i.e., the adjoint function only influences this small difference between \( \beta_{\text{eff}} \) and \( \beta_0 \), one only needs to know the adjoint function with 10% accuracy to get 2% accurate results for \( \beta_{\text{eff}} \).

Finally, it should be noted that a calculation of \( \beta_{\text{eff}} \) in this way is done by means of some minor bookkeeping in the code, which will give a result for \( \beta_{\text{eff}} \) in the same run with which one calculates \( k_{\text{eff}} \).

IV. \( \beta_{\text{eff}} \) Calculation

The effective delayed neutron fraction \( \beta_{\text{eff}} \) in PFBR is calculated by MCNP4C transport code using prompt method, which requires two calculations. According to \[5\] it is defined:

\[
\beta_{\text{eff}} \approx 1 - \frac{\langle \chi_p \nu_p \rangle}{\langle \chi_v \rangle} \approx 1 - \frac{k_p}{k} \quad \cdots (10)
\]

The required value of the effective multiplication factor \( k_{\text{eff}} \) taking both prompt and delayed neutrons into account was acquired in the straight calculation mode of MCNP4C calculation, using the data card KCODE. In the KCODE mode the mean values of both prompt and delayed neutrons (if these are included in the used cross-section libraries) are used in criticality calculations. To prevent the influence of the delayed neutrons, TOTNU data card with entry NO had to be used, to obtain the value of effective multiplication factor for prompt neutrons (\( k_p \)). A TOTNU card with NO as the entry causes \( \nu_p \) to be used, and consequently \( k_p \) to be calculated, for all fissionable nuclides for which prompt values are available. If the TOTNU card is used and has no entry after it, the total average number of neutrons from fission (\( \nu \)) using both prompt and delayed neutrons is used and the total effective multiplication factor (\( k \)) is calculated.
The entire PFBR core has been modeled in MCNP. In the model, several simplifications were considered:

1. Fuel pin level modeling has not been taken into consideration.
2. Various detectors like fission chambers etc. for power measurement during operation are not considered in the model.
3. All safety rods are in down position, ie core is subcritical.

The calculation has been performed using ENDF/B-VII.1 cross-section library. Spatial distribution of source neutrons was created using the KCODE data card. The source neutrons in each cycle are determined by the points generated in the previous cycle. For the initial cycle, the point neutron sources are necessary to specify. These are specified explicitly by KSRC data card. 5000 active cycles and 500 neutron generations were used in the calculations.

V. CALCULATION RESULTS:

The first calculation in KCODE mode with TOTNU card with NO, brought following value of effective multiplication factor for prompt neutrons: \( k_p = 0.91484 \pm 0.00077 \). The second calculation result was the value of total effective multiplication factor: \( k = 0.91811 \pm 0.00052 \). The final effective delayed neutron fraction for the model of PFBR, calculated using prompt method (10):

\[
\beta_{\text{eff}} = 1 - \frac{k_p}{k} = 1 - \frac{0.91484}{0.91811} = 0.00356 \pm 0.00025 \quad \text{(11)}
\]

Fig. 2 Nominal core configuration as modeled in MCNP

VI. DETERMINISTIC METHOD:

The 500 MWf FBR core design consists of 181 fuel subassemblies, 85 in the inner core and 96 in the outer core of a slightly higher enrichment as described earlier in this paper. There are 12 control rods out of which 9 rods are called the control and safety rods (CSR) and 3 rods are called the diverse safety rods (DSR). A cross sectional view of the core showing the fuel, control, blanket and shielding subassemblies are shown in Fig. 1. The R-Z view of the reactor is shown in Fig. 3.

A two-dimensional perturbation theory code NEWPERT [8] utilizing previously calculated fluxes and adjoint fluxes was used to estimate effective delayed neutron fraction for PFBR fresh core. The code NEWPERT is a modified version of PERTALCI code originally developed at Cadarache [9].
n(e) is the isotopic compositions of element ‘e’ in the region where ‘e’ represents the element and ‘k’ represent the delayed neutron group. 

\( \Phi_{opt} \) is the adjoint flux in the particular coarse group to which the \( k^\text{th} \) delayed neutron group belong.

1st order perturbation theory estimate of \( \beta_{\text{eff}} \) is found to be 355 pcm [10]. The result from the perturbation theory is in good agreement with the present Monte Carlo.

**Table 2: Delayed neutron fraction table.**

<table>
<thead>
<tr>
<th>k</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta_k ) (pcm)</td>
<td>8.2</td>
<td>76.8</td>
<td>66.9</td>
<td>128.4</td>
<td>57.6</td>
<td>17.2</td>
<td>355</td>
</tr>
</tbody>
</table>

**VI. CONCLUSION**

In this paper, possible determination methods of one main parameters of the reactor dynamics -the effective delayed neutron fraction \( \beta_{\text{eff}} \) are summarized and a calculation is made for PFBR using the stochastic transport Monte Carlo method based code MCNP. Delayed neutron fraction of PFBR has been calculated using the prompt method. The final value of the effective delayed neutron fraction 0.00356 with the standard deviation of 0.025% is matching with the delayed neutron fraction predicted by 2D deterministic code NEWPERT which is 0.00355.

**END NOTE**

Though Iterated Fission Probability (IFP) method which has been implemented in the codes like MCNPX, TRIPOLI, SERPENT, is more accurate compared to prompt method but prompt method is the simplest to be applied with MCNP code and does not require any modification of the code. Prompt method compares well with deterministic perturbation calculation. The IFP method also provides similar values of \( \beta_{\text{eff}} \) with increasing number of KCODE cycles, the uncertainties in determination of \( k_{\text{eff}} \) and \( k_{d1} \) cause uncertainty in \( \beta_{\text{eff}} \) results obtained with this method to increase [12]. IFP method and perturbation sampling methods are most suited when the effective contribution of the different delayed neutron groups needed to be investigated.

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