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Monte Carlo calculation of the effects of delayed neutron precursor transport in molten salt reactors

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Due to the motion of the fuel in molten salt reactors a portion of the delayed neutrons is born outside the reactor core, which decreases reactivity. The authors in their earlier papers presented a method which was developed in order to modify the program MCNP so that it can take into account the transport of the delayed neutron precursors, and therefore capable of calculating the reactivity loss of reactors with circulating fuel [1,2].

In the present paper, a further development of the method and its implementation in the MCNP code is presented, which makes it possible to radically reduce (by four orders of magnitude) the computer time needed to calculate the reactivity loss at the same accuracy. The method is based on the fact that the above mentioned decrease in reactivity is influenced by the delayed neutrons only, and can be outlined as follows. In the first of two consecutive criticality (KCODE) calculations the data describing the fission source (such as spatial coordinates of the fission points, delayed neutron parameters etc.) are recorded in a file, while in the second run only the random walk of the delayed neutrons is simulated using the data read from the file.

The applicability and efficiency of this variance reduction technique is illustrated by comparing calculations performed with the unmodified MCNP and the modified program, furthermore with some measured data.

The method is also applicable to the calculation of the effective delayed neutron fraction of static cases (i.e. solid fuelled reactors) at a high speed and accuracy.

KEYWORDS: molten salt, fluid fuel, fuel circulation, delayed neutrons, Monte Carlo method, criticality calculation, reactivity loss

1. Introduction

In the recent years a renaissance of the interest in molten salt reactors is observed. This fact played an important role in selecting the molten salt reactor as a Generation IV reactor type [3].

In molten salt reactors (or subcritical systems), the fuel circulates dissolved in some molten salt. The main advantage of this reactor type is the potential for continuous feed and on-line reprocessing.

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Due to the motion of the fuel, the precursor nuclei change their position between the fission and neutron emission events and decay may even occur outside the core. Therefore, the reactivity and effective delayed neutron fraction of these reactors are lower than those of solid fuel systems. The extent of the reactivity loss is primarily influenced by the velocity field of the fuel and the length of fuel recirculation cycle.

Since all of the presently operating power reactors utilize solid fuel, until recently little attention had been paid to the calculation of the reactivity loss caused by the circulation of the fuel. In the 1960s, measurements were performed on the Molten-Salt Reactor Experiment (MSRE) at the Oak Ridge National Laboratory and a theory was developed to determine the above mentioned reactivity loss [4]. When the interest toward such type of reactors started to grow a few years ago, research in this field gained a great impetus again. Efforts have been made to determine the reactivity loss by deterministic methods, such as the point kinetics theory and the one dimensional diffusion model presented in [5-7]. Though the deterministic theories are capable of describing the phenomena in full detail, they usually contain simplifications.

The problem can be efficiently studied with the aid of the Monte Carlo method since the motion of delayed neutron precursor nuclei can easily be accounted for by shifting the place of birth of the delayed neutrons. A further advantage of the Monte Carlo method is that tasks involving complex geometries and a large number of different materials can also be computed in an uncompromising manner. This is why it is reasonable to develop a method which enables certain general Monte Carlo neutron transport codes to perform criticality calculations on circulating fuel systems without any approximation.

The authors have presented [1,2] such a method and its implementation to the MCNP4C [8] code. With the aid of the modified version of MCNP, calculations were performed on a simple homogeneous reactor with cylindrical core. The method was also applied to perform calculations on the reactivity loss of the above mentioned MSRE reactor. The results obtained were in good agreement with the theoretical predictions and the measured reactivity loss values.

In this paper, after outlining the original method for the precursor transport simulation, a further development of the method capable for very effective variance reduction is presented. This advanced method makes it possible to radically reduce (by four orders of magnitude) the computer time needed to calculate the reactivity loss. The method is based on the fact that the above mentioned decrease in reactivity is influenced by the delayed neutrons only, and can be outlined as follows. In the first of two consecutive criticality (KCODE) calculations the data describing the fission source (such as spatial coordinates of the fission points, delayed neutron parameters etc.) are recorded in a file, while in the second run only the random walk of the delayed neutrons is simulated using the data read from the file.

The variance reduction technique is also applied to MCNP by modifying the source code. The applicability and efficiency of the method is demonstrated by carrying out calculations for the effective delayed neutron fraction of the GODIVA critical assembly and a hypothetical thermal lattice. As a practical application the reactivity loss in the MSRE is calculated, and the 3D effect of the velocity profile is investigated.

2. Method for the simulation of precursor transport

The method developed for the precursor transport simulation is based on the determination of the shift of the precursors from the velocity of the fuel and the sampled lifetime of the nuclide. The delayed neutron is born in this new position.

The above method is realized in MCNP4C. Although this is a highly flexible code and can

handle the delayed neutrons in every detail, it cannot account for the motion of delayed neutron emitters. Therefore, modifications were introduced into the code. With the aid of the modified version, the multiplication factor can be determined at different fuel velocities and different circulation cycle lengths.

The method can obviously be implemented for a given geometry, thus newer and newer versions of the program should be created when calculating reactors with different geometries. This is due to the fact that the motion of the neutron birth places should be described according to the geometry in question.

The above mentioned technique for the simulation of the delayed neutron emitter transport can most easily described by taking the case of a simple cylindrical homogeneous reactor core. The delayed neutron emitter is born at the place of fission, where a corresponding decay time is sampled. By use of the velocity, the length of time is determined in which the emitter nucleus would reach the upper plane of the cylindrical core. If this time is longer than that sampled for the emitter to decay, the distance traveled until the decay is calculated and the point of neutron creation is shifted with this distance parallel with the axis of the core. If the sampled decay time is longer than that needed for the emitter to reach the cover plane, the simulation takes the emitter off the core and it enters the primary (external) loop. In the next step it is determined whether the emitter can re-enter the core before it decays. If the sampled decay time is shorter than the time the emitter needs to reach the lower plane and then to re-enter the core, the neutron that would be generated by the delayed neutron emitter is not tracked. In the opposite case the emitter re-enters the core. The entrance position along the base surface is sampled uniformly. From now on, the emitter moves upward parallel with the axis of the core and the decay position can be modeled according to the algorithm described above. The above steps are repeated as long as the decay position of the emitter is not determined.

In the case of a more complex geometry the details of the algorithm are more complicated as well, however, the basic principle is the same as that described in the previous paragraph.

Two subroutines of the MCNP source code were modified: COLIDK (which generates the fission neutrons for the next cycle of the simulation) and SOURCK (which starts the required number of fission neutrons for the next cycle).

The applicability of the method has been demonstrated by performing different calculations with the modified MCNP [1,2]. For example, calculations have been made for the reactivity loss of a simple, cylindrical, homogeneous reactor as a function of fuel velocity and recirculation time. In order to prove that the method is applicable for complicated geometries as well, the reactivity loss of the MSRE reactor due to fuel circulation has been determined. With the aid of the method, three-dimensional effects such as the influence of the velocity profile of the MSRE and the shape of the bottom and upper plena of the reactor on the reactivity loss have been studied. The results obtained were in good agreement with the theoretical predictions and the measured reactivity loss values.

Nevertheless, it must be noted that a huge amount of CPU time was necessary in order to achieve the results with sufficiently low standard deviation. The intention to reduce this large computational requirement induced a further development of the method, by which significant variance reduction has been made possible.

3. Method for the reduction of the variance of the reactivity loss

3.1 Calculation of the reactivity loss due to fuel circulation

The loss in the effective multiplication factor (k_{loss}) due to the circulation of the fuel can be obtained by calculating the multiplication factors assuming a steady fuel case (k_{eff}) and a fuel

in motion case (k'_{eff}). The loss is obviously

$$k_{\mathrm{loss}} = k_{\mathrm{eff}} - k'_{\mathrm{eff}}\,, \tag{1}$$

or in terms of reactivity:

$$\rho_{\mathrm{loss}} = \rho - \rho' = \frac{k_{\mathrm{eff}} - 1}{k_{\mathrm{eff}}} - \frac{k'_{\mathrm{eff}} - 1}{k'_{\mathrm{eff}}} \approx \frac{k_{\mathrm{eff}} - k'_{\mathrm{eff}}}{k_{\mathrm{eff}}} = \frac{k_{\mathrm{loss}}}{k_{\mathrm{eff}}} \tag{2}$$

The approximation applied in Eq. (2) can be allowed since the relative difference between k_{eff} and k'_{eff} is in practical cases less than 1%.

Although with the aid of the unmodified MCNP and using the method described in Section 2 one can obtain accurate results for the k_{eff} and k'_{eff} values, respectively, a great disadvantage of this method is that the difference of the two numbers to be subtracted from each other is only a few tenth of a percent. In order that the standard deviation of k_{loss} be acceptable, k_{eff} and k'_{eff} must be computed to an extremely small variance. In the practical calculations only a few pcm standard deviation is tolerable. Therefore, the above outlined approach requires huge amounts of CPU time.

3.2 Variance reduction

The basis of the technique to increase the calculational efficiency is that the effective multiplication factor can be written as the sum of values:

$$k_{\mathrm{eff}} = k_{\mathrm{prompt}} + k_{\mathrm{delay}} \tag{3}$$

where k_{prompt} denotes the contribution of prompt neutrons to the multiplication factor, while k_{delay} is that of the delayed neutrons[a]. According to Eq. (1), k_{loss} can now be written as

$$k_{\mathrm{loss}} = k_{\mathrm{eff}} - k'_{\mathrm{eff}} = \left(k_{\mathrm{prompt}} - k'_{\mathrm{prompt}}\right) + \left(k_{\mathrm{delay}} - k'_{\mathrm{delay}}\right) \approx k_{\mathrm{delay}} - k'_{\mathrm{delay}} \tag{4}$$

Here again the quantities with and without prime correspond to the circulating fuel and steady fuel cases, respectively. The difference in the contribution of prompt neutrons (first bracket) is considered as negligible, since k_{prompt} compared to k'_{prompt} is only affected by the minor spatial redistribution of the fission source due to the moving precursors. Therefore, the difference (k_{loss}) is in fact determined by the expression in the second brackets. As it can be seen, the calculation described in the previous section spends the vast majority of computer time (about 99%, depending on the fuel composition and reactor structure) on the simulation of the transport of prompt neutrons, which is, in this context, actually a waste of time. Now one can easily conclude that if the values k_{delay} and k'_{delay} could be determined directly, the efficiency of the reactivity loss calculation would be improved with about four orders of magnitude. Moreover, since their relative difference is significantly larger than that of the two k_{eff} values, the numerical problems that had arisen in respect to the subtraction could also be avoided. Actually, in order to achieve the same accuracy, k_{delay} and k'_{delay} should be calculated with about hundred times smaller relative error than k_{eff} and k'_{eff}, which results in four orders of magnitude less computation time.

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[a] In the case when k_{eff} is equal to 1, k_{delay} is actually equal to the effective delayed neutron fraction.

In order that the values of k_{delay} and k'_{delay} can be directly calculated, the MCNP criticality calculations of both cases need to be divided into two consecutive parts. In brief, the first calculational step will yield a fission source term for the given system, while in the second step this source is used to start delayed neutrons only (with weights decreased proportional to the physical delayed neutron fraction) to estimate k_{delay}, and, in the case of circulating fuel, k'_{delay}. The scheme of this calculational process is shown in Fig. 1.

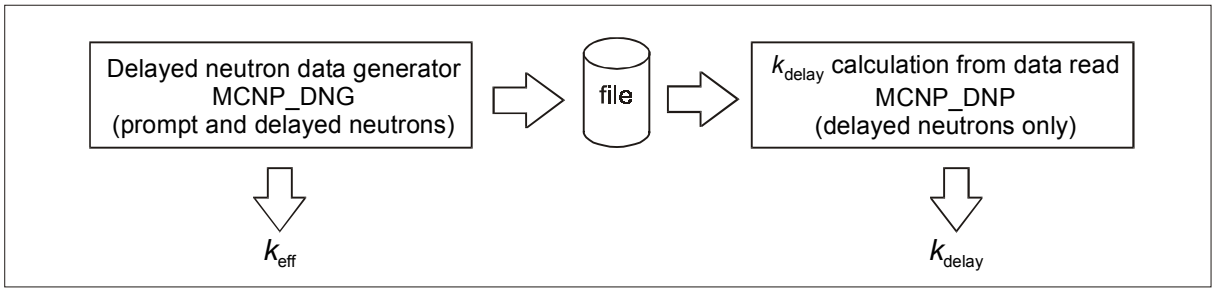

Fig. 1 Calculation scheme of the variance reduction method

In the first step, a „conventional" criticality run (KCODE calculation) is carried out, during which the data of all of the delayed neutrons are recorded in a file. The data stored are: the spatial coordinates of the place of birth of the delayed neutron, the delayed neutron fraction corresponding to the sampled nucleus and to the energy of the neutron that had induced the fission event, and the sampled energy of the delayed neutron. In the case of a steady fuel calculation, the place of birth of a delayed neutron is naturally the same as the point of the fission. However, in the case of a calculation involving fuel in motion, the coordinates stored are the shifted ones calculated by taking into account the sampled decay time of the precursor, the velocity field of the fuel and the geometry of the system. It should be noted that the actual random walk of the original MCNP criticality program flow is left unchanged.

In the second calculational step, a modified criticality run is performed, in which the source term is read from the file created in the first step. As a consequence, all the neutrons are delayed ones. The starting weight of the neutrons is multiplied by the corresponding physical delayed neutron fraction as read from the file. In this simulation, the fission event locations sampled according to the random walk of the original MCNP criticality program flow are discarded and only the data written to the file are used as source. The k_{eff} estimate provided by the modified MCNP in this way is k_{delay} or k'_{delay} for the steady fuel and circulating fuel calculations, respectively.

In order to implement the above presented variance reduction technique, modifications were introduced into the MCNP source code. According to the two calculational steps, two different source codes, named MCNP_DNG and MCNP_DNP were created. MCNP_DNG is used to produce the delayed neutron data file, while MCNP_DNP is applied to read these data and simulate the delayed neutron histories. In the case of MCNP_DNG, the MAIN program segment and the subroutines COLIDK, ACECOL and ACEDEL, while for MCNP_DNP MAIN, KCALC, COLIDK and SOURCK were modified.

It must be noted here that the above described variance description method is also applicable to the calculation of the effective delayed neutron fraction of static cases (i.e. solid fuelled reactors) at a high speed and accuracy.

4. Calculations

The applicability and efficiency of the above described variance reduction method has been verified by carrying out calculations for two static critical assemblies and one circulating fuel reactor. First, the k_{delay} values of the two solid fuel critical assemblies were calculated with the aid of the technique described in Section 3 and compared to the k_{delay} values computed using the „brute force" technique as provided by the unmodified MCNP. These latter calculations were performed such that the k_{prompt} values obtained from criticality calculations in which only prompt neutrons were simulated (an option provided by the standard MCNP) were subtracted from the k_{eff} values calculated in normal criticality runs.

The first of the above mentioned critical assemblies with solid fuel was the well known GODIVA experiment, which was a highly enriched uranium sphere of about 9 cm radius [9]. The other solid fuel assembly was a hypothetical light water moderated infinite lattice of fuel pins containing low enrichment uranium and plutonium.

The results obtained using the two different approaches for GODIVA and for the infinite thermal lattice are shown in Tables 1 and 2, respectively. One may conclude that the results obtained using the variance reduction technique (Section 3) agree very well with the data obtained in the „brute force" manner. However, the computer time needed to perform the calculation applying the variance reduction technique was four orders of magnitude shorter than that required by the "brute force" approach.

Table 1 Effective delayed neutron fraction (k_{delay}) results obtained for GODIVA critical assembly using the two different calculational methods

		Value	Standard deviation	Relative standard deviation
Unmodified MCNP ("brute force")	k_{eff}	0.99676	0.00003	
	k_{prompt}	0.99030	0.00003	
	$k_{delay,1} = k_{eff} - k_{prompt}$	0.00648	0.000042	0.65%
Variance reduction method (MCNP_DNG + MCNP_DNP)	$k_{delay,\,2}$	0.00644	0.000012	0.18%
Relative difference	$(k_{delay,1} - k_{delay,2}) / k_{delay,2}$	0.57%		

Table 2 Effective delayed neutron fraction (k_{delay}) results obtained for the hypothetical thermal lattice using the two different calculational methods

		Value	Standard deviation	Relative standard deviation
Unmodified MCNP ("brute force")	k_{eff}	1.00366	0.00004	
	k_{prompt}	0.99927	0.00004	
	$k_{delay,1} = k_{eff} - k_{prompt}$	0.00437	0.000057	1.29%
Variance reduction method (MCNP_DNG + MCNP_DNP)	$k_{delay,\,2}$	0.00433	0.000016	0.36%
Relative difference	$(k_{delay,1} - k_{delay,2}) / k_{delay,2}$	0.97%		

The third test case was the MSRE (Molten Salt Reactor Experiment, Oak Ridge, USA) [4]. Here the reactivity loss due to the fuel circulation was calculated by the variance reduction technique and compared to the measured values. The results are shown in Table 3 for the ^{233}U and ^{235}U load of the MSRE. The calculated values agree well with the measured ones. The exceptionally low standard deviations were achieved in a comparatively short computer time. In the earlier calculation aimed at the determination of the reactivity loss of the MSRE, in which the variance reduction technique was not applied, only a standard deviation of 0.00013 could be reached in a significantly larger amount of computer time [2].

Table 3 Comparison of the measured and calculated reactivity loss (ρ_{loss}) values obtained for the MSRE reactor.

Fuel	Variance reduction method (MCNP_DNG + MCNP_DNP)		Measurement [4]	
	Value	Standard deviation	Value	Uncertainty
^{235}U	0.00215	0.00002	0.00212	
^{233}U	0.00118	0.00001	0.00100	± 5%

The variance reduction method presented in the previous section makes it possible to investigate minor effects in full detail and to utilize all the capabilities of a 3D Monte Carlo code. In order to demonstrate this possibility, the above described calculational model for the MSRE reactivity loss was expanded with the fuel salt velocity profile. One can easily see that the higher velocity in the more important central region results in the removal of more precursors from the core and thus higher reactivity loss, as an earlier qualitative investigation of the authors has already shown [2]. It is known from the ORNL measurement on the full-scale model of the MSRE that the fuel velocity in the core can decrease 10-20% from the center to the vessel wall [10]. To simulate this effect, the fuel velocity (V_z) was defined as a function of the distance from the center (r):

$$V_z = A - Cr^2,$$

where the constants A and C were set to fulfill the following two criteria: preserve the flow rate through the core and set the ratio of the velocity in the center of the core (V_z^c) to the velocity along the wall of the vessel (V_z^w) equal to 1, 0.9, 0.8 and 0.7. This results in a set of velocity profiles from the completely flat to the slightly parabolic ones. The reactivity losses in the different cases can be seen in Fig. 2. One can conclude that according to the expectations higher velocity in the center results in higher reactivity loss, although the change is very small. It can be seen as well that due to the new variance reduction method the results are accurate enough to investigate such a minor effect.

5. Conclusion

For the reactivity calculation of molten salt reactors, it is vital to account for the effects due to the motion of the delayed neutron precursors. A new method has been developed and implemented by introducing modifications into the code MCNP in order to include the effect of the spatial transport of the precursors. The technique has proved to be viable, however, requires very long criticality runs. This condition induced the idea of a variance reduction

method by which the computer time needed can be reduced by four orders of magnitude. The method has been implemented by modifying certain subroutines of the MCNP. The applicability and efficiency of this variance reduction technique has been illustrated by comparing calculations performed with the unmodified MCNP and the modified program. Good agreement was shown between the results of the two approaches. As a practical application the reactivity loss in the MSRE was calculated. Due to the short running time the method allows of the simulation of minor 3D effects, as it was demonstrated on the MSRE fuel velocity profile. The investigation of huge and complicated geometries as the MSBR [11] or other full-scale MSR concepts becomes possible as well.

The technique developed is also applicable to the calculation of the effective delayed neutron fraction of static cases.

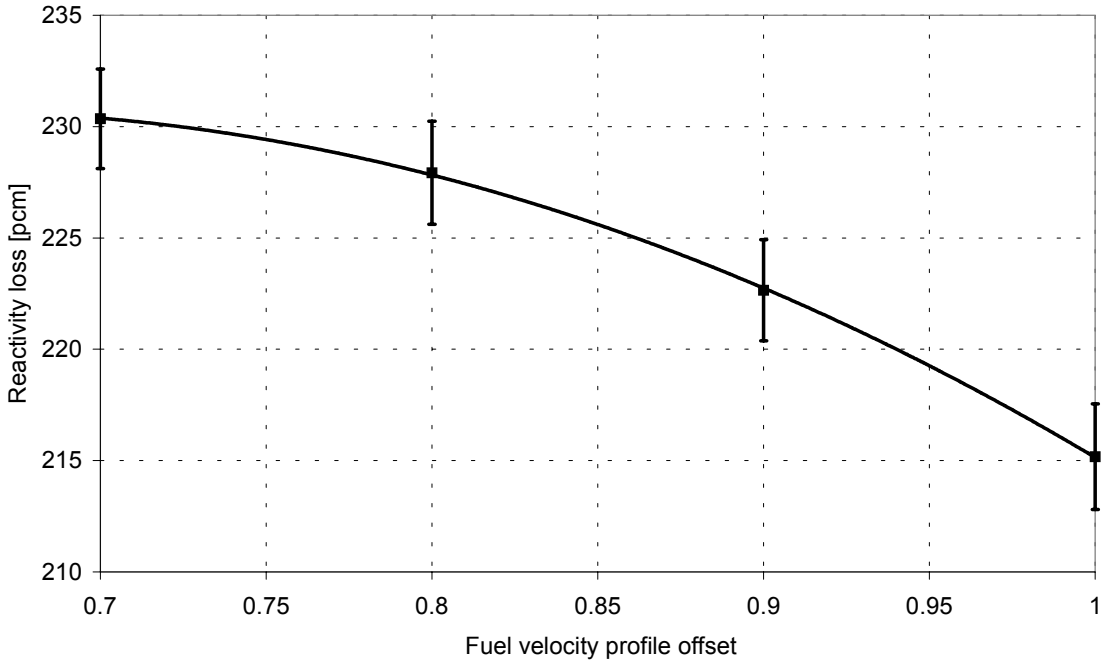

Fig. 2 Reactivity loss in the MSRE as a function of the fuel velocity profile offset (V_z^w / V_z^c)

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