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Current Status of the PSG Monte Carlo Neutron Transport Code

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Abstract

PSG is a new Monte Carlo neutron transport code, developed at the Technical Research Centre of Finland (VTT). The code is mainly intended for fuel assembly-level reactor physics calculations, such as group constant generation for deterministic reactor simulator codes. This paper presents the current status of the project and the essential capabilities of the code. Although the main application of PSG is in lattice calculations, the geometry is not restricted in two dimensions. This paper presents the validation of PSG against the experimental results of the three-dimensional MOX fuelled VENUS-2 reactor dosimetry benchmark.

KEYWORDS: PSG, Monte Carlo neutron transport, group constant generation, Woodcock tracking, pseudo-scattering, VENUS-2 benchmark

1. Introduction

Monte Carlo neutron transport codes are widely used for criticality safety analyses, validation of deterministic transport codes and for various tasks specifically requiring the detailed modelling of geometry and physics. Group constant generation for deterministic reactor simulator codes can be foreseen as one of the new applications of the method in the near future. Presently, this task is routinely carried out by second generation deterministic lattice codes.

Various studies have been made on the use of Monte Carlo methods for group constant generation (see e.g. [1, 2]), but the practical applications have so far been restricted by the lack of computer resources. The subject remains attractive because of its simplicity. The method provides an almost direct access to the evaluated nuclear data, which represents the best available knowledge on neutron interactions with matter. There is no need for the multi-group condensation of the cross sections or any special treatment for resonance self-shielding. The same code and data can be used for a wide range of applications.

A new Monte Carlo neutron transport code, specifically intended for lattice calculations, is being developed at the Technical Research Centre of Finland. The long-term goal of the project is to create a fast-running reactor physics code, capable of generating group constant data for deterministic reactor simulator codes using the Monte Carlo method and continuous-energy cross section data.

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The code development initially started in September 2004 and the project was given the working title "Probabilistic Scattering Game", or PSG. The first comparable results were attained in early 2005 and the project was included in a VTT research programme a few months later. The code capabilities and some preliminary results were introduced in two reactor physics conferences in year 2005 [3, 4].

The code was completely re-written by the end of 2005. New features, such as a thermal bound-atom scattering model and parallelisation using the message passing interface (MPI) were included. The results were considerably improved along with the new capabilities and the correction of some programming errors in the scattering routines. Code development during the first half of year 2006 has been focused on the calculation of diffusion parameters. A collaboration project has been initiated with the École Polytechnique de Montréal on the development of neutron leakage models for Monte Carlo based lattice calculations.

This paper presents the current status of the PSG project. The calculation methods, the interaction physics and the code capabilities are briefly introduced. Although the code is mainly designed for lattice-level calculations, the geometry description is not restricted in two dimensions. The capability to perform three-dimensional full-core calculations is valuable for code validation. In this study, the MOX fuelled VENUS-2 core [5] was modelled for such purpose.

2. Code Description

PSG is a three-dimensional, continuous-energy Monte Carlo neutron transport code, that uses analog Monte Carlo game for neutron transport and the criticality source (k-eigenvalue) method for simulating neutron generations. An alternative α-eigenvalue method has been developed in an effort to more consistently model systems far from criticality. This method has not yet been sufficiently tested and it will not be discussed here.

At its current stage of development, PSG has no capability to perform external source simulations. The applications are therefore restricted to reactor physics calculation and the simulation of a self-sustaining chain reaction. The main intended use is the group constant generation for deterministic reactor simulator codes and PSG can also be characterised as one of the first codes in the third lattice code generation.

2.1 Neutron Tracking

What differentiates PSG from the majority of similar Monte Carlo codes, is the method used for neutron transport. PSG implements a tracking procedure developed by Woodcock in the 1960's [6]. The Woodcock method is also used as an optional tracking method in the HOLE geometry package available for the MONK and MCBEND codes [7]. The technique is also known as the pseudo-scattering method and it is applied using this name in Monte Carlo codes MCU and VMONT [8].

The basic principle of the Woodcock method is simple. The conventional tracking procedure is modified by introducing so-called virtual collisions, in which the neutron energy and direction are not changed. This type of interaction is also called pseudo-scattering, because it is essentially a scattering reaction that does absolutely nothing for the incident neutron. It is easy to see that the virtual collision density can be freely adjusted without affecting the statistics, but a solid mathematical verification of the Woodcock method exists as well [9].

The reason to add the virtual collisions in the process is that the effective total cross section used for sampling the collision distances can be modified. If all the materials in the system share the same total cross section, there is no need to stop the tracking at the material boundaries, or even to calculate the distances to the boundary surfaces. It is instead sufficient to have

a geometry routine that can determine which material fills the cell at each collision point. This is considerably simpler than dealing with surface crossings. The procedure can result in a significant reduction in calculation time, especially in complex systems where the neutron mean free path is long compared to the characteristic dimensions of the geometry.

A natural choice for the modified effective total cross section (used for sampling the collision distances in all materials) is the majorant cross section, $\Sigma_{\mathrm{m}}(E)$, which at each tabulated energy point is set equal to the maximum total cross section in the system. The virtual collision cross section at the collision site is simply

$$\Sigma_0(\mathbf{r}, E) = \Sigma_{\mathrm{m}}(E) - \Sigma_{\mathrm{t}}(\mathbf{r}, E)\,, \tag{1}$$

where $\Sigma_{\mathrm{t}}(\mathbf{r}, E)$ is the physical total cross section of the material. This cross section determines the probability of a virtual collision:

$$P_0(\mathbf{r}, E) = \frac{\Sigma_0(\mathbf{r}, E)}{\Sigma_{\mathrm{m}}(E)}\,. \tag{2}$$

The tracking is continued until a real collision is sampled with probability $1 - P_0(\mathbf{r}, E)$, after which the procedure continues in the conventional way.

The main advantages of the Woodcock method are the simplicity of the geometry routines and the speed-up of calculation in certain types of complex geometries. The main drawback is that the track length estimate of neutron flux is not available and reaction rate integrals have to be calculated using the collision estimator. This results in a significant loss of efficiency in calculations involving reaction rates integrated over small, and especially optically thin volumes.

Another problem arises in geometries containing high-absorbing materials localised at relatively small regions of the geometry. An example of such case is a LWR fuel assembly with burnable absorber pins. At low energy, the majorant cross section is dominated by the absorption cross sections of the gadolinium isotopes, although the probability of a neutron hitting a burnable absorber pin is relatively low. This results in an increase in the virtual collision rate and computing time is wasted. The PSG code uses a simple procedure to overcome this problem in lattice geometries, and despite its limitations, the Woodcock method is seen to be well suited for lattice calculations.

2.2 Nuclear Data

The nuclear interaction data used by PSG is read from ACE-format cross section libraries. This data format is also used by MCNP [10]. The shared data format has the advantage that PSG results can be validated by MCNP calculations, without additional uncertainties emerging from the nuclear interaction data.

The original point-wise cross sections are adjusted to a new energy grid, which is used for all materials. This has the advantage that the cross section interpolation between two tabulated energy points has to be carried out only once, each time the neutron changes its energy. The result is a significant reduction in computing time. The drawback is that large amounts of computer memory are wasted by storing redundant data points. Such wasteful use of memory in an effort to gain efficiency is not seen as a serious problem, however, since the available computer memory is rarely a limiting factor today.

2.3 Interactions

Elastic scattering and inelastic level scattering are handled by solving the two-body collision equations in the centre-of-mass frame. Angular distributions and inelastic reaction Q-values

are read from the ACE libraries. The target velocity is sampled from a Maxwellian distribution when the incident neutron energy is low. This procedure is commonly known as the thermal free-gas treatment.

The combined energy-angle distributions for thermal bound atom scattering in moderator materials (parameters for the $S(\alpha, \beta)$-scattering laws), continuum inelastic scattering and (n,xn)-reactions are read from the ACE libraries. The interactions are modelled according to the corresponding ENDF reaction laws. Energy distributions of prompt and delayed fission neutrons and delayed neutron parameters (if available) are read from the ACE-format data.

2.4 Result Estimates

PSG calculates statistical estimates of effective and infinite multiplication factors, together with other integral parameters and homogenised few-group constants for an arbitrary energy group structure. The poor efficiency of the collision estimator is not a problem when reaction rates are integrated over the entire geometry, as is commonly done in lattice calculations.

Diffusion parameters are estimated directly from the transport process. Effective delayed neutron fractions are calculated using a method developed at the NRG [11]. Various types of detectors, or "tallies" in the common Monte Carlo terminology, can be set up by the user for the calculation of spectral and integral reaction rate parameters.

3. Example Results

So far, the group constant data generated by PSG has not been used for reactor simulator calculations. The main reason is the incapability to model fuel depletion and to produce homogenised data for burnt fuel. Some very promising results have been attained, however, in comparisons with other codes, such as the general-purpose Monte Carlo code MCNP [10] and the deterministic lattice code CASMO [12].

3.1 Lattice Calculations

In a previous study [4], a comparison to MCNP4C calculations using the same ENDF/B-VI based cross section libraries showed maximum differences in the order of few percent in two-group cross sections calculated for various LWR lattices. Discrepancies in k_∞ were in the order of few hundred pcm.

Since the last major modifications in the code, the differences in the group constants have been narrowed down to less than 0.5% and the differences in k_∞ to less than 100 pcm, compared to the MCNP calculations. The discrepancies are often comparable to the statistical accuracy of the Monte Carlo method, although certain anomalies still persist. PSG typically runs 2 to 12 times faster than MCNP, depending on the lattice type.

Comparison to CASMO results is not as straightforward, due to the differences in the calculation method and in the interaction data. There are typically differences in the order of a few percent between CASMO and MCNP results and similar discrepancies are observed in the PSG results as well. CASMO calculations have mainly been used for validating diffusion parameters. Fast and thermal diffusion coefficients are fairly consistent in the zero-buckling mode, but there is still work to be done for fundamental mode lattice calculations.

3.2 The VENUS-2 Reactor Dosimetry Benchmark

The VENUS facility (Vulcain Experimental NUclear Study) is a pool-type zero-power critical assembly located at SCK•CEN in Mol, Belgium. The VENUS-2 core configuration consists of three types of fuel pins, including a MOX fuel with 2.7 wt-% plutonium content. The fuel

is divided into separate regions and surrounded by a water reflector and various radial zones consisting of structural materials.

The three-dimensional VENUS-2 reactor dosimetry benchmark was initiated in 2004 [5] and the final report published in early 2006 [13]. VTT did participate the exercise [14], but not with the PSG code. The results presented here were calculated independently for the purpose of code validation. The main motivation for the study was to test the feasibility of PSG in the modelling of such a complex geometry. The capability to calculate detector responses was of special interest, since it was assumed to be problematic due to the limitations posed by the Woodcock tracking method.

A full-core PSG model was constructed, based on a previous MCNP geometry. In order to verify the quality of the original model, the calculations were repeated with MCNP4C. The MCNP results are not presented here. All calculations were carried out using new JEFF-3.1 based cross section libraries [15] and IRDF-90 based dosimetry cross sections. To assess the magnitude of uncertainties originating from the evaluated nuclear data, the calculations were repeated with ENDF/B-VI.8 based libraries.

The experimental measurements at the VENUS facility consist of integral parameters, axial and radial fission rate distributions and detector dosimetry data measured at various positions around the active fuel region. Selected results compared to PSG calculations are introduced in the following. All co-ordinates and pin and detector positions refer to the conventions used in the benchmark specification [5]. The geometry description is not repeated here.

A large number of neutron histories had to be run in order to compensate for the poor detector efficiency. A total of 200 inactive and 5000 active cycles of 120000 neutrons were run, which took about 100 hours on a 2.6 GHz AMD Opteron PC. The number of neutron histories in the MCNP calculation was much lower and it is hence not reasonable to compare the running times.

3.2.1 Integral Parameters

Since the VENUS-2 core configuration is a critical assembly, the experimental multiplication factor is assumed to be very close to unity. The k_{eff} reported by most of the benchmark participants ranges from 0.99600 to 0.99900, depending on the calculation system and the cross section data [13]. The PSG result was 1.00304$\pm$0.00004 using JEFF-3.1 based cross section libraries and 0.99655$\pm$0.00004 using ENDF/B-VI.8 data. Reference MCNP4C calculations using the same ACE files yield very similar results. Although both values are relatively close to criticality, it can be seen that the origin of the cross section data may have a very significant impact on the outcome of the simulation.

All PSG reaction rates are normalised to the total fission rate, which was given the value 1.8384×10^{13} fissions per second in the benchmark specification. The accurate calculation of total core power is not trivial, since the average energy deposited per fission depends to some extent on both neutron and photon leakage. PSG uses a fixed value of 202.5 MeV for ^{235}U fission[a]. The energy yields for the other fissile isotopes are adjusted according to the fission Q-values. The calculated total core power was 599.5 W, which is well consistent with the 600 W reference value. The result is not significantly dependent on the cross section data.

[a] This value includes both the energy deposited at the fission site and an estimate of the average recoil and photon energy absorbed in (n,γ)-reactions. The value should not be confused with the fission Q-value ($\sim$200 MeV) or the maximum recoverable fission energy ($\sim$195 MeV).

Table 1: The C/E values of axial fission rate distributions in 6 pin positions of the VENUS-2 core. Minimum and maximum values are emphasised.

pin type	2.0/2.7 MOX		4.0/0.0 UO_2		3.3/0.0 UO_2	
Pin position	(-27,-12)	(-22,-2)	(-15, 2)	(-13,-12)	(-11, 2)	(-6,-6)
Pin number	325	240	131	115	74	30
z-pos. (cm)	C/E values of relative fission rates					
110.0	0.9746	1.0034	0.9989	1.0092	1.0117	0.9983
112.0	1.0041	0.9944	1.0022	**1.0185**	0.9902	1.0017
114.0	**1.0316**	1.0350	1.0013	1.0058	1.0105	0.9939
116.0	1.0090	**1.0456**	**1.0129**	0.9905	1.0057	1.0127
118.0	1.0199	1.0003	0.9935	1.0006	0.9905	0.9889
120.0	0.9828	0.9929	1.0064	1.0150	**1.0138**	1.0005
122.0	1.0084	1.0247	0.9955	0.9985	0.9910	1.0070
124.0	1.0008	1.0059	1.0045	1.0042	0.9912	1.0053
126.0	0.9912	0.9910	**0.9904**	1.0076	0.9944	1.0033
128.0	1.0200	1.0208	0.9979	1.0004	1.0123	0.9980
130.0	1.0097	1.0173	1.0071	1.0161	1.0061	**1.0175**
132.0	1.0001	0.9856	1.0065	0.9835	1.0008	1.0045
134.0	1.0143	0.9882	1.0005	0.9974	1.0013	0.9999
136.0	0.9900	0.9831	0.9978	0.9838	0.9989	1.0018
138.0	0.9986	0.9853	0.9924	1.0051	0.9987	1.0083
140.0	0.9938	0.9918	0.9963	1.0021	1.0012	1.0001
142.0	0.9969	0.9953	0.9988	1.0064	0.9957	1.0055
144.0	1.0125	0.9978	1.0002	0.9866	0.9998	0.9952
146.0	0.9884	**0.9666**	0.9993	**0.9751**	0.9923	0.9857
148.0	**0.9516**	0.9830	0.9987	1.0027	1.0038	0.9851
150.0	0.9800	0.9955	1.0002	0.9932	**0.9893**	**0.9635**
Mean	0.9990	1.0002	1.0001	1.0001	1.0000	0.9989

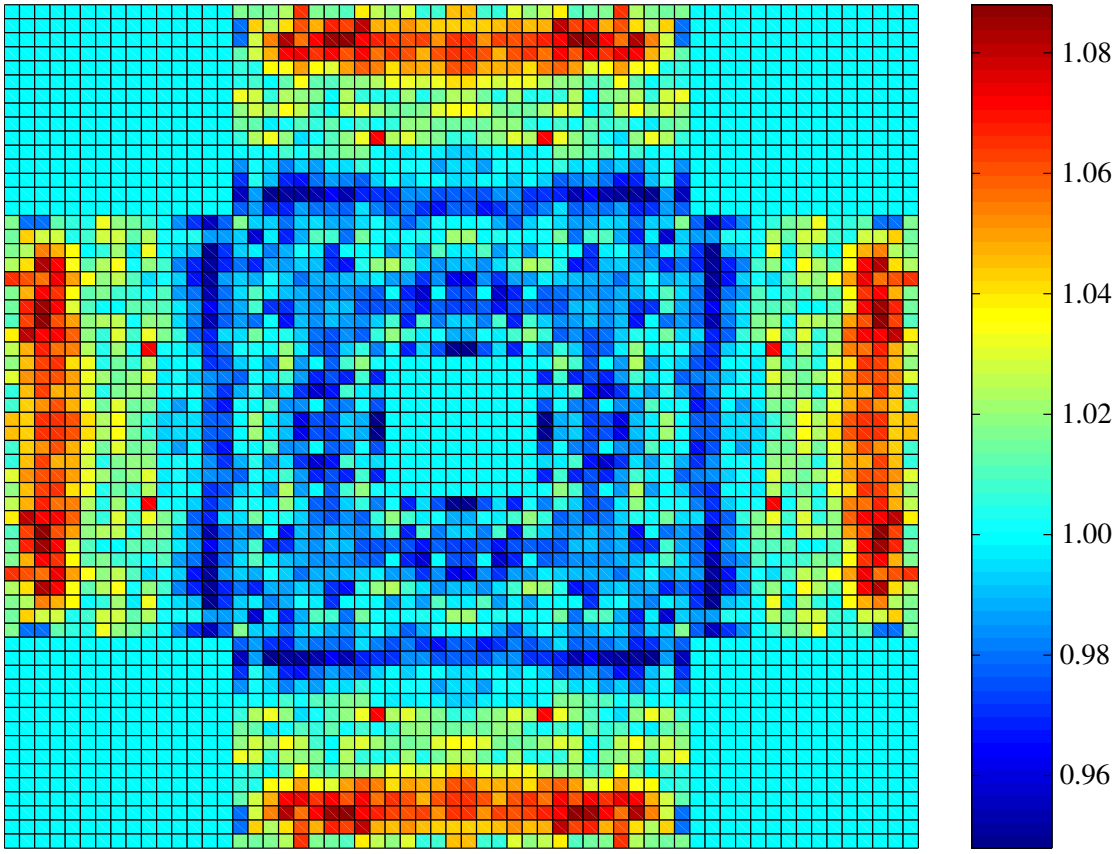
3.2.2 Fission Rate Distributions

The measured radial fission rate distribution at core mid-plane and the axial distributions at six pin positions are given in the VENUS-2 benchmark specification [5]. The calculated axial distributions relative to the experimental results are presented in Table 1. The comparison of the radial distribution is plotted in Fig. 1.

The fission rates were calculated as volume- and energy-integrated values in 2 cm high segments of the fuel pins. The volumes of the regions are small compared to the core dimensions and the efficiency of the collision estimator is not very good. The largest relative statistical errors are in the order of two percent, despite the large number of neutron histories run.

The axial distributions are well consistent with the experimental data. The results for the radial distribution are not much worse either: almost 90% of the values are within 5% and over 50% of the values within 2% of the experimental result. It seems, however, that there is a systematic trend in the discrepancies, as the fission rate is slightly over-estimated near the core periphery. The results are not particularly sensitive to the origin of the cross section data.

Figure 1: The C/E values of radial fission rate distribution at the VENUS-2 core mid-plane.



3.2.3 Detector Calculations

The equivalent fission fluxes of ^{58}Ni(n,p), ^{115}In(n,n'), ^{103}Rh(n,n'), ^{64}Zn(n,p), ^{237}Np(n,f) and ^{27}Al(n,α) detectors were experimentally measured at various positions at the core mid-plane. The equivalent fission flux of a detector responding to reaction i is defined as

$$\phi_{\mathrm{f},i} = \frac{\int_0^\infty \sigma_i(E)\phi(E)dE}{\overline{\sigma}_{\mathrm{f},i}}, \tag{3}$$

where $\sigma_i(E)$ is the microscopic cross section of the reaction, $\phi(E)$ is the neutron flux at the detector position and $\overline{\sigma}_{\mathrm{f},i}$ is the average dosimeter cross section of the detector, i.e. the microscopic cross section of reaction i integrated over ^{235}U fission spectrum.

The detectors were modelled using spherical cells of 2.4 cm in diameter. The microscopic cross section libraries were prepared from IRDF-90 dosimetry data files using NJOY-99 [16]. The processing failed for ^{237}Np and the standard dosimetry data provided with the MCNP4C code [10] was used instead. All average dosimeter cross sections were taken from a previous VTT study [14].

The results of the PSG calculation are compared to the experimental measurements in Table 2. In most cases, the differences are in the order of few percent, but larger discrepancies exist as well. Both JEFF-3.1 and ENDF/B-VI.8 based transport cross section libraries yield similar results. A review of the VENUS-2 final report [13] shows that the PSG results are generally well comparable to the results of the benchmark participants.

Table 2: The C/E values of equivalent fission fluxes of the 6 detector types in various measurement positions. Minimum and maximum values are emphasised.

Core region	Detector position (cm)	^{58}Ni (n,p)	^{115}In (n,n')	^{103}Rh (n,n')	^{64}Zn (n,p)	^{237}Np (n,f)	^{27}Al (n,α)
Inner Baffle	(-4.41, -0.63)	**0.9470**	0.9244	0.9054	0.9081	1.0106	0.9285
	(-4.41, -4.41)	0.9488	0.9196	0.9271	0.9161	1.0114	0.9429
Outer Baffle	(-39.69, -0.63)	0.9765	0.9690	–	0.9526	–	0.9217
	(-39.69, -5.67)	0.9893	–	0.9654	–	–	–
	(-39.69, -11.97)	0.9828	0.9751	0.9733	0.9756	1.0524	0.9071
	(-39.69, -18.27)	1.0033	0.9666	0.9756	0.9980	1.0244	1.0471
	(-37.17, -20.79)	0.9744	0.9400	0.9579	–	–	0.9557
	(-30.87, -20.79)	0.9616	–	–	–	–	–
	(-24.57, -20.79)	0.9611	0.9336	0.9245	0.9428	0.9970	0.9653
Barrel	(-49.77, -0.63)	1.0384	**0.9906**	0.9955	0.9983	–	1.1456
	(-49.77, -9.45)	1.0071	0.9444	0.9514	0.9496	1.0244	0.8972
	(-47.25, -18.27)	1.0136	0.9604	0.9715	0.9591	1.0600	1.0183
	(-45.99, -22.05)	0.9718	0.9404	0.9574	0.9366	1.0709	1.0484
	(-44.73, -24.57)	1.0030	0.9856	0.9805	0.9427	–	0.8768
	(-42.21, -28.35)	0.9941	0.9407	0.9500	0.9573	1.0399	1.0052
	(-38.43, -33.39)	1.0343	0.9665	0.9444	1.0080	1.0289	1.0899
	(-35.91, -35.91)	1.0410	0.9710	0.9763	1.0078	1.0526	0.9661
Neutron Pad	(-58.54, -22.47)	1.0434	0.9419	–	0.9925	0.9946	0.9742
	(-46.60, -41.95)	–	0.9402	–	1.1001	**0.9932**	0.9103
Water Gap	(-54.36, -9.59)	1.0250	–	0.9431	–	–	–
	(-52.89, -15.80)	1.0460	0.9818	0.9525	0.9588	–	1.0274
	(-51.53, -19.78)	1.1294	0.9684	0.9614	**1.2829**	–	**1.1583**
	(-50.03, -23.33)	**1.1572**	0.9787	0.9648	1.0434	–	1.0110
	(-48.74, -25.91)	1.1144	0.9803	0.9605	1.0387	–	0.8582
	(-46.29, -30.06)	0.9943	0.9197	0.9292	**0.8895**	–	0.6282
	(-44.08, -33.22)	0.9593	–	–	–	–	–
	(-42.29, -35.48)	1.1072	–	0.9690	0.9807	–	**0.5777**
	(-39.03, -39.03)	1.1464	0.9690	0.9463	0.9736	1.0446	1.0861
Reflector	(-23.31, -23.31)	0.9702	0.9090	**0.9994**	–	1.0305	0.9399
	(-25.83, -25.83)	0.9767	**0.8978**	0.9250	0.9428	1.0756	0.9003
	(-28.35, -28.35)	0.9832	0.9052	0.9219	0.9144	**1.0926**	0.9611
	(-30.87, -30.87)	1.0196	0.9353	0.9776	0.9424	1.0804	0.9573
	(-33.39, -33.39)	1.0277	0.8999	**0.8863**	–	–	0.8621

The earlier-discussed poor efficiency of the collision estimator is even more clearly seen in the detector calculations, as the target cells are located outside the active core region. The statistical accuracy is still much better than 5% in most positions, which is a fairly good indication of convergence. The number of collisions scored inside a detector cell depends not only on the distance from the neutron source, but also on the threshold energy of the response reaction.

This is the main reason why the ^{27}Al(n,α)-detector ($E_{\min} = 7.6$ MeV) gives such poor results. The relative statistical error exceeds 10% in most positions, which makes the quality of the results more or less questionable.

4. Conclusions

PSG is a new Monte Carlo neutron transport code, specifically designed for fuel assembly-level reactor physics calculations, such as group constant generation for deterministic reactor simulator codes. So far, the code has not been used for its intended task, but various comparison studies between PSG, MCNP [10] and CASMO [12] have been carried out for validation purposes [3, 4]. The calculations have covered mainly infinite, two-dimensional LWR lattice geometries. Recent results have been very promising, especially when compared to MCNP calculations using the same cross section libraries.

PSG uses the Woodcock method [6] (pseudo-scattering) for neutron tracking. This option disables the capability to calculate reaction rate integrals using the track length estimate of neutron flux and the less efficient collision estimator has to be used instead. The penalty is not significant when reaction rates are integrated over large volumes, which is the case in most lattice calculations. Problems are to be expected, however, in detector-type calculations, when the target cells are small compared to the geometry dimensions.

In this study, the recently completed VENUS-2 MOX-fuelled reactor dosimetry benchmark exercise [5, 13] was repeated using PSG. The initial motivation was to see if the code could be used for this type of complex calculation task at all, and if so, would it be possible to attain statistically converged results, despite the problems arising from the poor efficiency of the collision estimator.

It turned out to be possible to construct the geometry model from an existing MCNP input. The calculated integral parameters are consistent with both experimental results and reference MCNP calculations. As is often the case, the effective multiplication factor is strongly dependent on the origin of the nuclear interaction data. The rest of the results are less sensitive to the small discrepancies in the transport cross sections.

The comparison of radial and axial fission rate distributions shows differences in the order of few percent, compared to the experimental values. The results can be considered quite satisfactory. The poor efficiency of the collision estimator posed some problems with statistics, but a reasonable accuracy was attained by running a large number of neutron histories.

Statistical convergence was reached in the detector calculations. A clear exception was the ^{27}Al detector, for which the threshold energy of the response (n,α)-reaction was high. The results are fairly consistent with the experimental values and the overall differences well comparable to those reported by the VENUS-2 benchmark participants [13].

It is clear that the poor efficiency of the collision estimator restricts the applications of PSG to some extent and makes the code an impractical choice for routine detector response calculations. However, the capability to make comparisons to experimental results is extremely valuable for code validation, in which case the necessity to run even an excessively large number of neutron histories is not an issue. The outcome of the study is hence very encouraging, as it suggests that the PSG code could be used for other similar tasks in the future.

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