Leakage-corrected fast reactor assembly calculation with Monte-Carlo code TRIPOLI4r and its validation methodology

L. Cai, Y. Peneliau, J. Tommasi, J-F Vidal, C. M. Diop

PHYSOR 2014 - The Role of Reactor Physics toward a Sustainable Future
The Westin Miyako, Kyoto, Japan, September 28 - October 3, 2014, on CD-ROM (2014)

Leakage-corrected fast reactor assembly calculation with Monte-Carlo code TRIPOLI4® and its validation methodology

L. Cai, Y. Pénéliau, J. Tommasi and J-F Vidal
CEA, DEN, DER/SPRC
Cadarache, F-13108 Saint-Paul-lez-Durance, France
li.cai@cea.fr
yannick.peneliau@cea.fr
jean.tommasi@cea.fr
jean-francois.vidal@cea.fr

C. M. Diop
CEA, DEN, DANS/DM2S/SERMA
Saclay, F-91191 Gif-sur-Yvette Cedex, France
cheikh.diop@cea.fr

ABSTRACT

A leakage model based on B1 Homogeneous Equations has been recently implemented in continuous-energy Monte Carlo code TRIPOLI4®. This leakage model algorithm iterates between the point-wise Monte Carlo simulation and a B1 Homogeneous Equations solver till reaching a final critical state in Monte Carlo simulation. The two advantages of our leakage model compared with the others are: we use critical flux spectrum to generate the multi-group constants for solving the B1 Homogeneous Equations; the leakage coefficients calculated are considered in point-wise Monte Carlo simulation. This leakage model is validated by a pre-designed numerical experiment simulated with continuous-energy TRIPOLI4® and the obtained results are also compared with those from SERPENT leakage model and deterministic leakage model in ECCO code. Finally, our leakage-corrected multi-group constants are used in transport theory based core calculation and they give out consistent multiplicative factor and neutronic balance.

Key Words: **leakage model,critical buckling, TRIPOLI4®, Serpent, ECCO**

1. INTRODUCTION

The Monte-Carlo method is becoming more and more popular for reactor core design and analysis. It is particularly recommended for 3D whole core calculations graceful to its exact description for complex core geometry and its continuous energy dependent data library. These Monte-Carlo based advantages could also be used in the two-steps (assembly calculation & core calculation) methodology. The generation of few-group constants is an essential link between the two calculations steps. Till now, several teams [1–4] have paid attention to the research topic *multi-group constants generation with Monte-Carlo method*. For the moment, they mostly focus on producing

homogenized multi-group parameters for some diffusion theory based core simulation codes with consideration of time and memory consuming issues.

In the first assembly calculation step, the boundary condition is usually set as reflective or periodic. This approximation is more or less adequate for the thermal neutron reactor case where the neutron average free path length is much smaller than the assembly geometrical size. In contrary, for the fast neutron reactor case, the neutron average free path length is much more important with respect to the assembly geometrical size. The adjacent assemblies are more efficiently coupled among themselves. Thus, leakage effects need to be considered while dealing with a fast neutron assembly under reflective boundary condition.

Two different approaches exist principally to treat the leakage effect of every single assembly. The first one is a direct way which means a whole core is chosen to simulate the real critical state. Under this concept, most of the multi-group homogenized cross sections can be correctly produced by weighting on the intrinsic critical flux spectrum. However, the multi-group anisotropic scattering law needs more delicate treatment during the collapsing procedure [5]. The second one is to incorporate some leakage model within assembly calculation. The later concept aims at figuring out a critical steady-state for the assembly without knowledge of the exact operating conditions and materials surrounding it. Three different leakage models have been developed in Monte-Carlo environment thus far. The first model is based on the fundamental mode approximation *B1 Homogeneous equations*. This leakage model is originated from deterministic assembly codes. It was first introduced into the Korean Monte-Carlo code McCard at KAERI [2]. It was also used in the Finland Monte-Carlo code Serpent at VTT [1]. The second leakage model is proposed by another Korean research team from KAIST [6]. The main idea from this method is to search a critical spectrum via varying the reflection probability *albedo* for the neutrons which hit the boundary limit. The algorithm is implemented in the MCNP5 engine and coupled with MONTEBURNS code. The third leakage model is proposed by Yamamoto at Kyoto University with use of a complex-value for the neutron weight [7, 8]. The interest of this method is to link the leakage term with the propagation direction of neutron. Compared with the two previous methods, the last interpretation idea for neutron leakage rate is more appropriate because every single neutron has its own leakage probability during the continuous energy Monte Carlo simulation. In contrary, the two first leakage models assume that all the neutrons or the neutrons in each energy-collapsed group share the same escaping probability. Even though the last leakage model has its own physical advantage, it has some limitations related to the application issue. For example, it demands a symmetrical geometry in order to be able to cancel the imaginary part of the fission source.

Our study is aimed at developing a leakage model in the French Monte Carlo code TRIPOLI4® [9–12] in order to produce critical flux weighted multi-group constants for transport theory based deterministic core calculation. This work is based on our previous research step which lifted up the necessity to use In-Group Scattering Anisotropy correction at the end of assembly calculation [5]. The method chosen for the moment is always based on the *B1 Homogeneous fundamental equations*. However some different treatments for the group-wise leakage coefficients resolved from the *B1 Homogeneous fundamental equations* are proposed in our approach. These multi-group leakage parameters $d_g B^2$ are used in the continuous energy Monte Carlo simulation to modify the initial weight of the concerned neutron. The Monte Carlo simulation and the module in charge of solving the *B1 Homogeneous fundamental equations* are coupled and iterated till reaching a critical state in the continuous energy Monte Carlo simulation.

Another important issue concerned with Monte Carlo method is its validation work because Monte Carlo method itself is usually assumed to be the reference case compared with deterministic code. In this paper, a numerical experiment is designed as a natural leakage model to validate our implemented TRIPOLI4® leakage model. Meanwhile, comparisons are done between our leakage-corrected simulation results and those from SERPENT code and also from ECCO code [13, 14]. Finally, these multi-group cross sections weighted by the critical spectrum will be used in deterministic core simulation and also Monte Carlo multi-group simulation. Their simulation results will be compared with TRIPOLI4® continuous energy reference results.

2. METHOD

In this section, a review of the *B1 Homogeneous fundamental equations* is first proposed. We briefly remind the physics approximations used in the framework of fundamental mode. Secondly, we present the new algorithm of the leakage model and its implementation work in TRIPOLI4® code.

2.1. Revisit of B1 Homogeneous Equations

The solution of the transport equation applied to a homogeneous infinite multiplicative geometry is defined as fundamental mode. The assembly calculation is always performed under reflective or periodic boundary condition. In consequence, a leakage model needs to be introduced in the assembly to enforce $K_{eff} = 1$. In this context, the fundamental mode approximation is showing up which aims to represent the angular flux by a combination of two terms. One is a fundamental flux $\varphi(\mathbf{r}, E, \hat{\Omega})$ which is available within every single assembly wherever its position. The other one $f(\mathbf{r})$ is contributed to describe the spatial distribution in the whole core. Furthermore, $f(\mathbf{r})$ is assumed to be the solution of a Laplace equation (1) which is characterised by the geometrical buckling B^2:

$$\nabla^2 f(\mathbf{r}) + B^2 f(\mathbf{r}) = 0 \tag{1}$$

A generic solution of the above equation is: $f(\mathbf{r}) = \alpha e^{i\mathbf{B}\cdot\mathbf{r}}$. In addition, the spatial dependence in each assembly is eliminated under the homogeneous situation. Finally, the angular flux is expressed as $\phi(\mathbf{r}, E, \hat{\Omega}) = \varphi(E, \hat{\Omega}) e^{i\mathbf{B}\cdot\mathbf{r}}$. After substituting this factorized flux into the continuous energy transport equation and with use of linearly anisotropic collision approximation, we obtain the homogeneous B1 equation (2):

$$[i\hat{\Omega}\cdot\mathbf{B} + \Sigma_t(E)]\varphi(E,\hat{\Omega}) = \int_\infty dE' \frac{1}{4\pi}\{\Sigma_{s0}(E'\to E)\varphi(E') + 3\Sigma_{s1}(E'\to E)\hat{\Omega}\cdot\mathbf{J}(E')\} + \frac{\chi(E)}{4\pi K_{eff}}\int_\infty dE'\nu\Sigma_f(E')\varphi(E') \tag{2}$$

In order to convert the above angular flux into scalar flux with consideration of the manipulation facility in assembly calculation code, $Eq(2)$ and $Eq(2)\times\hat{\Omega}$ are integrated over the full solid angle 4π. Then, after collapsing the continuous energy parameters into multi-group form, we finally

obtain the two coupled multi-group *B1 Homogeneous equations* (3) & (4):

$$\Sigma_{t,g}\varphi_g + d_g B^2 \varphi_g = \sum_{g'=1}^{G} \Sigma_{s0}^{g'\to g}\varphi_{g'} + \frac{\chi_g}{K_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\varphi_{g'} \tag{3}$$

$$d_g = \frac{1}{3\Sigma_{t,g}\gamma_g}\{1 + 3\sum_{g'=1}^{G} \Sigma_{s1}^{g'\to g}\frac{\varphi_{g'}}{\varphi_g} d_{g'}\} \tag{4}$$

with the definition of γ_g:

$$\gamma_g = \begin{cases} \frac{1}{3}\frac{\frac{B}{\Sigma_{t,g}}\arctan\frac{B}{\Sigma_{t,g}}}{1-\frac{\Sigma_{t,g}}{B}\arctan\frac{B}{\Sigma_{t,g}}} & \text{if} \quad B^2 > 0 \\ \frac{B^2}{3\Sigma_{t,g}}\frac{\ln\frac{\Sigma_{t,g}+Im(B)}{\Sigma_{t,g}-Im(B)}}{2Im(B)-\Sigma_{t,g}\ln\frac{\Sigma_{t,g}+Im(B)}{\Sigma_{t,g}-Im(B)}} & \text{if} \quad B^2 < 0 \\ 1 + \frac{4}{15}\left(\frac{B}{\Sigma_{t,g}}\right)^2 - \frac{12}{175}\left(\frac{B}{\Sigma_{t,g}}\right)^4 + \cdots & \text{if} \quad B^2 \approx 0 \end{cases} \tag{5}$$

In the above *B1 Homogeneous equations*, the multi-group cross sections as $\Sigma_{i,g}$, $\Sigma_{s0}^{g'\to g}$, $\Sigma_{s1}^{g'\to g}$ and χ_g are all available parameters. They are calculated from continuous-energy TRIPOLI4® simulation. Their definitions vary according to their different properties.

- For one-dimensional cross sections, for example: total collision, absorption, fission

$$\Sigma_{i,g} = \frac{\int_{E_{g-1}}^{E_g} \Sigma_i(\mathbf{r},E)\varphi(\mathbf{r},E)}{\int_{E_{g-1}}^{E_g} \varphi(\mathbf{r},E)dE} \tag{6}$$

- For double-differential cross sections eg: the 0^{th} and 1^{st} order scattering cross sections

$$\Sigma_{s0}^{g'\to g} = (\Sigma_{t,g'} - \Sigma_{a,g'}) \times P(g' \to g) \tag{7}$$

with $P(g' \to g) = \frac{\int_{E_{g'}}^{E_{g'-1}} \int_{E_g}^{E_{g-1}} (\Sigma_s(E'\to E) + X\Sigma_{(n,Xn)}(E'\to E))\phi(E')dE'dE}{\int_{E_{g'}}^{E_{g'-1}} (\Sigma_s(E') + X\Sigma_{(n,Xn)}(E'))\phi(E')dE'}$: the energy transfer probability from group g' to g.

$$\Sigma_{s1}^{g'\to g} = \Sigma_{s0}^{g'\to g} \times \int_{-1}^{1} P_1(\mu)f(\mu)d\mu \tag{8}$$

with $P_1(\mu)$: the first order moment of the Polynomial Legendre series; $f(\mu)$: the discrete probability distribution function of the angular deviation μ obtained from continuous energy TRIPOLI4® simulation.

2.2. Implementation Algorithm in TRIPOLI4® code

This part is specified to determine the unknowns (φ_g, d_g and B^2) in the above *B1 Homogeneous equations* and also its coupling methodology into TRIPOLI4® code. The fission power iteration procedure is necessary to obtain the multi-group solutions. The iteration loops are separated into two levels: the inner loop which is executed with fixed B^2 value in order to get the converged φ_g and K_{eff}; the outer loop which is designed to vary the B^2 value according to certain rule (Eq (9)) until $K_{eff} = 1$.

$$B^2_{(n+1)} = B^2_{(n)} + (\frac{1}{K^{expected}_{eff}} - \frac{1}{K^{(n)}_{eff}})\frac{\overline{\nu\Sigma_f}^{(n)}}{\overline{d}^{(n)}} \tag{9}$$

- n: the index for the outer iteration loop;
- $K^{expected}_{eff}$: the expected multiplicative factor given out by user;
- $\overline{\nu\Sigma_f}^{(n)} = \frac{\sum_g \nu\Sigma_{f,g}\varphi^{(n)}_g}{\sum_g \varphi^{(n)}_g}$: the n^{th} loop converged flux weighted average production cross section;
- $\overline{d}^{(n)} = \frac{\sum_g d^{(n)}_g \varphi^{(n)}_g}{\sum_g \varphi^{(n)}_g}$: the n^{th} loop converged flux weighted average diffusion coefficient

The resolution procedure of *B1 Homogeneous equations* is presented in the right part of Figure (1). This module is coupled and iterated with the continuous energy TRIPOLI4® simulation (the left part of Figure (1)) via offering its obtained multi-group leakage coefficients $d_g B^2$ and taking use of the multi-group cross sections from TRIPOLI4® simulation. Then $d_g B^2$ are considered as multi-group macroscopic cross sections of a fictive nuclei mixed homogeneously in the whole assembly. It should be distinguished in two difference cases. When $d_g B^2$ is positive, it is considered as a fictive absorption cross section. In contrary, if $d_g B^2$ is negative, it is considered as fictive production cross section. This is equivalent to correct the neutron weight with the formula $W' = W \times \frac{\Sigma_t(\mathbf{r},E)}{\Sigma_t(\mathbf{r},E)+d_g B^2}$. The later idea was used by MARTIN [15] in a multi-group Monte Carlo code. The whole simulation ends till the below condition is reached: $|K_{eff} - K^{expected}_{eff}| < 100pcm + 3\sigma$. Our advantage compared with them is that the leakage coefficients are used in the continuous energy Monte Carlo simulation until it reaches a critical state at the end. For the moment, the case of $B^2 < 0$ is not yet treated. According to authors, this negative situation is not yet justified physically.

3. VALIDATION

This section is contributed to validate our implemented leakage model in TRIPOLI4® code. As pointed out before, problem of validating a Monte Carlo code is still ambiguous and there hasn't been a clear validation procedure so far. Here, we propose a numerical experiment under continuous energy TRIPOLI4® simulation which consists of a 1D homogeneous critical geometry. Graceful to its natural criticality, its flux spectrum, reaction rates, and produced multi-group cross

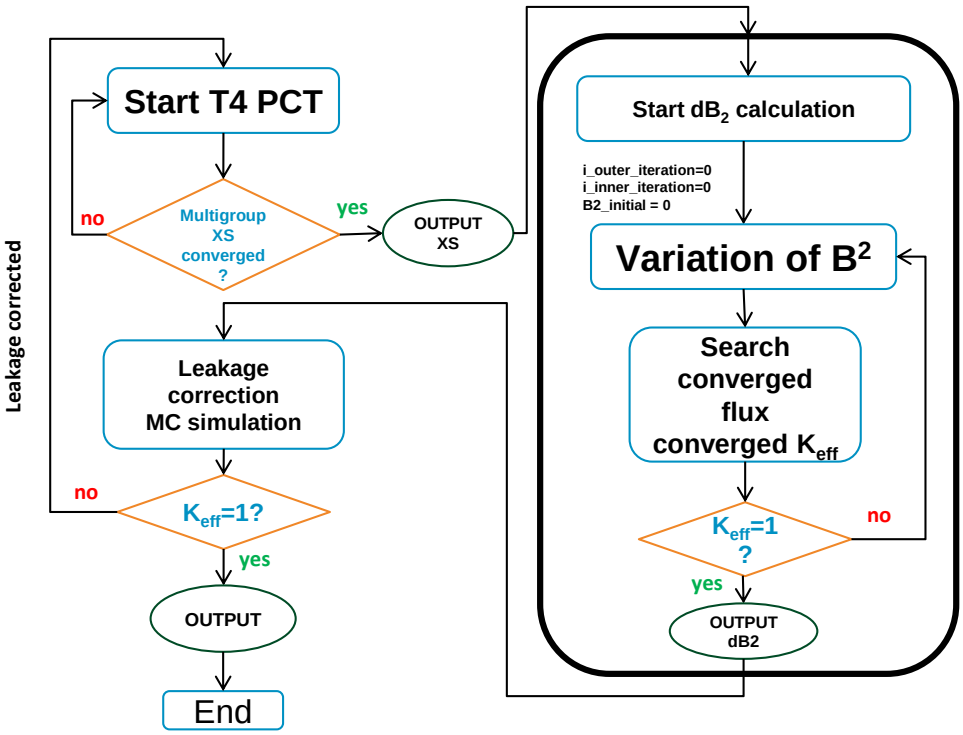

Figure 1. Leakage model algorithm in TRIPOLI4® code

sections will be used as references for those artificial leakage models implemented in different codes: TRIPOLI4®(Monte Carlo), Serpent (Monte Carlo) and ECCO (deterministic).

The validation works will be performed with use of the homogeneous assembly from Zero Power Plutonium Reactor Double Column Fuel (ZPPRDCF) [16]. This configuration represents an important leakage probability (42%) with its infinite multiplicative factor $K_{\text{inf}} = 1.67$. This feature makes the leakage treatment work more complicated. Several parameters (B^2; D_g; ϕ_g) calculated with the four above-talked methods will be compared. To make sure the results are comparable among them, the same library JEFF3.1.1 [17] with probability tables are used in the different codes. At the end, the multi-group cross sections produced by our leakage model will be used in core calculation codes: TRIPOLI4® (multi-group Monte Carlo) and Paris [18] (deterministic). Their simulation results (K_{eff}, neutronic balance) will also be compared with the reference values from the numerical experiment.

3.1. Critical Buckling Value Comparison

To calculate a critical buckling value is not difficult for the assembly calculation codes including leakage model. Though, the challenge here is to find out the reference value from the numerical experiment. The question turns to figuring out the macroscopic distribution function $f(\mathbf{r})$ in Eq (1). Mostly, $f(\mathbf{r})$ is considered as the flux $\phi(\mathbf{r})$ integrated over the whole energy domain. It is perfectly valid only in the context of the fundamental mode approximation applied over a global reactor featuring a periodic lattice of unit cell or assemblies. Even though, experimenters use always the

macroscopic reaction rate (eg: fission of Pu^{239}) to deduce B^2 that is equal to use the global flux $\phi(\mathbf{r})$.

The detailed formulation concerning about how to calculate $f(\mathbf{r})$ in a critical homogeneous core is given in Appendix. The deduction shows that $f(\mathbf{r})$ is in fact an inner product of two fluxes described in Eq (10).

$$f(\mathbf{r}) = \int_0^\infty \varphi^+(E)\phi(\mathbf{r}, E)dE \tag{10}$$

- $\varphi^+(E)$: the adjoint fundamental mode flux in a critical homogeneous assembly; independent of space.
- $\phi(\mathbf{r}, E)$: the direct flux in a critical core; dependent on space and energy

In our test, $\varphi^+(E)$ is calculated under 1968-groups by two different methods. One is the newly developed functionality in TRIPOLI4® code which enables to calculate continuous energy adjoint flux with Monte Carlo method and then collapses them into multi-group flux [19]. It is a reference method to obtain adjoint flux. Though, this new functionality cannot be used for a critical geometry with reflective or periodic boundary condition. So the only approximation used here is that we neglect the difference between an infinite adjoint flux spectrum and a critical one. The other method to obtain 1968-groups adjoint flux is done by two steps within ERANOS [20, 21] code. ECCO code is at first used to generate 1968-groups leakage-corrected cross sections and the critical buckling value. Then a reflective homogeneous core is calculated with consideration of the above critical buckling by BISTRO [22] code which is able to give out the 1968-groups adjoint flux. As for the second flux $\phi(\mathbf{r}, E)$, it is easy to obtain via continuous energy TRIPOLI4® simulation.

The two sets of adjoint flux are then used as microscopic cross sections in a continuous energy TRIPOLI4® simulation. The fictitious reaction rates representing $f(\mathbf{r})$ are scored in different positions along the pre-defined direction z. In our numerical experiment, the geometry is simplified to one dimension, which means $f(\mathbf{r})$ turns into $f(z)$. And the later function respects a cosine distribution in axis z as described in Eq(11). In contrary, with knowledge of the distribution curve, we can deduce the corresponding buckling value with help of a cosine function fit.

$$f(z) = c \cdot cos(Bz) \tag{11}$$

The two curves obtained respectively with TRIPOLI4® (left) and ERANOS (right) adjoint flux are showed in **Figure 2**. The dots are our measured scores and the lines correspond to their fitting curves. The critical height of the homogeneous assembly ZPPRDCF is at 51.40 cm. In order to ignore the edge impact, the cosine fit is done within the region [-20; 20] cm. The results are presented in **Table I** which contains also the critical B^2 values calculated with the artificial leakage models in TRIPOLI4®, SERPENT2.1.16 and ECCO codes under 33-groups.

In **Table I**, the value extracted from the curve 2 is used as the reference one. A tiny difference of 0.52% is observed between the two curves. This probably comes from the infinite adjoint flux spectrum calculated by TRIPOLI4®. As for the results from the three leakage model codes, TRIPOLI4®

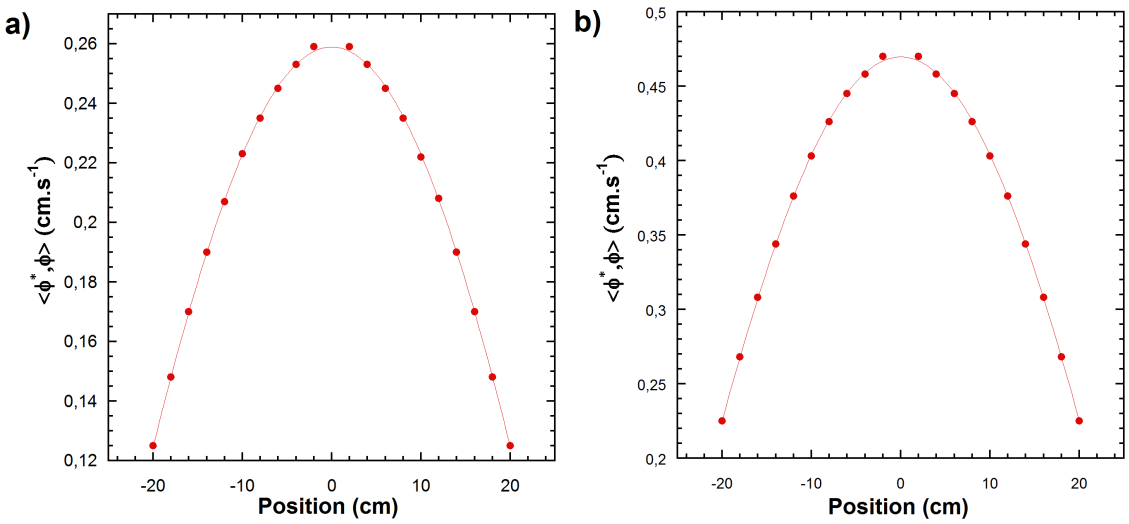

Figure 2. a) Axial distribution of TRIPOLI4® calculated adjoint flux weighted reaction rates b) Axial distribution of ERANOS calculated adjoint flux weighted reaction rates

Table I. Critical buckling comparisons among different leakage model codes and numerical experiments.

	numerical experiment curve a)	curve b)	TRIPOLI4®	SERPENT	ECCO
$B^2(10^{-3} \cdot cm^{-2})$	2.854	2.869	2.812	2.807	2.747
Rel. diff (%)	-0.52	——	-2.0	-2.2	-4.25

gave the closest value with respect to the reference one. This is graceful to our iteration algorithm between the continuous-energy Monte Carlo simulation and the routine for solving the *B1 Homogeneous Equations*. This procedure ensures a final critical state with the original simulation code. It means that in TRIPOLI4® leakage model, a critical flux weighted multi-group constants are used to resolve the *B1 Homogeneous Equations* while in SERPENT, multi-group constants are weighted by infinite flux spectrum. Another reason for explaining the difference between TRIPOLI4® and SERPENT results is their standard deviations associated with the produced multi-group cross sections. In this fast spectrum assembly case, important uncertainties show up in the thermal groups which give out some unreliable cross sections. Thus, these low energetic group cross sections impact the deterministic resolution of the *B1 Homogeneous Equations*. In order to confirm this deduction, perspective study on the spread of uncertainties of multi-group cross sections to the critical buckling value need be pursued. Otherwise, greater discrepancy (4.25%) is found between ECCO calculation and the reference value.

3.2. Comparisons of Critical Flux Spectrum, D_g and Leakage Rate

3.2.1. Critical Flux Spectrum Comparison

In Figure 3, we compare the critical flux spectrum calculated with different leakage model codes as well as the one extracted from the numerical experiment (no error bars given out for the numerical experiment because it is well converged and the standard deviations are around 0.01%). These flux spectra are normalized to attain $\sum_{g=1}^{G} \phi_g = 1$ with $G = 33$: the total number of energy meshes tested. Globally, all the four curves have the same tendency which proves that the leakage models in TRIPOLI4®, SERPENT and ECCO are able to reproduce the form of a realistic critical flux spectrum. The grey zone plotted in **Figure 3.b)** indicates the energy domain of interest, containing more than 95% of neutron production.

The relative differences between each leakage model result and the reference one in the interesting energy domain are plotted in **Figure 3.c)**. We find that on the high energy half part, the three leakage models have under-estimated the flux. And on the left half part, the leakage models have in contrary over-estimated the critical flux compared with the numerical experiment result.

3.2.2. Diffusion Coefficient Comparison

Obtaining the diffusion coefficient is not our original goal because transport core calculation will be fed with our produced multi-group cross sections, not a diffusion core calculation. However, we could always compare the obtained diffusion coefficients from different codes in order to evaluate the artificial leakage rates with respect to the real leakage terms from the numerical experiment.

Figure 4.a) shows the 33-groups diffusion coefficients obtained respectively with TRIPOLI4® continuous energy calculation ($TRIPOLI\_PCT\_trans$), TRIPOLI4® leakage model ($TRIPOLI\_MF$), SERPENT and ECCO calculations. To be marked, $TRIPOLI\_PCT\_trans$ result is obtained with $P1$ approximation formula:

$$D_g = \frac{1}{3\Sigma_{tr,g}} = \frac{1}{3(\Sigma_{t,g} - \overline{\mu}_g \Sigma_{s,g})} \tag{12}$$

with $\Sigma_{t,g}$, $\Sigma_{s,g}$ and $\overline{\mu}_g$ obtained with Monte Carlo simulation while the three leakage models take use of the B1 approximation. Therefore, it is normal that the red line differs a little bit from the others. At first, a similar tendency is shown by the three leakage model curves. However, there are some important discrepancies in the epithermal energy domain ($1eV \sim 100eV$) which come from poor statistic scores and do not enter into our interest zone.

The grey zone attracts more attention with the same reason as for the above critical flux spectrum and so is especially plotted in **Figure 4.b)**. We can tell that the leakage model curves agree rather well among themselves even with the $P1$ transport approximation calculation.

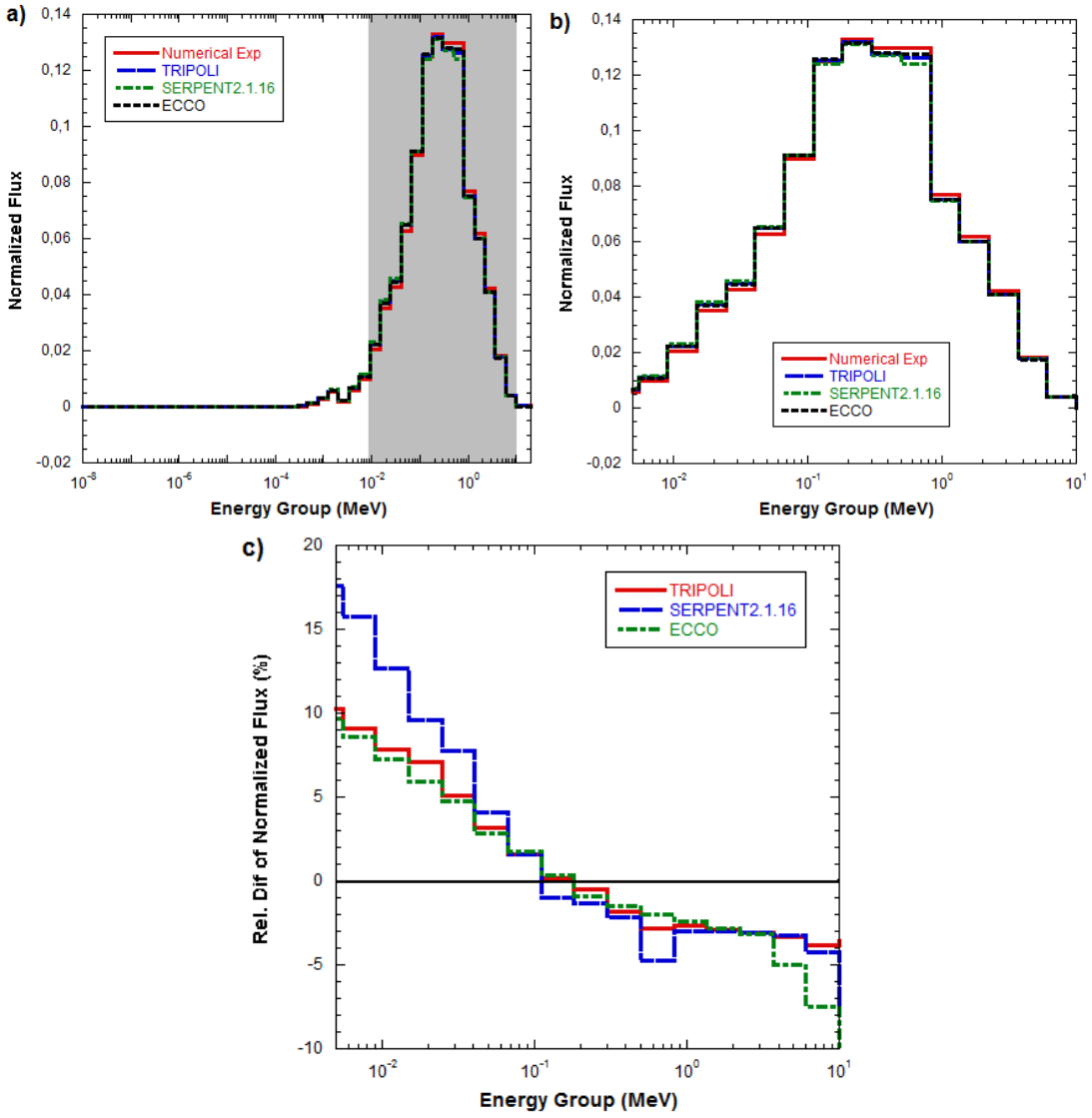

Figure 3. Normalized critical flux spectrum comparison

3.2.3. Leakage Rate Comparison

Previously, we focused on comparing every single parameters calculated from leakage models. However, the physical motivation of leakage model is trying to simulate artificially the approximated leakage rates ($d_g B^2 \phi_g$) in a correct manner. In order to verify the reliability of our implemented leakage model, we are going to compare the simulated leakage rates to the real one which is the score of neutrons travelling through the boundary surface in the numerical experiment.

In **Figure 5**, the discrepancies of leakage rates between the three leakage models and the numerical experiment are plotted versus energy groups. We observe that for all the 3 codes there exists a compensation effect between the higher energy part (over-estimated leakage) and the lower energy part (under-estimated leakage). The absolute discrepancies in each group are less than $500pcm$. This effect comes from the intrinsic approximation of B1 fundamental mode which assumes that

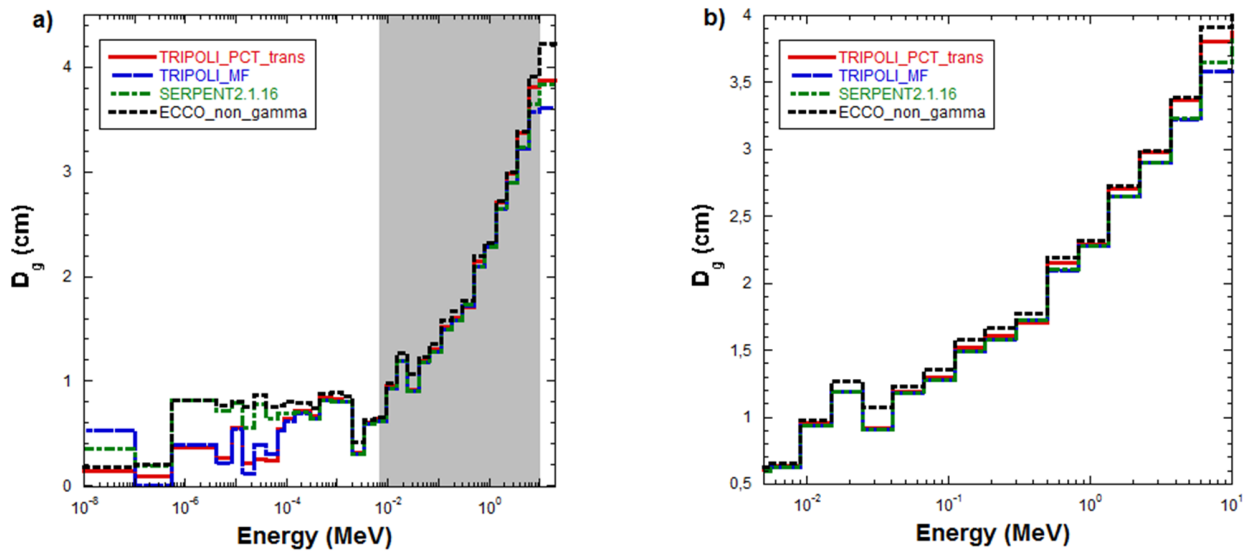

Figure 4. Diffusion coefficient comparison

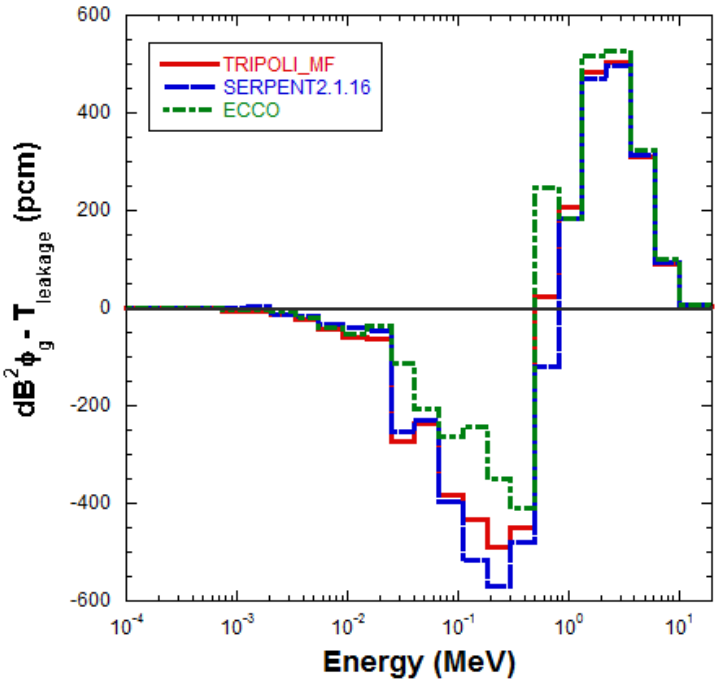

Figure 5. Leakage rates comparison

the neutron spectrum is not depending on the position in the assembly. It is not the case in a real assembly where the neutron spectrum is harder on the edge than in the center which represents better the fundamental mode case. Thus, there are less fast neutrons escaping on the edge of a real geometry. This explanation matches well with the over-estimation peak around 2 MeV.

3.3. Application of leakage-corrected cross sections in deterministic core calculation

In this section, we return back to the original motivation of this work: performing core calculations with the leakage-corrected multi-group cross sections. These constants can be used directly in a Monte Carlo based TRIPOLI4® multi-group calculation or converted to a compatible format and then used in a S_N method based PARIS calculation.The obtained multiplicative factors and their discrepancies compared with the numerical experimental reference value are showed in **Table II**. Through the ΔK_{eff} values and their corresponding standard deviations, consistent results are found between the two transport theory based core calculation codes with using the same TRIPOLI4® leakage model produced multi-group constants.

Meanwhile, another set of multi-group cross sections are directly produced for the critical experiment geometry which are considered as reference values and used in the same core codes. Their K_{eff} results are given out in **Table III**. So if we compare the K_{eff} values in **Table II** & **III** vertically, a good agreement is deduced between our leakage model produced cross sections and the ones directly generated from critical geometry because both of them can be used to calculate similar multiplicative factors. To be noticed that all the multi-group constants used in core calculations are always treated with In-Group Scattering Anisotropy Correction to guarantee their adequate performance in core calculation.

Table II. Comparison of K_{eff} values with use of 33-groups cross sections produced by TRIPOLI4® leakage model

	Numerical Experiment	TRIPOLI4® MG	PARIS (P_5)
K_{eff}	0.99923 ± 0.00005	0.99657 ± 0.00012	0.99574
ΔK_{eff} (PCM)	——	-266 ± 13	-349 ± 5

Table III. Comparison of K_{eff} values with use of 33-groups cross sections produced with critical experiment geometry

	Numerical Experiment	TRIPOLI4® MG	PARIS (P_5)
K_{eff}	0.99923 ± 0.00005	0.99685 ± 0.00017	0.99581
ΔK_{eff} (PCM)	——	-238 ± 13	-342 ± 5

Moreover, detailed analysis is done for the flux spectrum and neutronic balance. **Figure 6.a)** shows the normalized flux spectra from multi-group TRIPOLI4®(using leakage-corrected constants produced by itself) simulation and the reference numerical experiment simulation. The two curves are well superimposed. **Figure 6.b)** shows the reaction rate discrepancies. The multi-group TRIPOLI4® simulation has globally under-estimated the production rate and in contrary over-estimated the leakage rate. The oxygen resonance peak located at 400 KeV induced about $-50pcm$ of production. Another resonance peak situated around 130 KeV is probably from the structure element (Fe56; Cr52). However, the discrepancies compared to reference reaction rates are less than 60 pcm in any group.

In addition, we want to compare our produced leakage-corrected multi-group constants with those from ECCO code. The basic idea is using them in PARIS calculation. In **Table IV**, results from

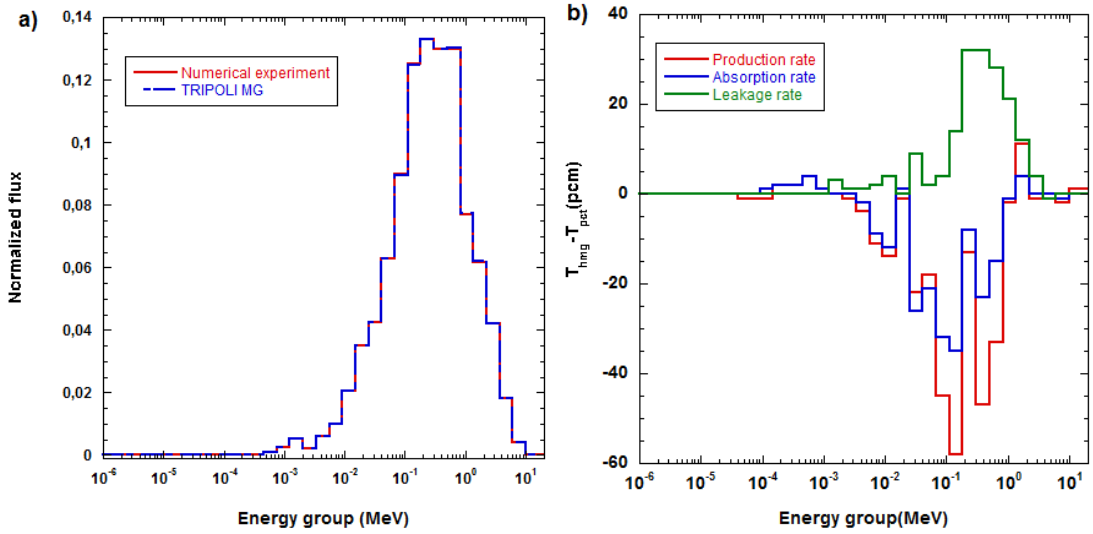

Figure 6. Normalized flux spectra and neutronic balance comparison between multi-group TRIPOLI4® simulation and reference results

ECCO-PARIS and TRIPOLI4®-PARIS calculations are respectively compared with the reference one. A consistent estimation of K_{eff} is obtained with TRIPOLI4® leakage model generated multi-group constants compared to those produced by ECCO.

Table IV. Comparison of K_{eff} values with use of ECCO and TRIPOLI4® leakage model produced multi-group cross sections

	Numerical Experiment	ECCO-PARIS(P_1)	TRIPOLI4®-PARIS(P_1)
K_{eff}	0.99923 ± 0.00005	0.99447	0.99440
ΔK_{eff} (PCM)	——	-476 ± 5	-483 ± 5

In order to better understand where the difference comes from, we compare respectively the production rate in TRIPOLI-PARIS and ECCO-PARIS simulations to the reference one from numerical experiment in **Figure 7.a)**. Generally, the two simulations have both under-estimated the production rate which is consistent with the multi-group TRIPOLI4® simulation. Though, ECCO-PARIS calculation showed more discrepancies than TRIPOLI4®-PARIS simulation in the high energy domain. Then if we move on to analyze the normalized critical flux spectra from the two simulations (**Figure 7.b)**), they match rather well with the reference spectrum.

4. CONCLUSION

A *B1 Homogeneous Equations* based leakage model has been implemented recently in the continuous-energy Monte Carlo code TRIPOLI4®. This leakage model makes use of the MC method generated multi-group cross sections to solve the *B1 Homogeneous Equations* in order to get the few-group leakage coefficients. The innovative point of our method is that these few-group leakage coefficients are re-used in a continuous-energy Monte Carlo simulation iteratively with coupling of the

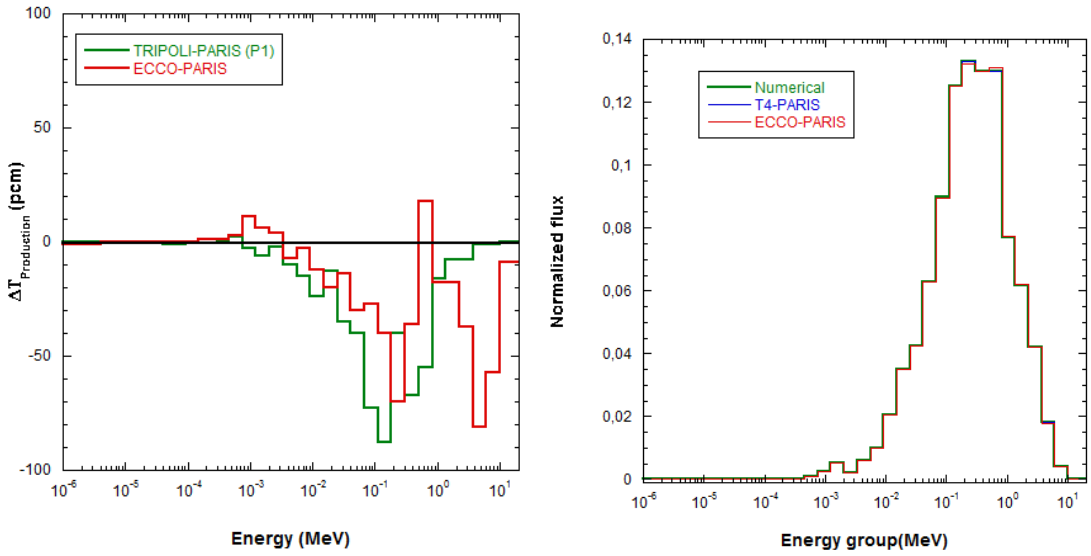

Figure 7. Production rates and normalized flux spectra from TRIPOLI4®-PARIS and ECCO-PARIS simulations and the their comparisons to numerical experiment results

resolution of *B1 Homogeneous Equations* till reaching a critical state according to MC simulation. Meanwhile, multi-group constants are produced which can be used in transport theory based core calculations.

Then a complete validation work is performed with using a critical geometry based numerical experiment as reference case. In particular, a high leakage rate ($\sim 42\%$) assembly geometry is tested. Various leakage characteristic parameters are compared between our leakage model calculations and those from SERPENT2.1.16 and ECCO. Globally, there is a good agreement among the three leakage model codes as well as the numerical experiment case. However, a methodology default is revealed while comparing the leakage model simulated multi-group leakage rates with a realistic reference one. This non-completely consistent phenomenon is related to the intrinsic approximation from the fundamental mode. To be able to answer this question, a more physical representative leakage model need to be investigated in the future.

ACKNOWLEDGMENTS

This work has been supported by CEA. Authors are thankful to the LEPh colleagues, especially to Pr. Gérald Rimpault, who gave us technical suggestions and discussions on this research work.

REFERENCES

[1] J. Leppänen. *SERPENT: a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code*. VTT Technical Research Centre of Finland (2013).

[2] Ho Jin Park *et al.* "Generation of few group diffusion theory constants by Monte Carlo code McCARD." *Nuclear Science and Engineering*, **172(1)**: pp. 66 – 77 (2012).

[3] J. E. Hoogenboom, V. A. Khotylev, and J. M. Tholammakkil. "Generation of multi-group cross sections and scattering matrices with the Monte Carlo code MCNP5." In: *Joint International Topical Meeting on Mathematics & Computations and Supercomputing in Nuclear Applications*. Monetery, USA, APRIL 15 - 19 (2007).

[4] S. C. van der Marck, J. C. Kuijper, and J. Oppe. "Homogenized group cross sections by Monte Carlo." In: *Physor The Role of Reactor Physics toward a Sustainable Future*. Vancouver, Canada, SEPTEMBER 10 - 16 (2006).

[5] Li Cai *et al.* "P1 adaptation of TRIPOLI-4 code for the use of 3d realistic core multigroup cross section generation." In: *Joint International Conference on Supercomputing in Nuclear Application and Monte Carlo*. Paris, France, October 27 - 31 (2013).

[6] Nam Zin Cho, Sunghwan Yun, and Jaejun Lee. "Generation of homogenized nodal parameters by Monte Carlo method with non-zero leakage spectra in global-local iteration framework." *Transactions of the American Nuclear Society*, **101**: pp. 707 – 710 (2009).

[7] T. Yamamoto. "Monte carlo method with complex weights for neutron leakage-corrected calculations and anisotropic diffusion coefficient generations." *Annals of Nuclear Energy*, **50**: pp. 141 – 149 (2012).

[8] Toshihiro Yamamoto. "Improvements and new findings in Monte Carlo method with complex-valued weights for neutron leakage-corrected assembly calculations." In: *Joint International Conference on Supercomputing in Nuclear Application and Monte Carlo*. Paris, France, October 27 - 31 (2013).

[9] J.-P. Both *et al.* "A survey of TRIPOLI4." In: *Int. Conf. on Radiation Shielding*. Arlington, USA (1994).

[10] E. Brun *et al.* *Overview of TRIPOLI4 version 7 Continuous-energy Monte Carlo Transport Code* (2011).

[11] J.-P. Both and Y. K. Lee. "Computations of homogenised multigroup cross sections with the Monte Carlo code TRIPOLI4." In: *SARATOGA JIC MM SNA*. Saratoga Springs, USA (1997).

[12] "NEA-1716 TRIPOLI-4 VERS. 8.1." URL http://www.oecd-nea.org/tools/abstract/detail/NEA-1716/ (2013).

[13] G. Rimpault. "Algorithmic features of the ECCO cell code for treating heterogeneous fast reactor assemblies." In: *Int. Conf. on Mathematics and Computations, Reactor Physics, and Environmental Analyses*. Portland, USA, May 1-5 (1995).

[14] M. J. Grimstone, J. D. Tullett, and G. Rimpault. "Accurate treatments of fast reactor fuel assembly heterogeneity with the ECCO cell code." In: *Int. Conf. on the Physics of Reactors: Operation, Desing and Computation-PHYSOR 90*. Marseille, FRANCE, April 23-27 (1990).

[15] Nicolas Martin and Alain Hébert. "Adaptation of the B1 leakage model to Monte Carlo criticality calculations." In: *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M& C 2011)*. Rio de Janeiro, BRAZIL, May 8-12 (2011).

[16] Toshio Sanda. *A 1,000 MWe-Class Sodium-cooled MOX-Fueled FBR Homogeneous Core Mock-up Critical Experiment in the state of removal of one of eighteen half-inserted control rods, where enriched uranium is used with the shape of a sector in the outer core*. NEA/NSC/DOC(2006)1.

[17] "THE JEFF-3.1.1 NUCLEAR DATA LIBRARY OECD/NEA 2009." URL https://www.oecd-nea.org/dbdata/nds_jefreports/jefreport-22/nea6807-jeff22.pdf (2009).

[18] L. Gastaldo *et al.* "High-order discrete ordinate transport in non-confirming 2d cartesian meshes." In: *Int. Conf. on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*. New York, USA, May 3-7 (2009).

[19] G. Truchet *et al.* "Continuous-energy adjoint flux and perturbation calculation using the iterated fission probability method in Monte Carlo code TRIPOLI-4 and underlying applications." In: *Joint International Conference on Supercomputing in Nuclear Application and Monte Carlo*. Paris, France, October 27 - 31 (2013).

[20] Gérald Rimpault *et al.* "The ERANOS code and data system for fast reactor neutronic analyses." In: *Int. Conf. PHYSOR*. Seoul, Korea, October 7 - 10 (2002).

[21] J. M. Ruggieri *et al.* "ERANOS 2.1: International code system for gen iv fast reactor analysis." In: *Int. Conf. ICAPP'06*. Reno, Nevada, June 4 - 8 (2006).

[22] G. Palmiotti. "Optimized two-dimensional Sn transport(BISTRO)." *Nuclear Science and Engineering*, **104**: pp. 26 – 33 (1990).

APPENDIX A. Fundamental Mode in the Center of a Homogeneous Core

In the central part of a homogeneous assembly geometry, the diffusion equation are written in both direct and adjoint forms:

$$D(E)\nabla^2\Phi(\mathbf{r},E)-\Sigma_t(E)\Phi(\mathbf{r},E)+\int_0^\infty dE'\Sigma_s(E'\rightarrow E)\Phi(\mathbf{r},E')+\chi(E)\int_0^\infty dE'\nu\Sigma_f(E')\Phi(\mathbf{r},E')=0 \tag{13}$$

$$D(E)\nabla^2\Phi^+(\mathbf{r},E)-\Sigma_t(E)\Phi^+(\mathbf{r},E)+\int_0^\infty dE'\Sigma_s(E'\rightarrow E)\Phi^+(\mathbf{r},E')+\chi(E)\int_0^\infty dE'\nu\Sigma_f(E')\Phi^+(\mathbf{r},E')=0 \tag{14}$$

The two above equations can be simplified with the diffusion operator M and its adjoint operator M^+ as following:

$$\nabla^2\Phi(\mathbf{r},E)+M\Phi(\mathbf{r},E)=0 \tag{15}$$

$$\nabla^2\Phi^+(\mathbf{r},E)+M^+\Phi^+(\mathbf{r},E)=0 \tag{16}$$

The eigenvalues and the corresponding vectors of M and M^+ are:

$$M\varphi_i(E)=\lambda_i\varphi_i(E) \tag{17}$$

$$M^+\varphi_i^+(E)=\lambda_i\varphi_i^+(E) \tag{18}$$

with $i=0,1,2\cdots$; $\int_0^\infty dE\varphi_i^+(E)\varphi_j(E)=<\varphi_i^+,\varphi_j>=0$, when $i\neq j$.

If we develop $\Phi(\mathbf{r},E)$ and $\Phi^+(\mathbf{r},E)$ respectively with their eigenvectors:

$$\Phi(\mathbf{r},E)=\sum_i f_i(\mathbf{r})\varphi_i(E) \tag{19}$$

$$\Phi^+(\mathbf{r},E)=\sum_i f_i^+(\mathbf{r})\varphi_i^+(E) \tag{20}$$

with $f_i(\mathbf{r})=\frac{<\varphi_i^+,\Phi>}{\varphi_i^+,\varphi_i}$; $f_i^+(\mathbf{r})=\frac{\Phi^+,\varphi_i}{\varphi_i^+,\varphi_i}$.

After substituting Eq(19) and Eq(20) into the first two diffusion equations, we obtain:

$$\sum_i[\nabla^2 f_i(\mathbf{r})+\lambda_i f_i(\mathbf{r})]\varphi_i(E)=0 \tag{21}$$

$$\sum_i[\nabla^2 f_i^+(\mathbf{r})+\lambda_i f_i^+(\mathbf{r})]\varphi_i^+(E)=0 \tag{22}$$

It means that: $f_i(\mathbf{r})\propto f_i^+(\mathbf{r})$, and $\nabla^2 f_i(\mathbf{r})+\lambda_i f_i(\mathbf{r})=0$ where $\lambda_0=B^2$.

So for $i=0$, we get:

$$\nabla^2 f_0(\mathbf{r})+B^2 f_0(\mathbf{r})=0 \tag{23}$$

with $f_0=\int_0^\infty dE\varphi^+(E)\Phi(\mathbf{r},E)=\int_0^\infty dE\varphi(E)\Phi^+(\mathbf{r},E)$. The detailed definitions of the different flux are given below:

- $\varphi^+(E)$: the adjoint flux in a critical homogeneous assembly;
- $\varphi(E)$: the direct flux in a critical homogeneous assembly;
- $\Phi(\mathbf{r},E)$: the direct flux in a critical core;
- $\Phi^+(\mathbf{r},E)$: the adjoint flux in a critical core.