Using Green's Functions to Compute 3 Dimensional Neutron Flux Maps - 16016

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ABSTRACT

The knowledge of the radionuclide content of radioactive waste is of utmost importance for safety and waste management reasons. Numerical simulations are used by EDF-DP2D to anticipate dismantling and radioactive waste management.

The main numerical activation schemes include the computing of a 3 dimensional neutron flux map, obtained on the basis of a neutron propagation calculation. The codes used solve the transport equation called the Boltzmann equation without simplification. The Monte Carlo method is used to solve the Boltzmann equation. Random series of numbers are used to simulate the lives of millions of neutrons. The codes follow each neutron individually, from its birth to its disappearance by leakage, absorption, or fission, and then the neutron flux map is calculated at the nominal power rating conditions.

The main drawback of the Monte Carlo codes is the large computing time needed to converge within acceptable statistical criteria. This extended time period is incompatible with the multiple fuel managements used by EDF to operate its NPPs because it is necessary to make a Monte Carlo calculation for each fuel loading pattern. The solution developed by EDF-DP2D is to use the importance factors of Green's Functions to simplify the computing of the 3 dimensional neutron flux maps. Physicists talk about Green's Functions where mathematicians talk about elementary solutions of linear equations with constant coefficients.

With an activation scheme based on the Green's Functions approach the 3D neutron flux is obtained on the basis of the convolution of the normalized source contributions (i.e. normalized response matrices) with the neutrons emitted by the fuel assemblies. The response matrices to unitary sources are computed with the Monte Carlo code MCNP for different tallies of interest and the neutron sources emitted by the fuel are computed with a core code for different fuel loading patterns.

The principal interest of this approach is the calculation of the response matrices to unitary sources that can be used for all power distributions, thus limiting the Monte Carlo computing time.

INTRODUCTION

The knowledge of the radionuclide content of radioactive waste is of utmost importance for safety and waste management reasons.

State of EDF nuclear reactor fleet

The EDF nuclear reactor fleet consists of 58 pressurized water reactors (PWRs) spread across 19 sites. Currently, three types of reactor can be noted, 34 "900 MW", 30 "1300 MW" and 4 "1450 MW".

In order to optimize the use of the fuel assemblies and to limit the vessel neutron fluence (i.e. neutron flux integrated in a period of time), different fuel loading patterns were defined for each reactor. Each fuel loading pattern is linked with a particular 3 dimensional power distribution.

The radioactive inventories of the vessel and the internals due to neutron flux activation are a result of the history of the different power distributions.

As EDF is the only operator of the French nuclear power plants (with regard to the French regulations), EDF is responsible for dismantling the French NPPs. Numerical simulations are used by DP2D (i.e. decommissioning branch of EDF) to anticipate dismantling and radioactive waste management. For this, DP2D developed a calculation scheme including the mapping of the 3 dimensional neutron flux, and radioactive inventory calculations (Ref. [1]).

Radioactive waste management in France

A waste classification can be set according to the radioactive inventory of each component or subcomponent and the waste classification criteria.

In France, 5 classes of nuclear waste are defined. Each refers to a particular level of specific activity and radio-toxicity. The different classes from the least to the most penalizing are : "Very Low Activity", "Low Activity Short Life", "Low Activity Long Life", "Intermediate Activity Long life", and "High Activity Long Life".

Typically it is necessary to know the radioactive inventory in terms of specific activity (Bq/g) based on a list of 143 radionuclides.

Due to the types of particles emitted, most of these radionuclides cannot be measured, this is why numerical simulations must be made. Then during the dismantling work, gamma measurements are made on the wastes. Depending on the measured values, the results of the calculated radioactive inventory can be corrected.

Classical calculations of the radioactive inventory

The main numerical activation schemes comprise a calculation of the 3 dimensional neutron flux map obtained on the basis of neutron propagation calculations. The codes used solve the transport equation called the Boltzmann equation without simplification. The Monte Carlo method is retained to solve the Boltzmann equation. Random series of numbers are used to simulate the lives of millions of neutrons. The codes follow each neutron individually, from birth to disappearance by leakage, absorption, or fission. Then the neutron flux map is calculated at the nominal power rating conditions.

The main drawback of the Monte Carlo codes is the large computing time needed to converge within acceptable statistical criteria. This computing time is incompatible with the multiple fuel managements used by EDF to operate its NPPs because a Monte Carlo calculation is necessary for each fuel loading pattern.

The solution developed by EDF-DP2D is to use the importance factors of Green's Functions to simplify the computing of the 3-dimensional neutron flux maps.

DESCRIPTION

The principal interest of using the importance factors of Green's Functions is that the normalized source contributions matrices can be used for all the power distributions, and thus reducing the Monte Carlo computing time.

Theoretical background of Green's Functions approach

Physicists talk about Green's Functions where mathematicians talk about elementary solutions of linear equations with constant coefficients.

Formally, using the Lebesgue integral notation (i.e. integral of a function over a measure space), the definition of a neutron detector response is given by the following relation :

$$R_k(Z) = \int_z s_k(P) . \Phi(P) \, dP \qquad\qquad \text{(Eq. 1)}$$

where $\quad P \quad = $ point in the phase space $\left(\vec{r}, E, \vec{\Omega}\right)$

$\qquad\qquad s_k \quad = $ sensitivity coefficient of detector k
$\qquad\qquad\qquad$ (for example macroscopic cross section)

$\qquad\qquad \Phi(P) = $ neutron flux at point P

$\qquad\qquad Z \quad = $ response space

The flux $\Phi(P)$ is given by :

$$\Phi(P) = \int_{z'} S(P') \, G(P' \to P) dP' \qquad\qquad \text{(Eq. 2)}$$

where $\quad G(P' \to P) \quad \equiv G\left(\vec{r'}, E', \vec{r} \in Z, E\right)$
$\qquad\qquad\qquad\qquad\qquad = $ Green's Function associating the emission position $\vec{r'}$ of the particle at energy E' to its arrival position $\vec{r}$ at energy E when tallying

$\qquad\qquad S(P') \qquad\qquad = $ neutron source emitted at point the P' in the region Z'

Relations /1/ and /2/ give :

$$R_k(Z) = \int_z \ s_k(P) \, dP \ \int_{z'} S(P') \, G(P' \to P) \, dP' \qquad\qquad \text{(Eq. 3)}$$

Changing the order of integration leads to :

$$R_k(Z) = \int_{z'} S(P') \, dP' \ \int_z \ s_k(P) \, G(P' \to P) \, dP \qquad\qquad \text{(Eq. 4)}$$

Using $\Phi^+(P')$, the adjoint flux that satisfies the adjoint Boltzmann equation, equation /1/ becomes :

$$R_k(Z) = \int_{z'} S(P') \ \Phi^+(P') \, dP' \qquad\qquad \text{(Eq. 5)}$$

With an adjoint source equal to the detector response $s_k(P)$, relations /4/ and /5/ finally give :

$$\Phi^+(P') = \int_{z'} s_k(P) \, G(P' \to P) \, dP \qquad\qquad \text{(Eq. 6)}$$

Equations /5/ and /6/ show the possibility of performing parametric calculations of the response $R_k(Z)$ against the core source distribution. The adjoint flux $\Phi^+(P')$ is currently obtained by solving the Boltzmann equation.

In this paper the Green's Functions importance factors are built by the Monte Carlo code MCNP.

The principle of the detector response calculation from the Monte Carlo Green's Functions is based on the calculation of Green's Functions importance factors between the source points and the response scoring space (denoted Z and being either a volume or a surface boundary).

The response of a detector k scored into Z is calculated by the following equation :

$$R_k(Z) = \int_{\vec{r}'} \ \int_{E'} \ \int_{\vec{r} \in Z} \ \int_E \ \frac{S(\vec{r}')}{S_0(\vec{r}')} \, s_k(\vec{r}, E) \ G\left(\vec{r}', E', \vec{r} \in Z, E, S_0(\vec{r}')\right) dE \, d\vec{r} \, dE' \, d\vec{r}' \qquad \text{(Eq. 7)}$$

where   E', E   = emission and arrival energies (the emission energy is the energy of the source particle, and the arrival energy corresponds to the energy of the particle when it scores in the Z area)

           $\vec{r}'$ = emission position of the source particle

           $S_0(\vec{r}')$ = number of source particles emitted per volume unit and energy unit at position $\vec{r}'$ in the reference Monte Carlo simulation

           $S(\vec{r}')$ = number of source particles emitted per volume unit and energy unit at position $\vec{r}'$ when using Green's Functions

$s_k(\vec{r}, E)$ = energy sensitivity coefficient of the detector k at position $\vec{r}$ and energy E

It can be noted that :

- the function G includes the parameter $S_0(\vec{r}')$;
- the description of the geometry, materials, temperatures and biasing options (i.e. variance reduction options) are the same in the reference simulations (i.e. $S_0(\vec{r}')$) and when using Green's Functions (i.e. $S(\vec{r}')$).

Any variation of the source can then be integrated in the calculations using the Green's Functions data. The tallies are built as shown in equation /7/. Flux, reactions rates, or dose equivalent rates can all be calculated from this. The statistical quality of the tallies derived from the Green's Functions directly depends on the statistical quality achieved in the reference simulation.

To reduce the computing time in the calculation of 3D neutron flux map associated with several 3D neutron sources, it can be helpful to calculate source contributions from Green's Functions related to fuel assemblies.

For any neutron source distribution S_i (i the index associated with the spatial mesh of the source region V_i), the response link to the detector k into the area Z is given by :

$$R_k(Z) = \sum_i S_i\, J_{ik}(Z)$$ (Eq. 8)

where $\quad S_i \quad = \quad \int_{V_i} S_i(\vec{r}')\, d\vec{r}'$

$\qquad\qquad\qquad$ = neutron source distributions

$\qquad J_{ik}$ = normalized source contributions related to k

With $R_{0k}(Z)$ related to the Monte Carlo reference simulation characterized by the neutron source distribution $S_{0i}(\vec{r}')$ the response can be written as :

$$R_{0k}(Z) = \sum_i S_{0i}\, J_{ik}(Z)$$

$$\qquad\quad = \sum_i C_{0ik}(Z)$$ (Eq. 9)

where $\quad S_{0i} \quad = \quad \int_{V_i} S_{0i}(\vec{r}')\, d\vec{r}'$

$\qquad\qquad\qquad$ = reference neutron source distribution

The normalized source contributions $J_{ik}(Z)$ can be deduced from the contributions $C_{0ik}(Z)$ performed from the reference Monte Carlo simulation results :

$$J_{ik}(Z) = \frac{C_{0ik}(Z)}{S_{0i}}$$ (Eq. 10)

Finally, relations /8/ and /10/ give :

$$R_k(Z) = \sum_i \frac{S_i}{S_{0i}} \, C_{0ik}(Z)$$
(Eq. 11)

Equation /11/ shows that the calculation of the normalized source contributions $C_{0ik}(Z)$ associated to the reference neutron source distributions S_{0i} is sufficient to know the response $R_k(Z)$ associated to any other neutron source distribution S_i. The use of equation /11/ can be simplified if using unitary sources (i.e. $S_{0i}(\vec{r}') = 1$).

The comparison between equations /7/ and /11/ shows the link between the source contributions $C_{0ik}(Z)$ and the associated Green's Function :

$$C_{0ik}(Z) = \; s_k(\vec{r}, E) \;\; G\left(\vec{r}', E', \vec{r} \in Z, E, S_0(\vec{r}')\right)$$
(Eq. 12)

The main difficulty of this approach is to compute the matrix $C_{0ik}(Z)$ of the normalized source contributions. In fact, its size directly depends on the number of sources.

Numerical activation scheme using Green's Functions

Figure 1 presents the numerical simulation scheme based on Green's Functions approach used by EDF-DP2D to calculate the activation by neutron flux.

This scheme comprises five steps :

- Step 1 : Computing of 3-dimensional response matrices to unitary sources. These matrices (i.e. normalized source contributions or importance factors of Green's Functions) are built for each tally of interest. The code used is MCNP (Ref. [2]). It was developed by the American Los Alamos National Laboratory to solve the Boltzmann equation. The input data covers the microscopic cross-sections, the 3-dimensional geometry, the chemical compositions with no impurities and the neutron unitary sources emitted by the fuel assemblies.

- Step 2 : Computing of a 3-dimensional multigroup neutron flux map. The neutron flux mapping is obtained on the basis of the convolution of the response matrices to unitary sources (step 1) with the neutron sources emitted by the fuel assemblies. The neutrons emitted by the fuel assemblies are computed with the core code COCCINELLE (deterministic code developed by EDF). The matrix convolution is made by using the Python language. The neutron flux maps are calculated for the nominal power rating conditions, and each flux is homogenized into a limited number of energy groups.

- Step 3 : Calculation of the activities. The activities are calculated for each component or sub-component of interest. The code used is DARWIN-PEPIN (Ref. [3]). It was developed by the French laboratory Commissariat à l'Energie Atomique (CEA) to solve a system of Bateman equations. The input data covers the 3-dimensional neutron flux maps calculated in step 2, the microscopic cross sections, the radioactive decay series associated with the radioactive half lives, the chemical compositions including impurities and the

irradiation history resulting from the daily power production. The output data is the radioactive inventory of each component or sub-component of interest limited to a list of 143 radionuclides.

- Step 4 : Comparisons between calculated results and measured results. For this, we need results of measurements and results of calculation linked with the measurements. The comparisons are based on calculation measurement ratios (i.e. "C/M"). A value greater than 1 corresponds to an overestimated calculation, and a value less than 1 corresponds to an underestimated calculation. Depending on the results, the input data may be redefined to make a new simulation.

- Step 5 : Waste classification. By using the radioactive inventory of each component or sub-component, and the waste classification criteria, a waste classification can be made. The criteria are based on specific activity and radiotoxicity levels of 143 radionuclides. The distinction between the "Long Life" and the "Short Life" waste is based on a list of specific activity limits for 40 radionuclides. If none of these limits are crossed, a weighted specific activity level is used to separate "Very Low Activity" and "Short Life" waste. The weighted specific activity value is obtained by taking into account the specific activity levels balanced with the levels of radio-toxicity of 143 radionuclides.
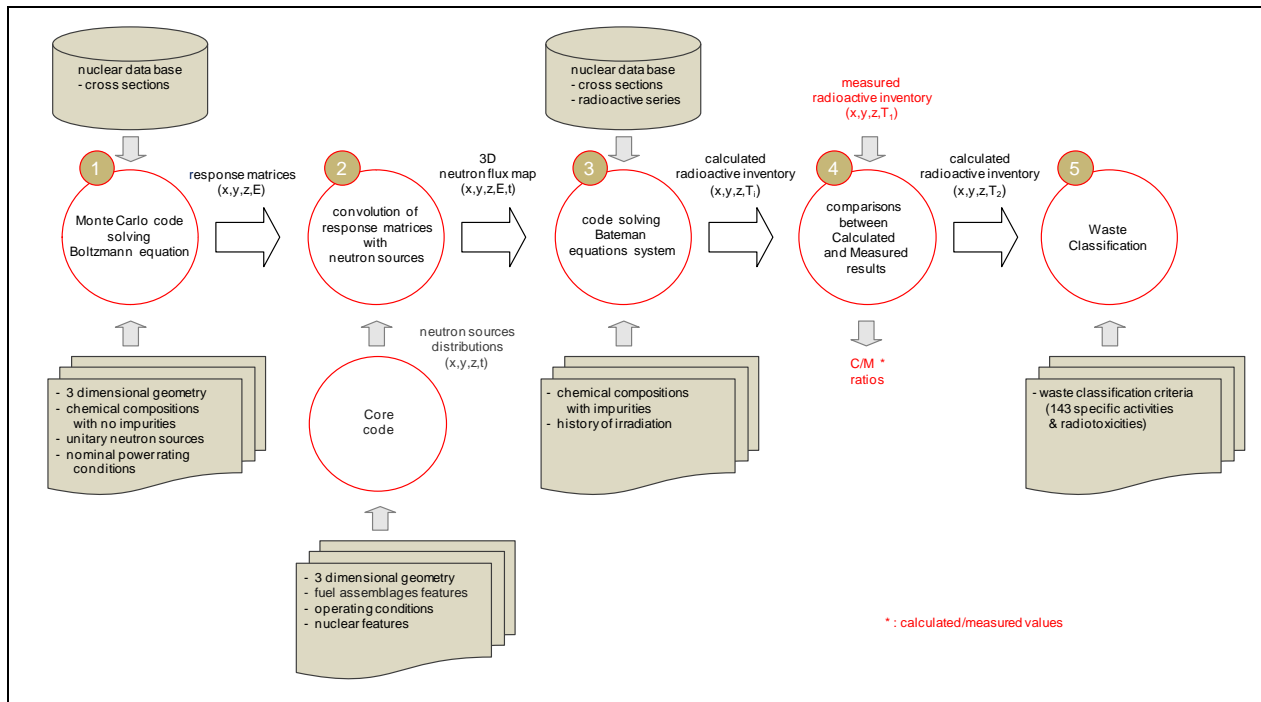

FIGURE 1
Numerical activation scheme based on Green's Functions

RESULTS

This paper uses the example of "Bugey 2", a "900 MW" PWR plant.

Principal hypothesis of the simulations

A 3-dimensional geometry was taken into account in the Monte Carlo code to compute the mapping of the neutron source contributions (see Figure 1, step 1). Depending on the tally localization, the fuel assemblies are described pin by pin or homogenized. If the propagation distance is high ($\gg$ 1 meter) the fuel must be homogenized to reduce the simulation time and the output data size. Therefore, the array fuel assemblies are homogenized for calculations concerning the vessel. In the same way regarding the control rods, the bottoms of the fuel assemblies are homogenized. All the internals are fully described 3-dimensionaly, including the different plates, the control rods and the guide tubes. The security absorbers are fully extracted from the core, whereas the control rods are partly extracted from the core (i.e. lower boundary operating zone). Three temperatures are defined for the primary water (core inlet, fuel assembly zone, core outlet).

The neutron sources calculated with a core code (see Figure 1, step 2) are given pin by pin according to axial distributions.

The isotopic compositions are reduced to the major chemical elements to calculate the neutron flux because impurities or traces do not affect the neutron propagation code (see Figure 1, step 1). However, to calculate the activation (see Figure 1, step 3), it is necessary to use the complete chemical compositions including impurities and traces as these minor impurities could directly impact the waste classification.

The flux mapping is calculated at the nominal power rating conditions (see Figure 1, step 2) while the isotopic evolution uses the irradiation history (see Figure 1, step 3). However this history was simplified to a limited number of steps, corresponding to the fuel campaigns.

Responses to unitary source distribution

Figure 2 presents graphical outputs of contribution sources (i.e. response matrices) of a "900 MW" PWR peripheral control rod tally and a "900 MW" PWR vessel tally respectively. Every colored point corresponds to a neutron source. Red illustrates a high contribution, yellow a intermediate one and green a low one. To simplify the use of equation /11/, these matrices correspond to the propagation of unitary sources.

To reduce the size of the matrix $C_{0ik}(Z)$ (i.e. normalized source contributions), the fuel assemblies are partially homogenized. The level of homogenization depends on the tally considered. So for the vessel tallies all the internal fuel assemblies are homogenized whereas the peripheral fuel assemblies were described pin per pin. For the control rods the lower part of the fuel assemblies are homogenized whereas the upper part of the fuel assemblies are homogenized.
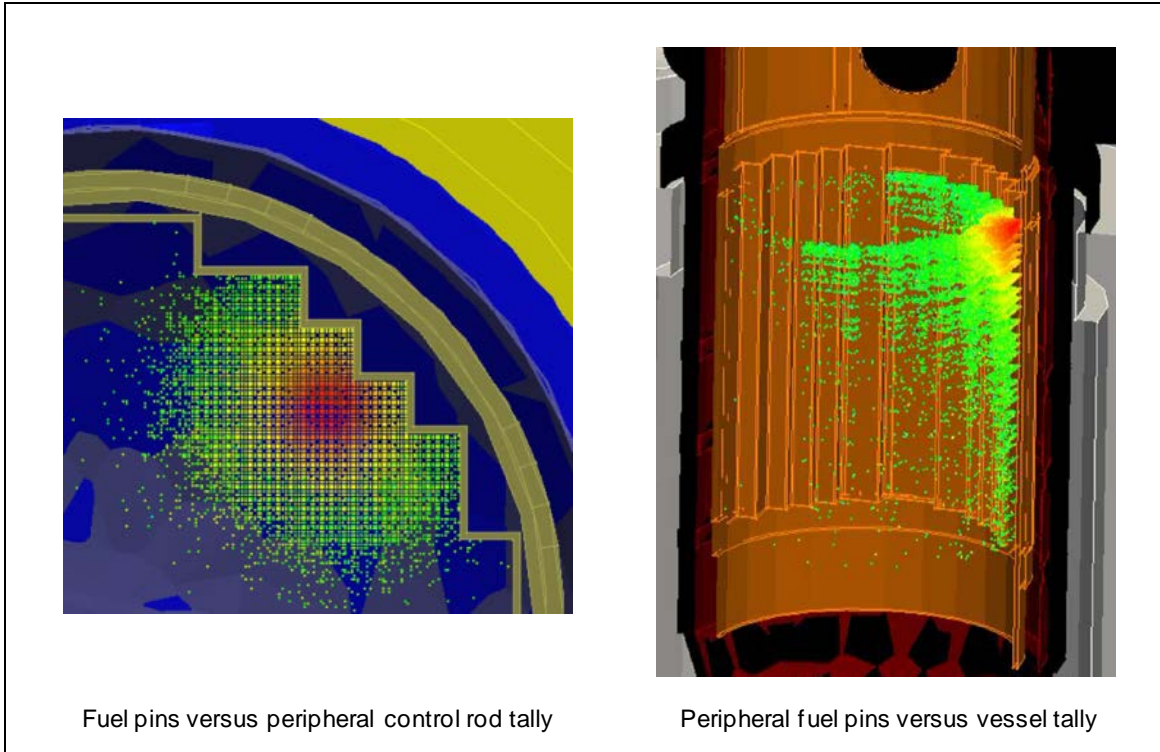
| Fuel pins versus peripheral control rod tally | Peripheral fuel pins versus vessel tally |

FIGURE 2
Graphical outputs of source contributions (i.e. response matrices)

Fuel assembly power distributions

Figures 3 and 4 illustrate our theoretical fuel assembly power distributions. Each corresponds to a specific fuel loading pattern (i.e. fuel assembly positions linked to a fuel campaign).

Typically at each refueling, up to one third of the fuel assemblies are replaced. Without going into the detail, for the first loading patterns the fresh fuel was disposed in the peripheral core positions (see Figure 3) and progressively irradiated fuel assemblies were disposed in the peripheral positions to reduce the vessel fluency (see Figure 4). Basically each fuel loading pattern is linked to a particular 3 dimensional power distribution. As the radioactive inventory is the result of the history of the different power distributions, each of the loading patterns must be considered for the simulations.

One of the features of the French fuel management is its flexibility. To optimize the dates of refueling, some plants stop before the normal end of the campaign, others stop normally and some stop after a stretch-out period. The consequence of this strategy is that the burn-up of the fuel assemblies changes for each fuel cycle. Also after each refueling, the power distribution changes, and it is necessary to use the real power distributions rather than the theoretical ones to make the simulations.
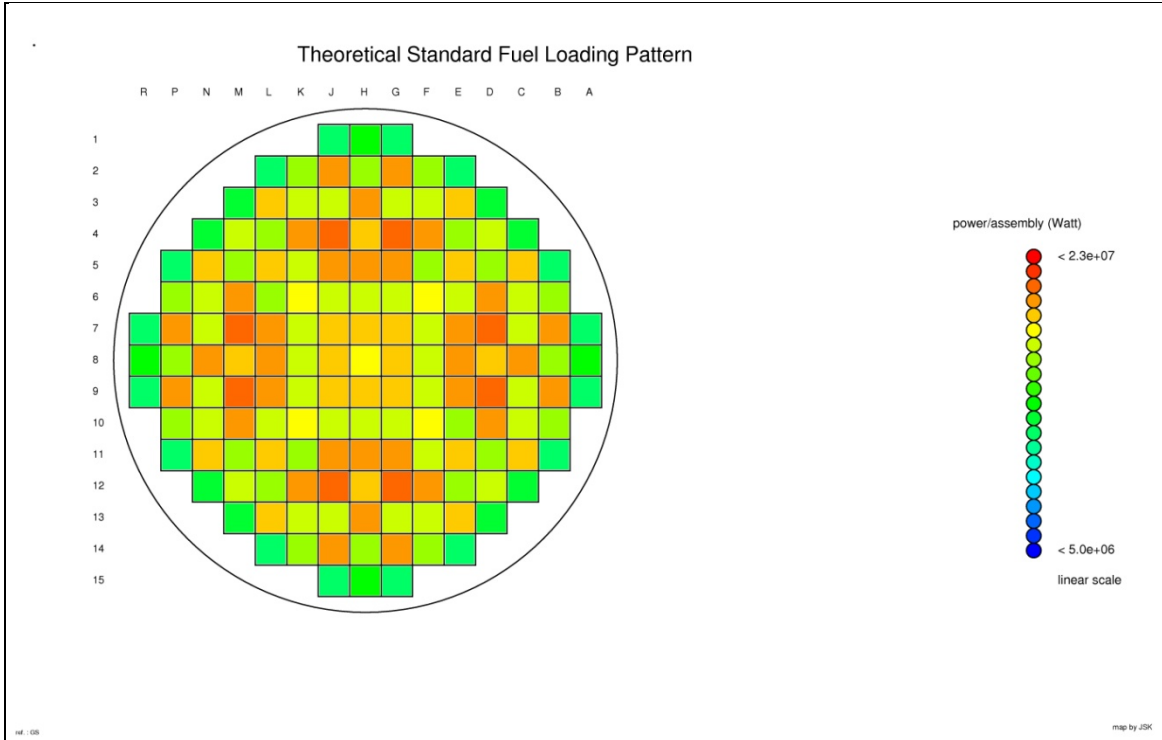
FIGURE 3
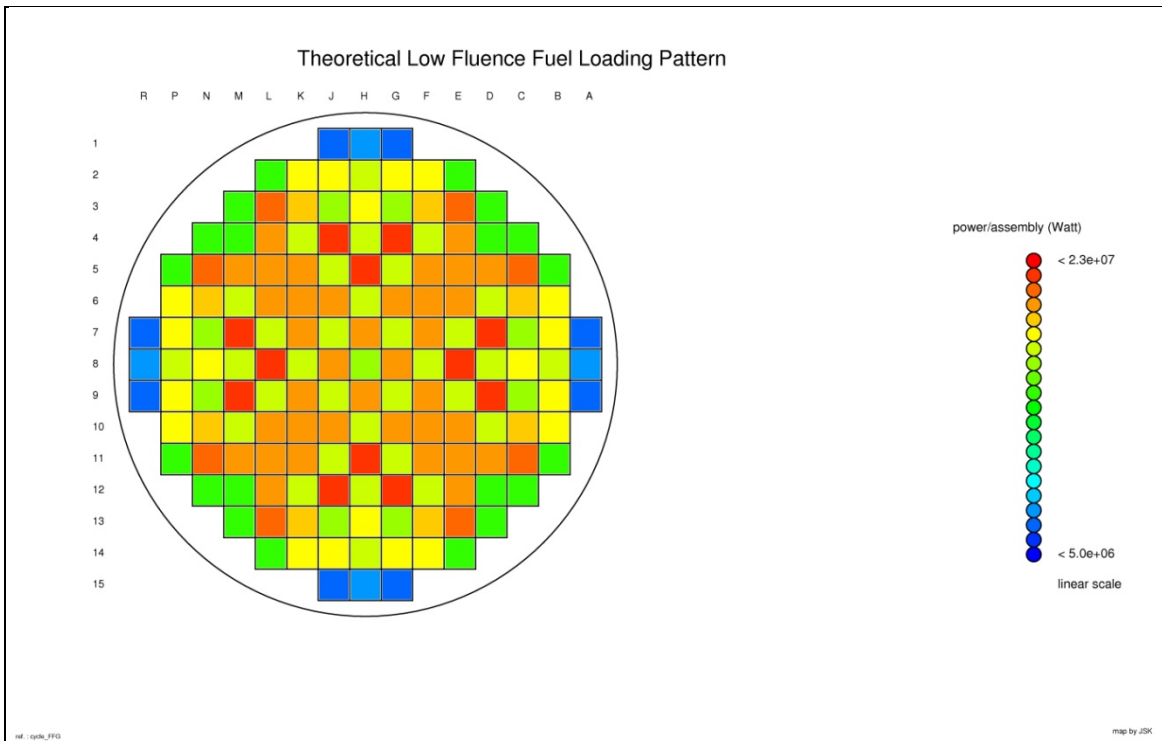*Power distribution of the "900 MW" PWR theoretical standard fuel loading pattern*

FIGURE 4
Power distribution of the "900 MW" PWR theoretical low fluence fuel loading pattern

Validation of the use of Green's Functions approach

An overall validation of the numerical simulation scheme can be made by using the activation of "standard" chemical elements (Ref. [1]). Certain criteria must be satisfied in order to qualify a chemical element as "standard" : high concentration, activation into large cross section range, low concentration uncertainties, production of radionuclide having significant half life (greater than several months) and no difficulties measuring the radionuclide produced.

The validation of the use of Green's Functions approach is based on the activation of "Bugey 2" control rods. "Bugey 2" is a "900 MW" PWR. Its control rods are composed of a mixture of "Silver", "Indium" and "Cadmium". "Silver" was retained as the "standard" chemical element, and the γ emitter measured by γ spectrometry is the Ag-108m ($T_{1/2}$ = 418 years).

The reason for our choice of control rods validation is that our PWR plants are still in operation. So the only possibility of validating the method is to use items that are irradiated in a limited period of time.

DISCUSSION

Comparison between calculated and measured values

Seven control rod storage cases were measured. Each case contained between 5 and 11 control rods. Before storage, the control rods were irradiated during 3 to 10 fuel cycles, in different core positions (i.e. radial positions), at different depths in the core (i.e. axial positions) and in different periods of time. All of these parameters were used in our simulations.

Table I provides the Calculated/Measured values (C/M) relative to the 7 measured cases. It can be noted that the numerical simulation produces a slight overestimation of the Ag-108m inventory (+30%).

Table I
Calculation/Measurement ratios

case n°	number of rods	average irradiation time [years]	average cooling time [years]	Ag-108m C/M
1	11	11	23	1.0
2	8	10	8	1.0
3	5	4	18	1.5
4	11	11	25	1.7
5	10	9	14	0.9
6	11	11	22	1.3
7	11	8	17	1.2
average value				**1.3**

The reasons for these overestimations are directly linked to the measurement uncertainties, the nuclear data uncertainties, the Monte Carlo statistical uncertainties and the hypotheses retained for the irradiation conditions history (like the position of the control rods, the temperature of the primary water, the average monthly power level, etc). However, it is difficult to give a weighting to each of these parameters.

Interest of using the Green's Functions

Whatever the method used (direct calculation versus Green's Functions approach), the 3D neutron flux maps are similar. This point is discussed in the Theoretical Background section of this paper. Numerical validations were also made through several MCNP simulations using both approaches.

The main interest of the Green's Functions is the calculation of response matrices based on unitary sources that can be used for all power distributions, enabling a reduction in the MCNP computing time. In fact, the use of Green's Functions in our calculation scheme allows us to carry out parametric studies where the aim is to determine the incidence of a source variation on the neutrons flux. A reference simulation performed once, is used to compute response matrices. These matrices are then convoluted with the different neutron source distributions to obtain the neutron flux.

Table II shows CPU times (i.e. Central processing Unit) needed to calculate the fluxes of our nuclear fleet considering respectively direct Monte Carlo calculations and then the use of Green's Functions. In the case of Bugey 2 (one reactor associated with 40 fuel loading patterns), the direct Monte Carlo calculations would need approximately 7 years compared with 4 months using the Green's Functions. I think these values speak for themselves. As the Green's Functions are made with unitary sources, the response matrices are completely independent of the fuel loading patterns, and they can be used whatever the power distribution.

Table II
MCNP CPU time period for approximately 100 tallies per reactor

type of reactor	number of reactors	number of power distribution maps *	MCNP CPU time	
			direct calculations	Green's Functions
900 MW	1 **	40 / reactor	~ 7 years	4 months
900 MW	34 (fleet)	40 / reactor	~ 200 years	4 months
1300 MW	20 (fleet)	40 / reactor	~ 100 years	4 months
1450 MW	4 (fleet)	40 / reactor	~ 30years	4 months

* : i.e. number of fuel campaigns per reactor   ** : i.e Bugey 2

It can be noted that the Green's Functions approach is useful whenever the number of the power distribution maps is greater than 2. It can also be noted that the CPU time depends on the number of tallies and the statistical uncertainties targeted.

The use of the Green's Functions approach enables the limitation of the Monte Carlo neutron propagation simulations. Even though the EDF nuclear reactor fleet consists of 58 PWRs, it is necessary to make just 3 simulations, 1 per type of design (i.e. "900 MW", "1300 MW" and "1450 MW").

CONCLUSION

Knowing the radionuclide content of radioactive waste is of utmost importance for safety and waste management reasons. Numerical simulations are used by EDF-DP2D to anticipate dismantling and radioactive waste management.

The main numerical activation schemes include the computing a 3 dimensional neutron flux map obtained on the basis of a neutron propagation calculation. The codes used solve the transport equation called the Boltzmann equation, without simplification. The main drawback of the Monte Carlo codes is the large computing time needed to converge within acceptable statistical criteria. This computing time is incompatible with the multiple fuel campaigns used by EDF to operate its NPPs because a Monte Carlo calculation is necessary for each fuel loading pattern.

The use of Green's Functions in our calculation scheme allows us to conduct parametric studies where the aim is to determine the incidence of a source variation on the neutron flux. A reference simulation performed once, is used to compute response matrices. These matrices are then convoluted with the different neutron source distributions to obtain the neutron flux.

The Green's Functions approach was validated by the activation of "Bugey 2" control rods. "Bugey 2" is a "900 MW" PWR plant. The numerical simulation produces a slight overestimation of the Ag-108m inventory (+30%). This overestimation is not linked to Green's Functions but to the other parameters like to the measurement uncertainties, the nuclear data uncertainties, the Monte Carlo statistical uncertainties and the hypotheses retained for the irradiation conditions history (like the position of the control rods, the temperature of the primary water, the average monthly power level, etc).

The main interest of this approach is to reduce computing time without loss of quality for the results. Even though the EDF nuclear reactor fleet consists of 58 PWRs (resulting in 34 "900 MW", 20 "1300 MW" and 4 "1450 MW"), it is necessary to make just 3 simulations, 1 per type of design.

The next steps will be :

- to repeat the same procedure on the other "900 MW" materials, that means the vessel, the internals including the different plates, the guide tubes, and the in-core instrumentation.
- to expand the validation to our other types of pressurized water reactors.

The final goal will be to obtain the same overestimation levels as those observed for the "Bugey 2" control rods presented here.

REFERENCES

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