A Review of History Parameters in LWR core nalysis

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I. INTRODUCTION

The use of nodal methods has allowed in the past decades the development of very efficient core simulators to carry out 3D full core calculations for design and safety studies [1]. Major advances in homogenization and equivalence theory, which started from the late 70s, have provided the standard methodologies for modern nuclear computer codes [2, 3, 4, 5].

This work presents the standard methodologies of cross section preparation for the water-moderated nuclear reactors, which represent nowadays the majority of the power units operating worldwide. Specific attention is devoted to the history effects occurring during normal operation, such as control rod withdrawal after a prolonged insertion or other temporary situations where the exposure history may imply significant changes in the local isotopic content and in the neutron spectra.

A review of the different techniques suggested in literature to account for the history effects is here reported. A few topical cases provided by the OECD-NEA Burn-up Credit Criticality Benchmark, Phase-IID, are used to evaluate their performances [6]. A discussion about the implementation effort is also addressed in the conclusion.

II. FEW-GROUP CROSS SECTION MODELS

In general, core calculations are performed on coarse meshes and the thermal-hydraulic feedback is ensured by a few-group cross section model through non-linear iterations. The typical size of the cells (often called nodes) of the spatial mesh is about 10 cm, whereas the most used energy mesh employs only two groups with a cutoff energy of 0.625 eV. The few-group cross section model provides indeed the cross sections (XS) and the possible additional equivalence factors, like the assembly discontinuity factors for instance, homogenized in the coarse nodes and condensed in the few-group energy scheme. This entails a projection on the region R and on the energy group G of the cross section $\sigma_{X,G,R}$:

$$\sigma_{X,G,R} = \frac{\int_G \int_R (\sigma_X \phi)(\mathbf{r}, E) \mathrm{d}\mathbf{r} \mathrm{d}E}{\int_G \int_R \phi(\mathbf{r}, E) \mathrm{d}\mathbf{r} \mathrm{d}E}, \qquad (1)$$

where X stands for each reaction type of interest (fission, absorption, scattering, etc.)

The neutron flux ϕ used to produce the few-group constants comes from idealized 2D neutron transport calculations reproducing lattices of single or multiple fuel assemblies arranged in a periodic environment. Specifically, single assembly calculations with the white or the reflection boundary conditions are used to prepare data for all different types of fuel assembly loaded in the core plan, whereas calculations in detailed environments of multiple assemblies (colorset calculations) are quite common for the reflector modelling. The critical condition is achieved by a leakage model, although possible underestimation of fast neutrons has recently been underlined [7].

Since the tracking of all existing nuclides present in the reactor would prevent depletion calculations along fuel exposure due to an unaffordable computational effort, only a limited amount is considered with the introduction of reduced depletion chains. These have been enriched with more isotopes as long as the computational resources increased in time, showing now up to 150 isotopes in industrial calculations and yielding accurate fuel inventories. All actinides are generally accounted for, as well as the most important fission products and burnable absorbers.

In order to represent all possible reactor conditions at operation or in accidental situations, homogenized data are functionalized by means of given 'state parameters', which are selected according to their influence on the neutron reactivity, being reactor-dependent as well. Common choices of state parameters for water reactors show the thermo-dynamic properties of the coolant, as for instance the moderator temperature and/or its density, covering subcooled convection, nucleate boiling and di-phasic heat exchange, an average fuel temperature over the pins within the hosting node to reproduce the Doppler effect, the amount of ^{135}Xe at equilibrium with the power level, the burnup or exposure in EFPD and the amount of boron PPM diluted in water. Of course, these state parameters are expected as output quantities of other models employed in the core calculation to reproduce the coupled physics, i.e. the thermal-hydraulics and the isotopic depletion models.

Ordinarily, the core codes treat second order forms of the transport equations for neutrons, and SP_N solutions have become quite popular. Although its physical validity holds generally to asymptotic regimes, it can always yield a diffusion solution at the order 1 (with the P1-diffusion coefficient of $1/3\Sigma_{tr}$). Node-averaged macroscopic XS are the input data of the nodal equations. The amount of isotopes in the sum over the microscopic XS characterizes further the XS model. Early core codes, bound by limited memory constrains and with the strict need for computational savings, used to parameterize only macroscopic XS with just a few particularized isotopes, like ^{135}Xe and ^{135}I [8, 9]. By omitting the group G and the reaction type X, this means:

$$\Sigma = \Sigma^{ref}(\mathbf{p}) + \sum_{i=1}^{I} \sigma_i^{ref}(\mathbf{p})(N_i - N_i^{ref}(\mathbf{p})), \qquad (2)$$

with a small I, $\mathbf{p}$ as the vector of state parameters and the superscript *ref* for data computed by the lattice calculations. As more isotopes are treated explicitly by a core depletion model, a redefinition of the model is demanded to avoid the tabulation of all isotopes in $\mathbf{N}^{ref}$. This is the current choice of modern few-group cross section models, showing a unique residual material that lumps all minor isotopes, untracked by the code depletion solver. Eq. (2) becomes then:

$$\Sigma = \Sigma_{res}(\mathbf{p}) + \sum_{i=1}^{I} \sigma_i(\mathbf{p}) N_i, \qquad (3)$$

where the superscript *ref* is removed since now pointless. Recently, schemes like in Eq. (2) have been proposed again for homogenized pin-by-pin codes, due to the higher amount of data necessary with respect to classic quarter-assembly calculations [10].

The XS computed by lattice calculations are then stored in external data libraries to be accessed later on at core calculations. According to the specifications of the few-group cross section model, these libraries may contain other coefficients determined by smoothing the XS data with numerical polynomial-like fitting techniques. Provided an integer N of values per parameter and M state parameters, N^M calculations may be requested to map the XS space laying in $\mathbb{R}^M$, raising the problem of the curse of dimensionality. This last reveals in a considerable amount of data to store and calculations to run, increasing with both N and M, and rapidly preventing the feasibility of its implementation. The combination of projected maps in smaller subspaces is often adopted to overcome this limitation. This ends in tabulation with three state parameters at most, with the goal of describing dedicated operating conditions, as base load at hot full power, core shutdown and cold condition states, xenon transients while maneuvering, or others. The selected projections are mainly driven by experience or trial and error approaches.

The wide range of possible reactor states are estimated as perturbed conditions with respect to a reference configuration all along the fuel exposure, so that 'branch calculations' are derived from a 'base depletion history', where the only evolving parameter is the burnup (or fuel exposure). The other parameters are fixed at their 'nominal' values, being the most probable values during the entire fuel cycle. In fact, the weighting neutron spectra ϕ depends on the exposure history, and the nominal conditions ought to be the most reasonably representative of the average core history for attaining an accurate cross section representation.

Consideration of several base depletion histories is instead a very common feature for BWRs, due to the severe change of void fraction throughout the core's height and permanent controlled fuel assemblies on the lower region [11, 12, 13]. About PWRs, a single base history is usually chosen for the relatively short insertion periods of control elements at power operation. However, the need of load following capabilities has called for more controlled core patterns in PWRs, especially in France where the electrical power production is largely coming from nuclear power plants. And in addition, it is possible to remark as general trend in the design of new PWR units enhanced control by gray banks permanently inserted or with prolonged insertion, with the goal of reducing the operational costs of the chemical shim [14,15]. These innovations may need the introduction of more base histories in the cross section models of PWRs, motivating further the reason of this work.

Whenever temporary deviations from the nominal conditions are noticed along the real exposure observed in the nodes of the core calculations, the conditions of the local spectra may get farer from those simulated a priori at XS preparation. Prolonged insertion is just an example of these deviations, since controlled assemblies are only modelled with instantaneous insertion at given burnup values, and the flux used at depletion neglects any rod insertion. Unfortunately, this kind of situations are rather frequent in real calculations, and may generate considerable error in extreme cases as shown by Tomatis et al. [16] Eventually, it follows the need of history parameters to avoid unphysical XS modelling.

III. HISTORY PARAMETERS

The few-group data is affected by the neutron spectrum used at condensation and homogenization. In turn, this spectrum follows from self-shielded XS obtained with the current fuel inventory. Hence, the local spectral conditions can be influenced by the history incurred by the assembly prior to the considered time. This requires the introduction of the history parameters, in addition to the customary instantaneous ones.

In a thermal reactor, the depleting spectrum acts directly on the amount of fissile material, affecting the reactivity evolution. A harder spectrum promotes mainly savings of ^{235}U and ^{239}Pu by lowering the flux in the thermal groups, while keeping almost unchanged the plutonium production. It follows that the same target burnup is achieved with longer exposure in time, thus with a different isotopic history.

A standard approach from the literature to reproduce the history effects derives new parameters $\bar{X}$ as burnup-average quantities of the corresponding instantaneous parameters X, as:

$$\overline{X}(Bu) = \frac{\int_0^{Bu} X(Bu')\mathrm{d}Bu'}{\int_0^{Bu} \mathrm{d}Bu'}. \qquad (4)$$

For instance, the thermo-dynamic properties of the fuel or of the moderator are rigorously instantaneous parameters p (moderator density, control rod, fuel temperature, etc.) from which new historical parameters p_h can be defined. Although the burnup itself follows as integration in time of a reaction rate, fixing a depletion history, we do not consider it as a history parameter. The void fraction is not following the definition of Eq. (4), since it changes naturally with the different base histories.

Provided linear independence of all the state parameters in the model, the general functionalization of a XS becomes $\sigma(Bu, p, p_h)$. Many industrial code simulators show tabulations

extended to history parameters, like SIMULATE-4 [17], ARCADIA [18], NECP [19] or the applications of corrective terms determined numerically by empirical correlations, like in POLCA [20] or studied by Mosteller [21].

The introduction of the history parameters needs new base depletion histories to still allow the construction of a Cartesian domain. However, branch calculations may not be requested for all the base calculations, depending on the mapping strategy of the state parameters space. Of course, the choice is driven by feasibility reasons according to the available resources, as usual. For instance, the size of the data libraries for core calculations is estimated of the order of several Gb and even if a single lattice calculation is in the order of minutes, the library production time may become promptly prohibitive for the industrial workframe. It is also been frequently assumed that changes of the cross sections induced by the spectral variations are independent of the phenomena that caused it, in order to ease the implementation of the additional base histories.

In particular, for PWR modelling, the spectral history (*SH*) has been mentioned in several publications [22, 23, 24] being defined through the integration in the burnup of the ratio between the actual Spectral Index *SI* and the reference one SI_N from the base calculation:

$$SH = \frac{1}{Bu}\int_0^{Bu} \frac{SI}{SI_N}\mathrm{d}Bu' . \qquad (5)$$

The spectral index in the two-group model is the ratio of the fast flux to the thermal flux, $SI = \phi_1/\phi_2$. For example, in some early works (e.g. the NEREUS code), the macroscopic XS were corrected with quadratic terms of the kind $\Delta\Sigma_h = \sum_{i=0}^{2} a_i(Bu)(SH-1)^i$ [24].

Different definitions of the spectral index are noticed in literature, as

$$SI = \frac{\Sigma_{c1}}{\Sigma_{a1} + 0.5(\Sigma_{s12} + \Sigma_{s12}^{ref})} \frac{\Sigma_{c1}\phi_1}{\Sigma_{f1}\phi_1 + \Sigma_{f2}\phi_2}, \qquad (6)$$

with Σ_a, Σ_f and Σ_c respectively as absorption, fission and radiative capture XS. The first factor determines the probability of radiative capture of fast neutrons, basically temperature-dependent in the fuel, while the second factor estimates the production of plutonium normalized to the total energy production [25, 26].

An interesting work by Bilodid et Mittag uses relative differences of ^{239}Pu concentrations as history parameter [27]. This option was implemented in the code DYN3D [28]

$$\sigma = \sigma_{ref}(Bu, p)(1 + k(Bu)\Delta Pu^9 / Pu_{ref}^9),$$

$$k(Bu) = \frac{\sigma - \sigma^{ref}}{\sigma^{ref}} \frac{\sqrt{N_{Pu}^{ref}}}{\sqrt{N_{Pu}} - \sqrt{N_{Pu}^{ref}}}, \qquad (7)$$

where the coefficient *k* is obtained from at least two depletion histories. This technique does not undergo modifications when changing the adopted multi-group scheme.

The SCIENCE code package by Framatome used the ratio of total plutonium over ^{238}U to recover the spectral effects [29]. An off-nominal base history at a different moderator density allowed a linear fit for a correction term applying to the standard output of the data-table interpolation.

Instead of a burnup-average value, the code PHOENIX/ANC used the spectral index evaluated at HFP and HZP,

$$\sigma = \sigma^{ref}(Bu, p)\, f(SI / SI^{ref}), \qquad (8)$$

where the function *f* was a second order polynomial whose coefficients came by ordinary least square regression. This correction was applied only to the fission and to the absorption thermal XS of ^{235}U and ^{239}Pu [30]. The model was later enhanced to correct also the fast group data [31], and is reported in the Westinghouse's core package NEXUS aimed at general LWR simulation [32, 33].

I. Validation on topical cases

A few cases from OECD-NEA Burn-up Credit Criticality Benchmark (Phase-IID) are used in this section to validate the main history parameters introduced in section III. Other situations where the spectral effects are caused by varying moderator conditions, like at core inlet or outlet, are also reproduced by means of the same cases.

The results will be presented in the final paper.

II. Discussion

A discussion of the results obtained from the calculations with the tests of the different suggested history parameters will be addressed in this section.

Finally, the section will end with general remarks and with technical comments about the implementation of the different history parameters analyzed in this work.

III. Conclusion

A discussion of the results obtained from the calculations with the tests of the different suggested history parameters.

A. Appendix: lattice calculation

In this study, the APOLLO2 code [34] considers the Burn-up Credit Criticality Benchmark [6]. The flux calculations were performed using 281-group cross section library based on JEFF-3.1, with the step option of the MOC flux solver and the P_3 anisotropic scattering. The trajectories along which the MOC solves the balance and transmission equations were defined using the following parameters: parallel trajectories spacing equal to 0.05 cm, with the angular quadrature of product type, where the azimuthal spacing was π/24, with three polar angles following the Legendre quadrature between 0 and π/2. The depletion calculation is performed using the predictor–corrector scheme based on parabolic extrapolation /interpolation, while solving the Bateman equations with the fourth order Runge–Kutta method. At each depletion step the flux is recalculated with the new self-shielded cross-sections and the convergence is guaranteed by imposing a criterion of r = 0.025 as relative difference of isotopic concentrations and the

values of depletion matrix between the predictor and corrector steps.

The recommended self-shielding options of APOLLO2, based on Livolant-Jeanpierre formalism are used [35], [3]. Self-shielding is done for all actinide isotopes, the main fission products and the constituents of the cladding, burnable absorber pins and control rods: ^{107}Ag, ^{109}Ag, ^{110}Cd, ^{113}Cd, ^{241}Am, ^{243}Am, ^{nat}Cr, ^{133}Cs, ^{153}Eu, ^{nat}Fe, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{160}Gd, ^{115}In, ^{95}Mo, ^{143}Nd, ^{145}Nd, ^{nat}Ni, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{103}Rh, ^{101}Ru, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{99}Tc, ^{234}U, ^{235}U, ^{236}U, ^{238}U and ^{nat}Zr, where *nat* denotes the chemical elements with the natural isotopic abundances [36]. The options for the treatment of the resonance interferences (resonant mixtures model) are chosen for ^{235}U, ^{238}U, ^{239}Pu and ^{240}Pu. The B_1 fundamental mode is set as leakage model to obtain a critical flux for the depletion calculation [3].

The typical discretization that accurately reproduces the spatial variation of the effective cross sections due to self-shielding effect and the isotopic concentrations during the cycle, comprises the four annular regions in an ordinary fuel pin that contains different macroscopic XS. In the case of gadolinium bearing pins the pin volume is divided into eleven equivolumic rings. A typical spatial mesh of the MOC flux calculator is presented in Fig. 1.

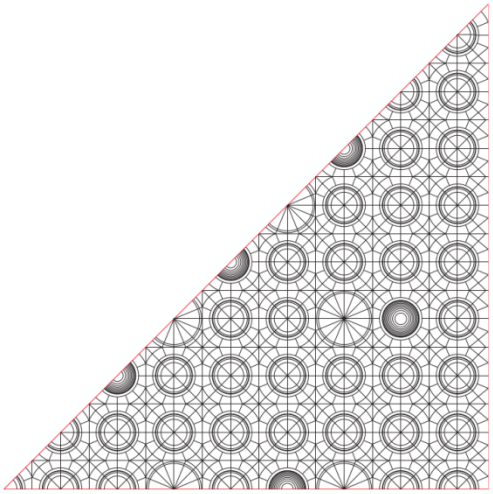

Figure 1. Spatial mesh of the MOC solver on a gadolinium assembly. One eighth of a 17 × 17 cell symmetric assembly is calculated.

Each ring of the pins depletes independently, while the sets of four (or eleven) self-shielded cross sections are shared between the pins that are gathered into groups according to pin position and environment. The number of different groups (self-shielding fuel pins) vary then between 5 for the simple UO_X assembly without control rods nor gadolinium pins, to 13 for gadolinium assembly.

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