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I. Ovdiienko, M. Ieremenko,
A. Kuchin, V. Khalimonchuk

State Scientific and Technical Center for Nuclear and Radiation Safety, Kyiv, Ukraine

Development of Cross-Section Library for DYN3D Code

At present time SSTC NRS uses the HELIOS code for generation of few-group cross-section libraries for WWER core calculations.

There is an actual problem choosing the appropriate approach to implement the cross-section library into the DYN3D code. The paper overviews the application of approaches used by SSTC NRS, such as a multidimensional table and polynomial dependences. The capabilities and possible extension of each approach are described with inherent advantages and disadvantages. In addition, the model development and cross-section preparation for the WWER-1000 radial reflector taking into account discontinuity factors are discussed. Brief results of calculations with the use of different approaches are presented.

Keywords: WWER; cross-section library; fuel assembly; reflector.

Ю. М. Овдієнко, М.Л.Єременко, А. В. Кучин, В. А. Халімончук

Розвиток бібліотеки нейтронно-фізичних констант для коду DYN3D

На даний час ДНТЦ ЯРБ використовує спектральний код HELIOS для підготовки малогрупових бібліотек нейтронно-фізичних констант тепловидільних збірок (ТВЗ) активних зон ВВЕР. У процесі розробки моделей ТВЗ виникає актуальна проблема вибору правильного підходу до реалізації бібліотеки констант у коді DYN3D. У даній роботі надано результати досліджень підходів, що використовує ДНТЦ ЯРБ, — реалізації бібліотеки у вигляді багатовимірної таблиці й поліноміальних залежностей. Розглянуто підходи ДНТЦ ЯРБ до вирішення проблеми розробки моделі та підготовки нейтронно-фізичних констант радіального відбивача для ВВЕР-1000 з урахуванням факторів розривності. Наведено короткі результати розрахункових досліджень при використанні різних підходів.

Ключові слова: ВВЕР; нейтронно-фізичні константи; тепловидільна збірка; відбивач.

The DYN3D code is widely used at SSTC NRS in licensing activities both for steady-state calculations in reviews of safety substantiation for fuel reloading and transient calculations for emergency modes of WWER reactors of Ukrainian NPPs.

Since 2006 SSTC NRS has been using the modern spectral HELIOS code for preparation of few-group cross-section libraries instead of the out-of-date one-dimensional NESSEL code. It allowed SSTC NRS to increase the accuracy in calculations of the entire complex DYN3D/cross-section library.

The basic parameterization of cross-sections in DYN3D is given in the following way:

$$\Sigma = \Sigma_0 \left\{1 + \alpha_s \left(\frac{1}{\sqrt{T_{\text{mod}}}} - \frac{1}{\sqrt{T_{\text{mod},0}}}\right)\right\} \times$$
$$\times \left\{1 + \beta_{s,1}\left(\gamma_{\text{mod}} - \gamma_{\text{mod},0}\right) + \beta_{s,2}\left(\gamma_{\text{mod}} - \gamma_{\text{mod},0}\right)^2\right\} \times$$
$$\times \left\{1 + \delta_{s,1}\left(C_b\gamma_{\text{mod}} - C_{b,0}\gamma_{\text{mod},0}\right) + \delta_{s,2}\left(C_b\gamma_{\text{mod}} - C_{b,0}\gamma_{\text{mod},0}\right)^2\right\} \times$$
$$\times \exp\left\{\gamma_s\left(\sqrt{T_f} - \sqrt{T_{\text{mod}}}\right)\right\},$$

where Σ is the actual cross-section; Σ_0 is the reference cross-section; α_s, $\beta_{s,1}$, $\beta_{s,2}$, $\delta_{s,1}$, $\delta_{s,2}$, γ_s are parameterization coefficients; T_{mod}, T_f, γ_{mod}, C_b are actual thermophysical parameters; $T_{\text{mod},0}$, $\gamma_{\text{mod},0}$, $C_{b,0}$ are parameters of reference state.

Each parameterization coefficient is represented as a second-order polynomial dependence versus fuel burnup B, as $P_i = P_{i,0}*(1+\alpha_{i,1}B+\alpha_{i,2}B^2)$.

In general, results with use of the basic parameterization of cross-sections are quite acceptable besides the reactivity coefficient on moderator temperature; particularly on hot zero power states where it shows low absolute values and relative errors more than 100 %.

The significant drawback of the basic cross-section library parameterization is the impossibility to use discontinuity factors. The use of discontinuity factors for WWER-1000 fuel assemblies does not have a significant effect. However, the cross-section for the radial reflector without discontinuity factors gives too high discrepancy in power distribution that can reach up to 10 % for peripheral assemblies. This occurs because the HELIOS library for fuel assemblies uses old parameterization for the radial reflector in which cross-sections were additionally adapted by auxiliary program for application without discontinuity factors.

Elaboration of basic XS parameterization. The parameterization was improved by adding the third-order polynomial dependence of moderator density β_3 and boron acid concentration δ_3.

$$\Sigma = \Sigma_0 \left\{1 + \alpha \left(\frac{1}{\sqrt{T_{\text{mod}}}} - \frac{1}{\sqrt{T_{\text{mod},0}}}\right)\right\} \times$$
$$\times \left\{1 + \beta_1\left(\gamma_{\text{mod}} - \gamma_{\text{mod},0}\right) + \beta_2\left(\gamma_{\text{mod}} - \gamma_{\text{mod},0}\right)^2 + \beta_3\left(\gamma_{\text{mod}} - \gamma_{\text{mod},0}\right)^3\right\} \times$$
$$\times \left\{1 + \delta_1\left(C_b\gamma_{\text{mod}} - C_{b,0}\gamma_{\text{mod},0}\right) + \delta_2\left(C_b\gamma_{\text{mod}} - C_{b,0}\gamma_{\text{mod},0}\right)^2 + \right.$$
$$\left. + \delta_3\left(C_b\gamma_{\text{mod}} - C_{b,0}\gamma_{\text{mod},0}\right)^3\right\} \times$$
$$\times \exp\left\{\gamma\left(\sqrt{T_f} - \sqrt{T_{\text{mod}}}\right)\right\}.$$

Additionally, the linear dependence of change in the moderator density with parameterization coefficients on boron acid concentration was introduced in form of $\delta_i = \delta_{i0} + a_{c_{ij}}(\Delta\gamma)$. The third-order polynomial dependence on fuel burnup $P_i = P_{i,0}(1 + \alpha_{i,1}B + \alpha_{i,2}B^2 + \alpha_{i,3}B^3)$ was also added.

The improved basic cross-section library parameterization allowed a slight increase in the accuracy of calculating the boron concentration and axial power distribution. However, the reactivity coefficient on moderator temperature remained unsatisfactory.

Further elaboration of the basic cross-section parameterization consisted in introducing the discontinuity factors and pin power distributions from the spectral code with the possibility to increase the calculation accuracy and extend the capabilities of DYN3D code.

XS library in form of multidimensional tables. The new cross-section library was prepared for WWER-1000 based on the OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark. This is a five-dimensional table of cross- section with dependence on burnup, moderator density, boron concentration, fuel and moderator temperature.

The accuracy of this multidimensional table cross-section library will depend on meshing of the whole range of thermo-hydraulic variables. The meshing should be based on balance between the error caused by linear interpolation of cross-sections and the reasonable total number of branch calculations that will define calculation time for library preparation. Based on this analysis, we chose 7 branches for moderator density, 4 branches for boron concentration and fuel temperature, and 3 branches for moderator temperature (Table 1). The total number of branches to cover the whole range of change in thermo-hydraulic parameter amounts to 336. Further meshing causes difficulties with calculation time for library preparation because adding of one branch increases the total number of branches by two times.

Table 1. Chosen parameters for multidimensional tables

№ burnup step	Burnup, MW× ×days/kgU	Moderator density, kg/m^3	Boron concentration, g/kg	Fuel temperature, K	Moderator temperature, K
1	0.0	200.0	0.0	293.0	293.0
2	0.5	400.0	4.0	793.0	563.0
3	1.0	500.0	8.0	1393.0	623.0
4	3.0	600.0	16.0	2593.0	–
5	6.0	700.0	–	–	–
6	9.0	800.0	–	–	–
7	12.0	1000.	–	–	–
...	...	Total 336 branches for different thermo-hydraulic parameters			
25	66.0				

Use of the multidimensional table cross-section library (with chosen parameters of branches) increases the accuracy of calculating neutron-physical characteristics of reactor core in comparison with the parameterization form of library, first of all accuracy of reactivity coefficient on moderator temperature at HZP (Table 2). It also covers the whole range of changes in core thermal-hydraulic parameters both for normal operation (hot and cold states) and for accidents with admissible accuracy.

Besides the much greater total number of calculating branches in comparison with the library with improved parameterization (336 vs. 44), this form of library has one more disadvantage. The use of multidimensional table library significantly increases the DYN3D calculating time — by approximately three times. Moreover, in some calculating cases, the iterations were not converged in contrast to the library with improved parameterization under the same convergence parameters.

Table 2. Reactivity coefficient on moderator temperature at HZP with different types of XS library

NPP unit and loading number	Experiment	BIPR	DYN3D (polyn. param.)	DYN3D (table param.)
KhNPP-2, loading № 1	−6.68(↓T) −7.38(↑T)	−6.93	−6.16	−5.41
KhNPP-2, loading № 2	−4.3	−5.73	−10.23	−6.47
KhNPP-2, loading № 3	−9.3	−9.16	−13.16	−9.40
KhNPP-2, loading № 4	−12.0	−11.10	−15.36	−11.65
ZNPP-1, loading № 22	−5.60	−4.23	−12.64	−8.96
ZNPP-1, loading № 23	−7.60	−5.54	−13.61	−9.96
ZNPP-1, loading № 24	−8.80	−9.09	−13.55	−9.66

Preparation of cross-section for radial reflector. The aim of preparing the advanced cross-section library for radial reflector is to increase the accuracy of power distribution in the core owing to more precise geometry of in-core components. Specifically, five different XS sets (Fig. 1) calculated by HELIOS were introduced into the library instead of one set in one-dimensional geometry calculated by the NESSEL code.

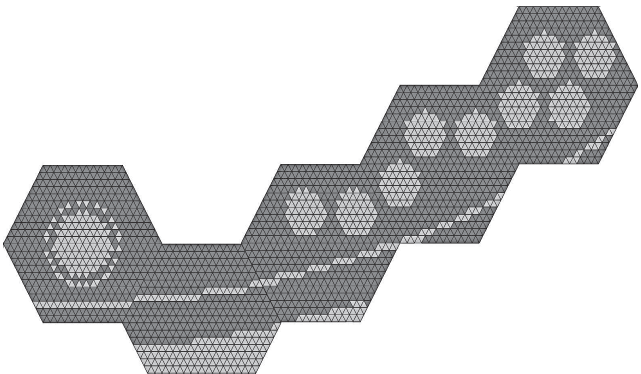


Fig. 1. Five reflector cells of advanced cross-section library for radial reflector

The advanced cross-section library for the radial reflector was supplemented with reflector discontinuity factors. The discontinuity factors were calculated by analytical solution of the

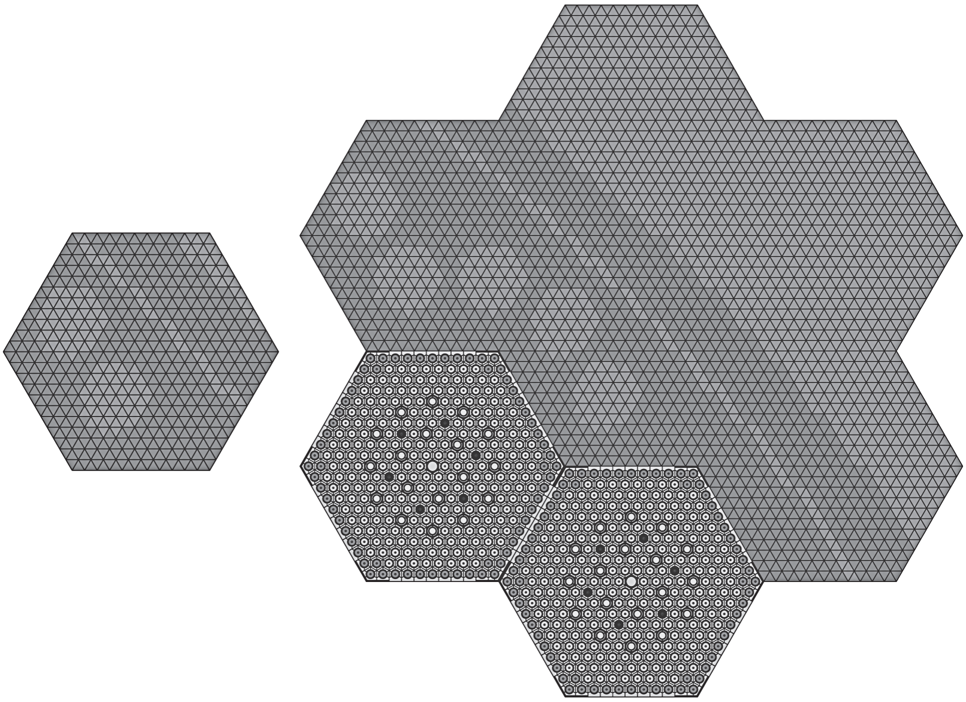


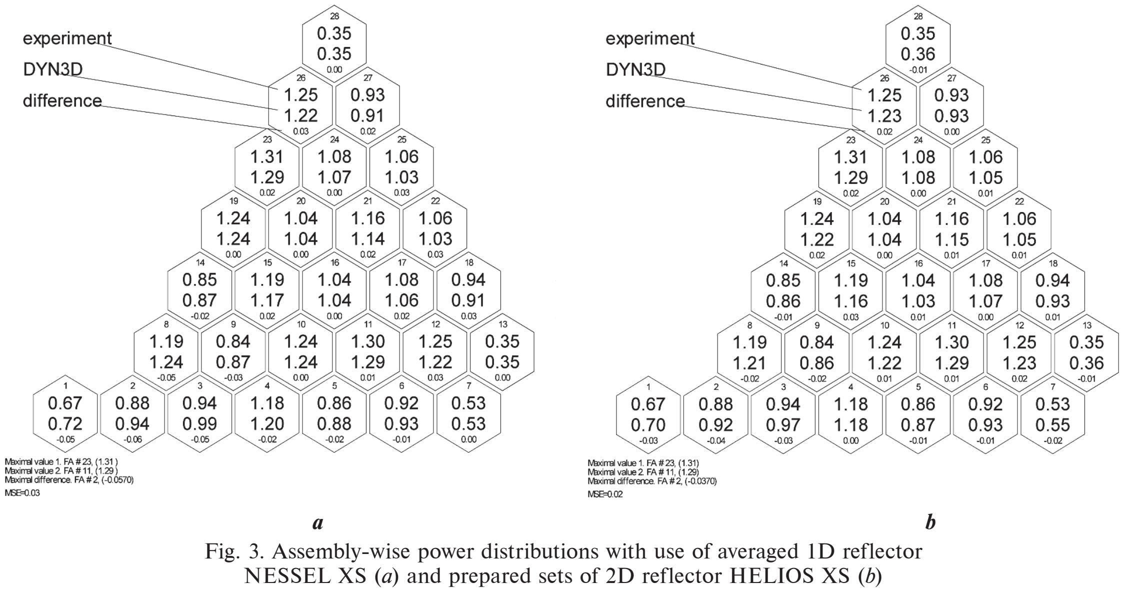
Fig. 2. One (third) cell of radial reflector and model with surrounded cells for HELIOS model

diffusion equation for two-dimensional hexagonal reactor geometry in non-multiplying material with the approach described in [4].

The model of each reflector cell for HELIOS calculations represents a macro cell of the considered cell surrounded by six neighboring ones, some of them (from 1 to 3) are fuel assembly cells (Fig. 2).

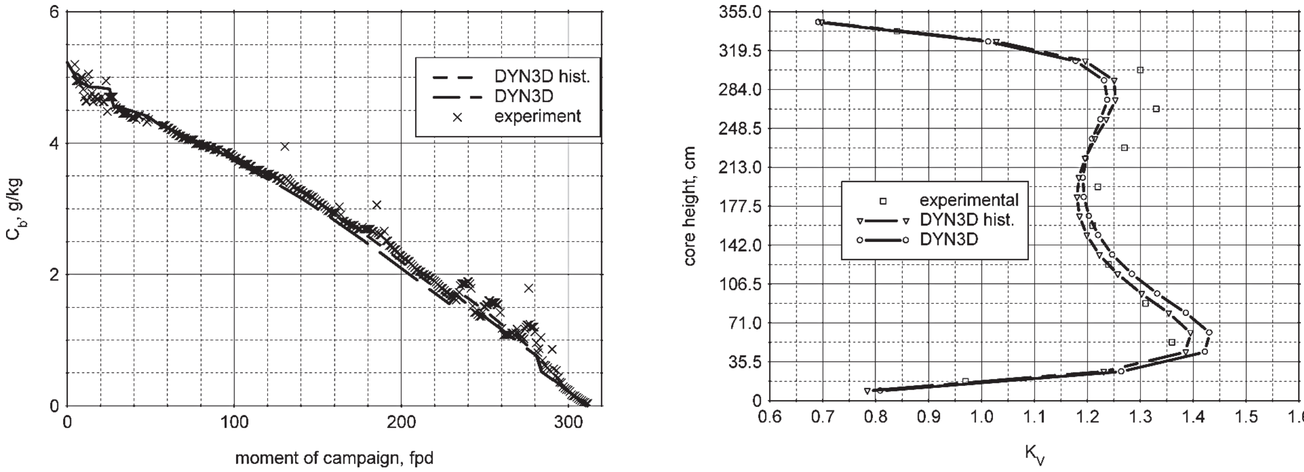
The RDFs calculated with the mentioned approach for introduction into the advanced cross-section for radial reflector were averaged over sides of the reflector cells neighboring the core. It is necessary to note that the cross-section with improved parameterization allows the introduction of RDF for each of the six hexagon sides.

Effect from the introduction of advanced cross-section for radial reflector was estimated for several fuel campaigns of Ukrainian NPPs. Typical assembly-wise power distributions with use of the averaged 1D reflector NESSEL XS and prepared sets of 2D reflector HELIOS XS are presented in Fig. 3. As follows from the figure, the prepared sets of XS do not only increase the accuracy of power distribution for peripheral assemblies, but also decrease its maximal discrepancy near the core center (for the case from $\delta k_q = 0.057$ up to $\delta k_q = 0.037$).



a ***b***

Fig. 3. Assembly-wise power distributions with use of averaged 1D reflector NESSEL XS (*a*) and prepared sets of 2D reflector HELIOS XS (*b*)



a ***b***

Fig. 4. Effect of accounting of spectral effect for boron acid concentration (*a*) and axial power profile in the most loaded FA (*b*) (AER-19 benchmark, first loading)

Accounting of historical effect. The multidimensional table cross-section library gives the possibility to take into account spectral effect during reactor core burnup calculation using the DYN3D code. The DYN3D code includes the approach for spectral effect accounting based on usage of plutonium-239 concentration as the spectral history indicator [5].

For this purpose, the multidimensional table cross-section library was supplement with an additional sub-library. The following parameters were prepared for the sub-library:

- ^{239}Pu and ^{238}U concentrations in standard depletion,
- microscopic cross-sections needed for ^{239}Pu calculation,
- history coefficients.

In the sub-library, these cross-sections and their historical coefficients are also given in multidimensional tables.

The consideration of spectral effect is quite appreciable already for the first fuel campaign, starting from zero fuel burnup (AER-19 benchmark, first loading, Fig. 4). The calculation accuracy increased not only for axial profile but also for boron acid concentration. The trend of distortion of axial power profile in the core upper part agrees well with results of direct accounting of spectral effect by moderator density for the fuel campaign presented in [6].

Conclusions

1. Use of the multidimensional table cross-section library (with chosen parameters of branches) increases the accuracy of calculating neutron-physical characteristics of reactor core in comparison with the parameterization form of library, first of all accuracy of reactivity coefficient on moderator temperature at HZP. It also covers the whole range of changes in core thermal-hydraulic parameters both for normal operation (hot and cold states) and for accidents with admissible accuracy.

2. The main disadvantages of the multidimensional table cross-section library include a much higher total number of calculating branches and worse convergence of iteration process, significantly increasing the DYN3D calculating time.

3. Introduction of advanced cross-sections for the radial reflector increases the accuracy of power distribution for peripheral assemblies and decreases its maximal discrepancy near the core center.

4. The accounting of spectral effect increases the calculation accuracy both for axial profile and for boron acid concentration and agrees with results of other approaches to spectral effect accounting.

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