MACROSCOPIC CROSS-SECTION PROCESSING FOR NESTLE CODE SYSTEM

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1. Introduction

The paper focuses on the development of macroscopic cross-section library for gas cooled fast reactor (hereinafter GFR 2400). Preparation of the appropriate neutronic library is a crucial part for 3D nodal neutron kinetics code simulators as PARCS or NESTLE [1]. The macroscopic cross-section data included in the libraries depends on multiple variables, e.g. fuel temperature, coolant temperature, coolant density, soluble absorber concentration or control rod insertion [2]. Nodal core simulators interpolate between these set of data points to obtain nodal parameters for instantaneous operational condition. SCALE sequence referred as TRITON is used to process macroscopic cross-section libraries [3, 4]. The NEWT deterministic code is called by the sequence TRITON to calculate the neutron flux in the investigated case. Finally, homogenized macroscopic multigroup cross-section library is prepared.

2. Geometry and Material Parameters

Currently, the development of GFR 2400 is in progress and the key material properties of the core design are under investigation. In the paper, the material properties are taken from literature [5, 6], where the authors were involved in GoFastR project [7]. The cross-sectional view of the fuel pin is shown in Fig. 1. Multiple material layers of cladding were homogenized for the purpose of faster convergence in deterministic code NESTLE (Fig. 2).

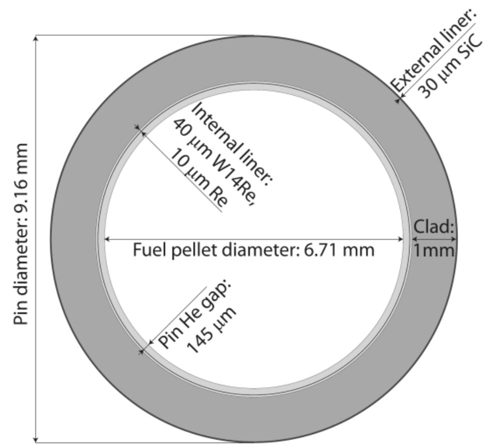

Fig.1: *Cross sectional view of the GFR 2400 fuel pin (height of the fuel pin - 165 cm) [5].*

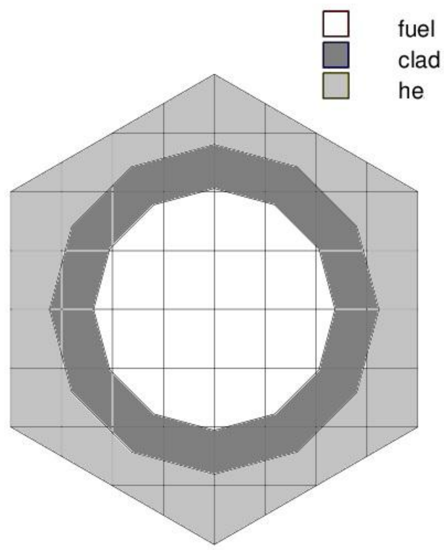

Fig.2: *Cross sectional view of the homogenized pin (lattice pitch - 11.57 mm).*

Mixture of uranium and plutonium carbide (U-PuC), with the average volumetric enrichment of Plutonium 15.84%, is used as the fuel material for the calculation of GFR 2400 core (more details are shown in Tab. 1). Main advantage of the carbide fuel is higher thermal conductivity in comparison with MOX fuel, which increases the heat transfer from the fuel to the coolant in the case of high power transient. However, the carbonization of the inner cladding wall may occur during fuel-cladding interaction. Therefore, thin W14Re and Re layer is included to prevent this effect. Moreover, refractory liners in the form of W14Re layer enhance the fission product retention of the cladding. On the other hand, this material introduces a significant neutronic penalty during normal operation. The cladding is made from reinforced silicon carbide (SiC_f/SiC). The main goal is to develop fully ceramic model which would satisfy all the ambitious GFR requirements. One of the most ambitious goal is the high temperature gradient in the ^{4}He coolant, which operates at the pressure 7 MPa, where inlet temperature is 400 °C and outlet temperature 780 °C. ^{4}He introduces practically no moderation to the GFR's neutron spectrum, making the GFR 2400 concept ideal for recycling all actinides, including minor actinides (MAs) [5].

The homogenous mixture of the cladding layers smeared with ^{4}He gap was prepared by a conservation of the volumetric mass fractions of the particular materials. The material composition of the homogenized cladding and the coolant is shown in Tab. 2. More information about the material properties can be found in former study [8].

The macroscopic cross-section processing by TRITON sequence is described in the next section.

Tab. 1. *Fuel material composition [5, 6].*

Fuel density [g.cm^{-3}]	10.9002
$\%_V$ in PuC	15.84
$\%_W$ in PuC	15.81
$\%_V$ in UC	84.16
$\%_W$ in UC	84.19
$\%_W$ Pu-238	0.4065
$\%_W$ Pu-239	8.4314
$\%_W$ Pu-240	3.8995
$\%_W$ Pu-241	1.1142
$\%_W$ Pu-242	1.0991
$\%_W$ Am-241	0.1054
$\%_W$ U-235	0.5770
$\%_W$ U-238	79.5684
$\%_W$ C-nat	4.7984

Tab. 2. *Coolant and cladding material composition [5, 6].*

Coolant density [g.cm^{-3}]	0.00487
$\%_W$ He-04	100
Pressure [MPa]	7
Homogenized cladding [g.cm^{-3}]	2.9579
$\%_W$ W-182	4.9824
$\%_W$ W-183	2.6942
$\%_W$ W-184	5.7989
$\%_W$ W-186	5.4380
$\%_W$ Re-185	1.9861
$\%_W$ Re-187	3.3588
$\%_W$ Si-28	48.7308
$\%_W$ Si-29	2.5611
$\%_W$ Si-30	1.7492
$\%_W$ He-04	0.0168
$\%_W$ C-nat	22.6838

3. TRITON model of GFR 2400

Cross-section data generated with TRITON/NEWT are used in a wide variety of applications, including generation of cross section library suitable for core calculations with NESTLE [3]. TRITON supports the ability to perform branch calculations during depletion calculations. Branch calculations allow for the quantification of changes in system responses of interest due to changes in system parameters [4].

The NESTLE treats macroscopic cross-section model as a Taylor series expansion in terms of coolant density, coolant temperature, effective fuel temperature and soluble poison density. Macroscopic cross-section is written in the form:

$$\hat{\Sigma}_{xg} = a_{1_{xg}} + \sum_{n=1}^{2} a_{(n+1)_{xg}} \left(\Delta\rho_c\right)^n + a_{4_{xg}} \Delta T_c + a_{5_{xg}} \Delta\left(T_{F_{eff}}\right)^{1/2} + \sum_{n=1}^{3} a_{(n+5)_{xg}} \left(\Delta N_{sp}\right)^n \qquad (1)$$

where $\hat{\Sigma}_{xg}$ represents a macroscopic cross-section for reaction type x and energy group g without transient fission products corrected to local conditions, $a_{j_{xg}}$ is an expansion coefficient, $\Delta\rho_c = \rho_c - \rho_c^{(0)}$ is a change in coolant density [g.cm^{-3}] from reference condition, $\Delta T_c = T_c - T_c^{(0)}$ stands for change in coolant temperature [°F] from the reference condition, $\Delta\left(T_{F_{eff}}\right)^{1/2} = \left(T_{F_{eff}}\right)^{1/2} - \left(T_{F_{eff}}^{(0)}\right)^{1/2}$ is a change in square root of effective fuel temperature [°F] from the reference condition and $\Delta N_{sp} = N_{sp} - N_{sp}^{(0)}$ represents a change in soluble poison number density [cm^{-3}.10^{-24}] from the reference condition [1]. Obviously, the dependency on soluble poison density is excluded for the case of ^{4}He coolant. The envelope formed by the branch conditions should cover the range of possible operational conditions [3]. The part of investigated states is shown in Tab. 3 for the GFR 2400 core.

The NEWT model of the investigated case was developed for proper macroscopic cross-section library processing by TRITON. The investigated geometry of 7 pins is shown in Fig. 3., where 20 coarse mesh intervals in each direction were used and 4 intervals were added to unstructured coarse-mesh finite-difference acceleration approach for the NEWTs convergence acceleration. The reflective boundary condition was assumed and the standard ENDF/B-VII.0-238 group library within the SCALE code package system was used for the NEWT calculation. Convergence criterion was set to the particular mixtures and for the eigenvalue ($\varepsilon_{keff} < 10^{-6}$). However, the absence of moderator had negative effect for inner iteration convergence, which was not established. Only the outer iteration process has converged. According to the list of branches in Tab. 3., the 2-group homogenized macroscopic cross-section library was prepared for NESTLE calculation by the TRITON sequence.

Tab. 3. *Calculation branches for GFR 2400.*

Fuel temp. [K]	Coolant temp. [K]	Density of coolant [g.cm^{-3}]
973.15	673.15	0.0049439
1073.15	773.15	0.0043126
1173.15	873.15	0.0038242
1273.15	973.15	0.0034350
1373.15	1073.15	0.0031177
1473.15	1173.15	0.0028540
1573.15	1273.15	0.0026314
1773.15	1473.15	0.0022763

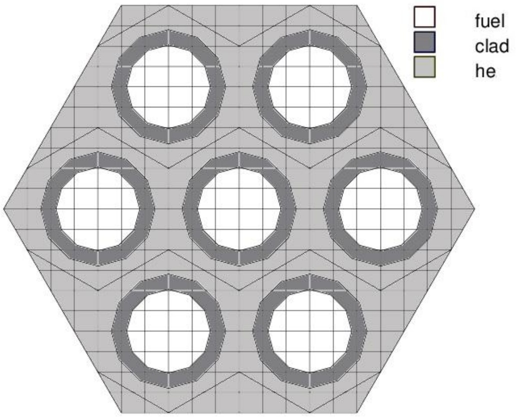

Fig.3: *7 pin geometry used for the macroscopic cross-section processing.*

The control model of the case in Fig. 3 was developed for KENO-VI Monte Carlo simulation to assess the deviation of the non-converged inner iteration in NEWT calculation. No corrections were applied for KENO-VI calculation and results of k_{eff} are shown in Tab.4.

Tab. 4. *Results of k_{eff} calculated by different software codes.*

	k_{eff}	σ
KENO-VI (v7-238)	1.22473	± 0.00077
NEWT (v7-238)	1.22349	-

4. NESTLE calculation of GFR 2400

The input data for NESTLE code were prepared from generated macroscopic cross-section library. The boundary conditions were set to *reflective* in radial direction and in axial direction to *zero flux*. The flowrate of the coolant at the pressure 7 MPa was set to 0.01083 kg.s^{-1} for one fuel pin and the reference power generation rate was 337.545 MW.m^{-3}.

The results of NESTLE calculation are compared with the former study [8], with the performed coupled CFD FlowVision calculation [9] with Monte Carlo code MCU, and with the study [6] (Fig. 4, Fig. 5 and Fig.6). Only small differences occur in axial temperature distribution of the coolant due to the same material properties with the same power generation rate within the fuel for all cases.

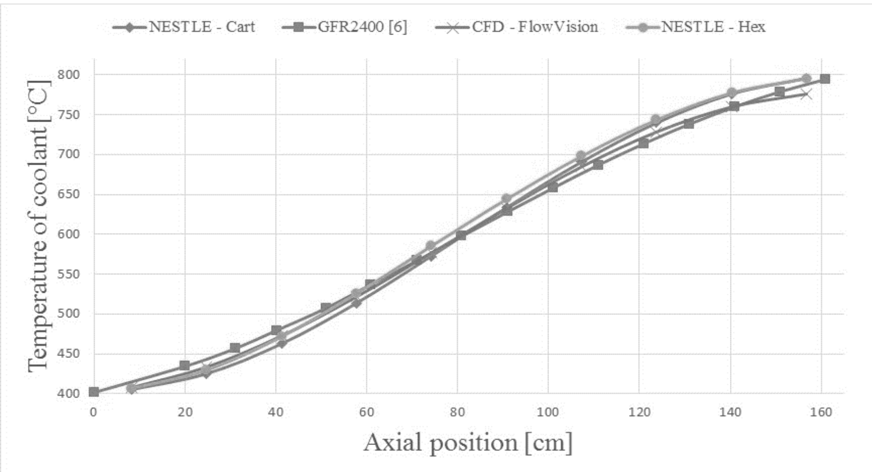

Fig.4: *Results of the coolant axial temperature distribution (Cart – the fuel pin is placed in rectangular lattice in NEWT simulation; Hex – the fuel pin is placed in hexagonal lattice).*

The axial offset of power generation peak in Fig. 5 is shifted to the bottom of the core. The possible reason is that the hexagon cell is more compact than the rectangular cell, thus the temperature increases more rapidly in the axial direction for the fuel (Fig. 6). All macroscopic cross sections are approximated in Eq. (1) with the linear function, however it must be noted that the relationship between instantaneous variables and neutronic parameters could not be simple; in fact, it is shown that they are mainly non-linear [10]. All performed simulations were calculated without the axial reflector and that is the reason of the deviation from the study [6] where authors calculated the model with the axial reflecting zones.

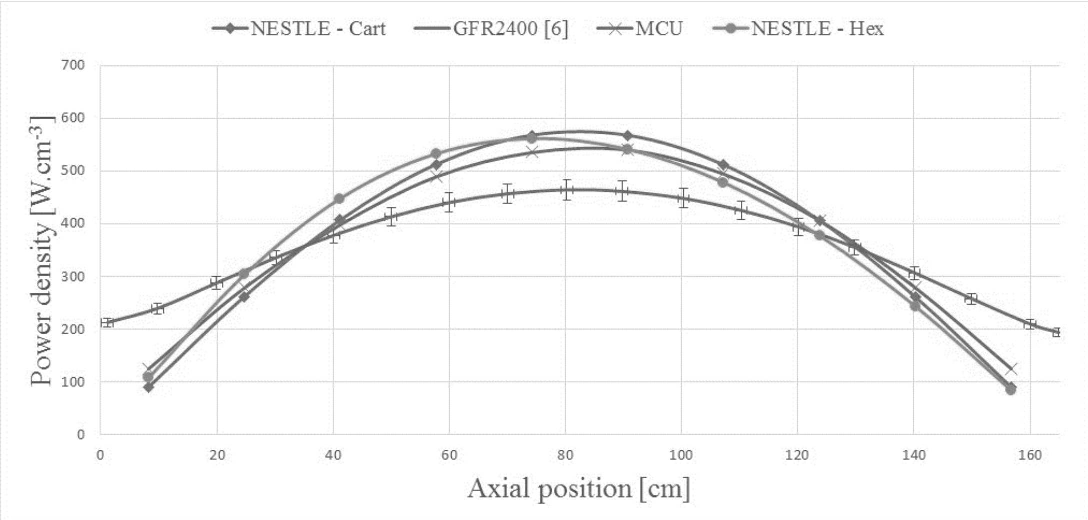

Fig.5: *Results of axial power distribution.*

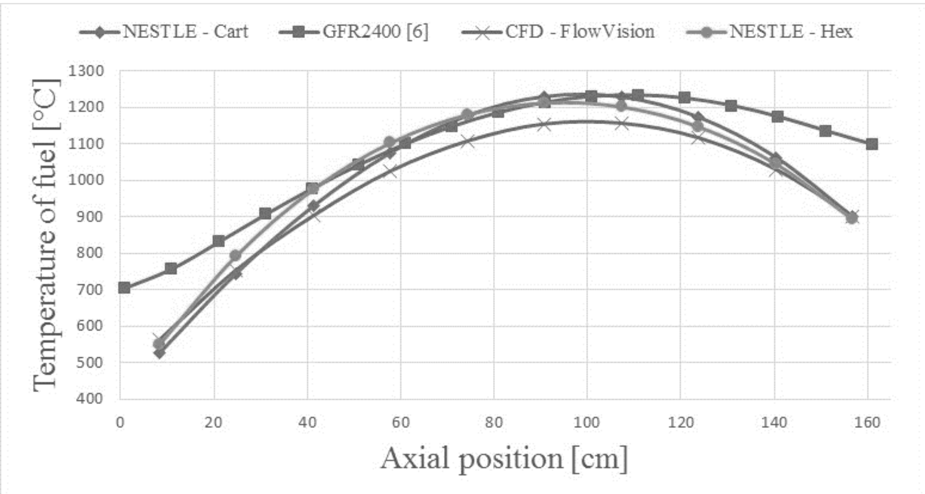

Fig.6: *Results of the fuel axial temperature distribution.*

5. Conclusion

The simplified model of the GFR 2400 fuel assembly is proposed in the paper. However, the performed calculation by deterministic code NEWT is not converging for the inner iteration step. The main reason is absence of the moderator in the model and this phenomenon has to be investigated in the future. The results of the NEWT calculation converge in outer iteration step, where the criterion is set to eigenvalue. The additional Monte Carlo simulation was performed by KENO-VI and the result of the k_{eff} in the NEWT calculation fall outside of the KENO-VI simulation with one sigma uncertainty. The homogenized multigroup macroscopic cross-section library was prepared by TRITON sequence for the 3D nodal neutron kinetics code simulator NESTLE. NESTLE calculation shows good agreement in the coolant axial temperature distribution. However, the new prepared library results in the axial shift of the power generation peak to the bottom of the GFR 2400 core.

The successful development of transient methodology calculation at the Institute of Nuclear and Physical Engineering (INPE) have potential to relevantly contribute to the nuclear safety in Slovakia. However, the first initial step is to prepare correct neutronic and thermal-hydraulic material models that are currently under investigation at the INPE.

Acknowledgement

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