Few group cross sections generation using MCU-PTR and Serpent for diffusion calculation of light water research reactor

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Abstract. Different methods of generating homogenized few-group cross sections using continuous energy Monte Carlo codes MCU-PTR and Serpent 2.1.27 for full core diffusion calculation of small-size light water reactor were studied. Few-group cross sections were used in core diffusion nodal simulator TIGRIS for the calculation of the simplified cores with fuel of CROCUS reactor and IRT-type reactor in light water reflector. Special attention is paid to the impact of diffusion coefficients on the results of diffusion calculation. Three different ways of diffusion coefficient generation were compared: usual “out-scatter” approximation, using of the hydrogen transport correction curve and migration area method.

1. Introduction
Many recent Monte Carlo codes have functionalities required for few-group cross sections (XS) generation. XS can be generated as in a unit cell or some colorset, as in full-scale reactor calculation with any complex geometry description. Few-group XS are then used in core diffusion simulator. Monte Carlo full-scale calculations also can be used as a reference solution. So generating few-group XS by Monte Carlo code allows for the estimation and reduction of the diffusion calculation errors because of group partition, leakage correction in unit cell calculation, cell environment modeling and diffusion coefficient definition, by the comparison with “exact” solution for the considered core without additional approximations of cell calculation.

This work is focused on few-group XS for small-size light water reactors (research reactors, LWR critical assemblies).

2. Models and codes
Model problems were calculated using continuous energy Monte Carlo codes MCU-PTR [1] and Serpent 2.1.27 [2]. Homogenized 4-group XS for the fuel assemblies (FA) and water reflector were generated (energy group boundaries – 10 MeV; 0.821 MeV; 5.53 keV; 0.625 eV). These XS were used in the calculations of the simplified cores with fuel of CROCUS reactor and IRT-type reactor in light water reflector using diffusion nodal simulator TIGRIS [4, 5].

For small-size light water systems with high neutron leakage diffusion coefficient calculation is an important problem [6, 7]. Serpent calculates the multi-group transport cross section using the “out-scatter” approximation as a default option, but since version 2.1.27 there is the possibility to use a
specific correction for the hydrogen transport cross section (TRC option). User-defined energy dependent transport correction curve represents the ratio of transport cross section to total cross section for this isotope. Correction procedure subtracts the non-corrected hydrogen transport cross section from transport cross section of a material mixture containing hydrogen, multiplies the total cross section for hydrogen with correction curve, and adds it back to the transport cross section of the mixture. This correction accounts for the anisotropic scattering for the hydrogen more appropriately than usual “out-scatter” approximation.

MCU-PTR calculates the diffusion coefficients from neutron migration area [8]. This parameter can be tallied directly in Monte Carlo simulation. In [9] it was demonstrated that similar procedure based on the cumulative migration method produces transport cross sections and diffusion coefficients consistent with the “in-scatter” approximation (with diffusion coefficients calculated directly by solving P1 equations).

3. Calculated results

3.1. Hydrogen transport cross section correction curve calculation
To calculate hydrogen transport cross section correction for Serpent, the infinite medium of light water with uniformly distributed fission source was modeled using MCU-PTR code. Transport cross section was calculated from neutron migration area. The calculated hydrogen transport cross section correction curve (transport cross section to total cross section ratio) is shown in figure 1. This curve is similar to the curve presented in [6].

![Figure 1. Transport cross section to total cross section ratio calculated using MCU-PTR code.](image)

3.2. Test problem with CROCUS reactor fuel
The model was built based on the assembly containing 16×16 fuel pins. The assembly fuel pitch is 1.837 cm loaded with UO₂ fuel (1.806 wt%-enriched) and light water moderated [7]. The core dimensions were 58.7 × 58.7 × 100 cm (width × length × height). The same reflector thickness (29.39 cm) was used and black boundary conditions were imposed in all three directions. Calculated neutron multiplication factor is shown in table 1. The results calculated using TIGRIS code are presented for three variants of XS: generated by MCU-PTR code, generated by Serpent code without TRC option, and by Serpent code with TRC option.
Table 1. Calculated results for the core 58.7 × 58.7 × 100 cm (2×2 FA).

| Code             | XS       | $k_{\text{eff}}$ | $\rho$, pcm | $\Delta$, pcm |
|------------------|----------|------------------|--------------|---------------|
| MCU-PTR          | -        | 1.06317          | 5942±20      | -             |
| TIGRIS           | MCU-PTR  | 1.0599           | 5651         | -291          |
| Serpent          | -        | 1.06677          | 6259±10      | -             |
| TIGRIS           | Serpent without TRC | 1.04825       | 4603         | -1656         |
| TIGRIS           | Serpent with TRC | 1.06615       | 6205         | -54           |

The difference in $k_{\text{eff}}$ between the diffusion and Monte Carlo calculation is 1700 pcm, 50 pcm and 300 pcm for the cases with the diffusion coefficients generated using “out-scatter” approximation (Serpent without TRC), corrected hydrogen transport cross section (Serpent with TRC), and migration area method (MCU-PTR), respectively. The results of the diffusion calculation with XS generated using Serpent code without TRC option and with TRC option are consistent with the results presented in [7].

3.3. Test problems for the core with IRT-3M fuel

The core with IRT-3M (LEU, 19.7 w/o, U-9%Mo) [10] fuel was considered. Two cores of 12 (3×4) and 16 (4×4) fresh FA were calculated (the core dimensions in horizontal plane were 21.5 × 28.6 cm and 28.6 × 28.6 cm, the core height was 58 cm). The same reflector thickness (29.39 cm) was used and black boundary conditions were imposed in all three directions. Calculated neutron multiplication factor is shown in tables 2 and 3.

Table 2. Calculated results for the core 28.6 ×28.6 × 58 cm.

| Code             | XS       | $k_{\text{eff}}$ | $\rho$, pcm | $\Delta$, pcm |
|------------------|----------|------------------|--------------|---------------|
| MCU-PTR          | -        | 1.0629           | 5916         | -             |
| TIGRIS           | MCU-PTR  | 1.0599           | 5650         | -266          |
| Serpent          | -        | 1.0642           | 6036         | -             |
| TIGRIS           | Serpent without TRC | 1.0077       | 762          | -5274         |
| TIGRIS           | Serpent with TRC | 1.0591       | 5583         | -453          |

Table 3. Calculated results for the core 21.5×28.6 × 58 cm.

| Code             | XS       | $k_{\text{eff}}$ | $\rho$, pcm | $\Delta$, pcm |
|------------------|----------|------------------|--------------|---------------|
| MCU-PTR          | -        | 0.9908           | -924         | -             |
| TIGRIS           | MCU-PTR  | 0.9886           | -1149        | -225          |
| Serpent          | -        | 0.9927           | -739         | -             |
| TIGRIS           | Serpent without TRC | 0.9333       | -7142        | -6403         |
| TIGRIS           | Serpent with TRC | 0.9870       | -1322        | -583          |

For the cores of the dimension of ~30 × 30 cm in horizontal plane and of 58 cm height, the difference in $k_{\text{eff}}$ between the diffusion and Monte Carlo calculation is up to 5000-6000 pcm for the cases with diffusion coefficients generated using “out-scatter” approximation. The using of the corrected hydrogen transport cross section or the migration area method enables to reduce this difference to 500-600 pcm.
Table 4 presents 4-group diffusion coefficients calculated using MCU-PTR code and Serpent 2.1.27 code for the core with 12 IRT-3M fuel assemblies.

| Group | MCU-PTR Water | MCU-PTR FA | Serpent with TRC Water | Serpent with TRC FA | Serpent without TRC Water | Serpent without TRC FA |
|-------|---------------|------------|-------------------------|---------------------|---------------------------|------------------------|
| 1     | 1.59          | 2.59       | 2.20                    | 2.30                | 3.05                      | 2.81                   |
| 2     | 1.03          | 1.06       | 0.92                    | 1.07                | 1.00                      | 1.13                   |
| 3     | 0.62          | 0.69       | 0.56                    | 0.75                | 0.55                      | 0.73                   |
| 4     | 0.15          | 0.23       | 0.15                    | 0.26                | 0.15                      | 0.26                   |

It should be noted that in the calculation of water reflector diffusion coefficients using MCU-PTR code by migration area method, the whole reflector of 29 cm thickness was selected as the tallied region. If the tallied region with the thickness of ~10 cm or less is selected, the diffusion coefficient of the first group (E > 0.821 MeV) may change significantly. Further verification of the reflector diffusion coefficients calculated by migration area method is necessary.

Also the impact of the cell environment on few group XS and the results of diffusion calculation was investigated. In the calculations described above, XS for the fuel and water were generated in the whole reactor calculations using MCU-PTR code and Serpent 2.1.27 code. In addition, XS for fuel were generated in single-assembly lattice calculation with reflective boundary conditions (BC). The difference in \( k_{\text{eff}} \) between the diffusion calculations with XS from the cell calculation and the whole reactor calculation is shown in Table 5. For the cores of the dimension of 28.6 \( \times 28.6 \) cm in horizontal plane and of 58 cm height, this difference is ~600 pcm. It means that fuel XS generation in infinite lattice is suitable for the considered core (for 4 group energy structure).

| Code    | Fuel XS                  | \( k_{\text{eff}} \) | \( \rho \), pcm | \( \Delta \), pcm |
|---------|--------------------------|----------------------|-----------------|-----------------|
| MCU-PTR | -                         | 1.0629               | 5916            | -               |
| TIGRIS  | MCU-PTR, whole reactor calculation | 1.0599               | 5650            | -266            |
| TIGRIS  | MCU-PTR, single FA with reflective BC | 1.0664               | 6227            | 311             |

4. Conclusion

4-group diffusion XS generated using MCU-PTR and Serpent 2.1.27 for small-size cores with IRT-3M fuel were tested. The difference in \( k_{\text{eff}} \) between the diffusion and Monte Carlo calculation is approximately the same for the cases with diffusion coefficients generated using Serpent code with TRC option and using MCU-PTR code resorting to migration area method. This difference is less than 600 pcm. It was shown that diffusion coefficients calculated by migration area method are suitable for the diffusion calculations of the cores with IRT-type fuel. Further investigations are needed for generating reflector (water, beryllium) XS by migration area method.

References

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