

# New cross section processing methodology for HFIR core analysis

Germina Ilas\*, Jess C. Gehin, R. T. Primm, III

*Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA*

---

## Abstract

The High-Flux Isotope Reactor is an 85 MW, very high flux reactor operated at the Oak Ridge National Laboratory to support neutron scattering experiments, isotope production, and materials irradiation research. As part of an ongoing engineering design study on the conversion of the reactor from the currently used, highly enriched uranium to a low enriched uranium fuel, work was initiated to develop a new cross section processing methodology. The aim of the study was to ensure an accurate representation of the cross section data for the fuel regions located near the edges of the fuel elements. These regions are characterized by larger in-leakage of thermal neutrons than other parts of the core and neutron flux spectra much different from the average flux in the fuel elements. The new methodology is based on the TRITON/NEWT sequence available in the SCALE code system that allows two-dimensional depletion calculations for arbitrary-mesh geometries. The new cross section processing approach is described and the available results are presented and discussed in this paper.

---

## 1. Introduction

The High-Flux Isotope Reactor (HFIR) is an 85 MW, very high flux reactor operated at the Oak Ridge National Laboratory (ORNL) to support neutron scattering experiments, isotope production, and materials irradiation research. The HFIR, a pressurized light-water-cooled and moderated flux-trap type reactor, is currently fueled with highly enriched uranium (HEU). The reactor core consists of a series of concentric annular regions: a central flux trap containing vertical experimental targets surrounded by two fuel elements separated by a thin water region, a region containing two control plates, a beryllium reflector, and a water region to the edge of the pressure vessel, which is located in a pool of water. An engineering design study of the

conversion of the HFIR from HEU to low enriched uranium (LEU) fuel is ongoing as part of an effort sponsored by the U.S. Department of Energy's National Nuclear Security Administration Global Threat Reduction Initiative to support the minimization and, to the extent possible, elimination of the use of HEU in civilian research or testing involving nuclear applications. The conversion should be accomplished so that both the reactor performance and the ability to achieve the facility's missions are maintained.

### 1.1. Background on the LEU conversion study

The HFIR core consists of two annular fuel elements composed of many 1.27 mm thick involute-shape fuel plates that are separated by

---

\* Corresponding author, [ilasg@ornl.gov](mailto:ilasg@ornl.gov)  
Tel: +01 (865) 241 4672; Fax: +01 (865) 574 9619.

coolant channels with 1.27 mm thickness, as illustrated in Fig. 1. The plates are a sandwich-type design, with a fuel region enclosed in an aluminium-based clad. The fuel region currently contains a mixture of aluminium powder and  $U_3O_8$  with 93 wt %  $^{235}U$  enrichment. The thickness of the fuel meat inside the fuel region varies (is graded) along the width of the fuel plate. The fuel meat is the region that will need to be changed when replacing the current HEU fuel with LEU fuel. Two types of high-density LEU fuels have been under consideration and studied: a uranium-molybdenum (U-Mo) dispersion (in aluminium) fuel (Ellis et al., 2007) and a monolithic U-Mo alloy fuel (Ellis et al., 2006). Given HFIR's unique design, high power density, and the requirement that the impact of the fuel change on the core performance and operation be minimal, the conversion from HEU to LEU constitutes a complex and challenging endeavor. Such a task requires improvements in and extensions of the computational methodologies and tools currently used to support the operation of the reactor. Details of the reactor configuration and operation and results of previous studies on the conversion to LEU can be found elsewhere (Primm et al., 2006; Ellis et al., 2006; Ellis et al., 2007).



Fig. 1. HFIR fuel elements.

### 1.2. Computational tools

The analysis of the HFIR core performance for an LEU fuel has been carried out in previous studies (Primm et al., 2006; Ellis et al., 2006; Ellis et al., 2007) using a set of computational tools that includes the MCNP code (LANL, 2003) and the SCALE (ORNL, 2006) and BOLD VENTURE (Vondy, 1981) code systems. BOLD VENTURE is a three-dimensional (3-D) multigroup diffusion

theory code with depletion capabilities that is used to obtain the power profile and the peak fluxes in the target and reflector regions for various initial fuel distributions. The ability to provide fast solutions, perform depletion calculations, and allow changes in the geometry during depletion (i.e., changes in the control element locations) make BOLD VENTURE a suitable tool to perform fuel grading scoping studies. As for any other multigroup diffusion code, the use of a good set of cross section data appropriate for the configuration to be simulated is essential for the accuracy of the results obtained from the calculation. The cross section processing methodology used previously for fuel grading studies is based on a set of modules in SCALE that perform resonance processing (BONAMI, NITAWL) and one-dimensional (1-D) transport calculations (XSDRNPM) based on a radial representation of the core. The use of these cross sections with the BOLD VENTURE model resulted in relatively large differences, between 5 and 20% (Ellis et al., 2006), in power density near the top and bottom of the fuel elements as compared with the data calculated with an MCNP model. These regions of the HFIR core can be particularly challenging because of the significant changes in flux spectra near the radial reflector and the light-water coolant above and below the fuel elements. However, calculation of physics parameters for such relatively small volumes at the edges of the core with Monte Carlo codes requires considerable time. Completion, in a short time frame, of the numerous iterative design calculations required in the optimization of any new reactor fuel design—especially one for a reactor with fuel plates in which the fuel varies in thicknesses—requires a deterministic solution method. Therefore, an improved methodology to obtain cross sections better representing these spectral changes is needed.

### 2. 2-D cross section processing methodology

Work on development of a new cross section processing methodology for LEU fuel configurations started recently, with the aim of ensuring a more appropriate representation of the cross section data for the fuel regions located near the edges of the fuel element. The new methodology is based on the TRITON/NEWT sequence available in SCALE, which allows two-dimensional (2-D) depletion calculations for arbitrary-mesh

geometries. This sequence couples the 2-D arbitrary polygonal mesh, discrete ordinates transport code NEWT to the point depletion and decay code ORIGEN-S. It is expected that the 2-D cross section processing approach will provide a better representation of the spatial dependence of the neutron flux. A better representation is especially important for the fuel regions at the top and bottom of the fuel elements. These regions are characterized by large leakage from fuel-bearing to non-fuel-bearing regions and neutron flux spectra much different from the average flux in the fuel element. Since coolant flow in HFIR is axial—top to bottom—improving the results of the BOLD VENTURE calculation also improves the accuracy of the thermal hydraulic analysis of the reactor core.

### 2.1. NEWT model

The 2-D NEWT model of HFIR represents an axial cross section of the reactor core that cuts the annular core into two equal halves. Due to symmetry, only one quarter of the axial cut is modelled, as illustrated in Fig. 2. Reflective boundary conditions are imposed on the left and bottom of the bounding surfaces, and vacuum boundary conditions are imposed on the other two edges of the configuration. As a first step, a simplified configuration is considered; no control elements or experiment targets in the beryllium moderator are included in the NEWT model. However, the fuel radial grading is modelled in detail, as used in the previous 1-D grading study (Ellis et al., 2006). Eight and nine radial regions of different fuel compositions to simulate the fuel grading are considered for the inner fuel element (IFE) and outer fuel element (OFE) in the core, respectively.

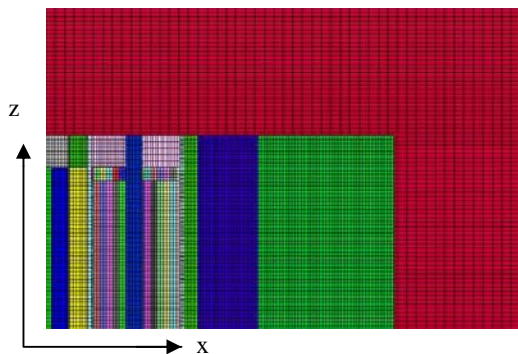


Fig. 2. 2-D NEWT model of HFIR.

For the purpose of cross section collapsing, multiple zones are specified in the axial direction for each fuel region with unique material composition. For each of the zones, NEWT calculates a zone-averaged neutron flux that is used to collapse the fine-group SCALE neutron transport cross section library to a few-group structure. Therefore, the effect of axial flux variation is included in the resulting microscopic cross sections as compared to the fuel element axially-uniform flux that is inherent in the 1-D cross section processing methodology. For simplicity, only two axial zones in the fuel elements are shown in Fig. 2. The actual model for generating cross sections used ten axial zones from the top to the center of the fuel element.

### 2.2. Verification of the NEWT model

A simplified three-dimensional (3-D) MCNP model of HFIR (relative to the complex model described in Primm, 2006), consistent with the NEWT model, was developed for comparison purposes. Continuous energy cross section data were used with MCNP whereas NEWT calculations employed a 238-group SCALE neutron transport library. Both sets of cross section data were based on ENDF/B-V nuclear data files. Trends in the thermal neutron flux and microscopic thermal fission cross section of  $^{235}\text{U}$  as a function of axial and radial location in the fuel element were determined using the 3-D MCNP model for a HFIR LEU configuration, with the purpose of establishing an optimum zoning of the fuel elements in the NEWT model for which cross section data are to be generated. All analyses in this work considered a monolithic U-10Mo LEU fuel with 19.75 wt %  $^{235}\text{U}$  enrichment.

A total of 170 tally regions were defined for the fuel elements in the MCNP model: 80 in the IFE (8 radial by 10 axial) and 90 in the OFE (9 radial by 10 axial). The thicknesses of the fuel regions in the axial direction are 0.5, 0.5, 1.0, 1.0, 1.4, 4.2, 4.2, 4.2, 4.2, and 4.2 cm from the top of the active fuel region to the core midline, for a total of 25.4 cm. The radii of the regions in the fuel elements and the material composition data for the LEU fuel are consistent with models used by Ellis et al. (2006).

The thermal (neutron energy  $< 0.625$  eV) flux variation along the axial direction for a constant radius, as obtained with MCNP, is shown in Figs. 3 and 4 for the IFE and the OFE, respectively. The radii specified in the figure legends for each of the

radial regions are outer radii; the radii for the left edge of the IFE and OFE are 7.14 and 15.15 cm, respectively.

The variations of the thermal flux as a function of radius for a constant axial location are presented in Figs. 5 and 6 for the IFE and OFE, respectively.

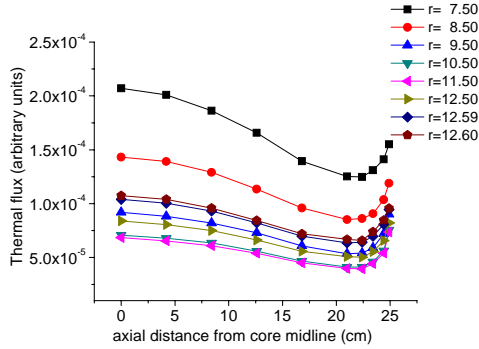


Fig. 3. Axial variation of thermal flux in IFE.

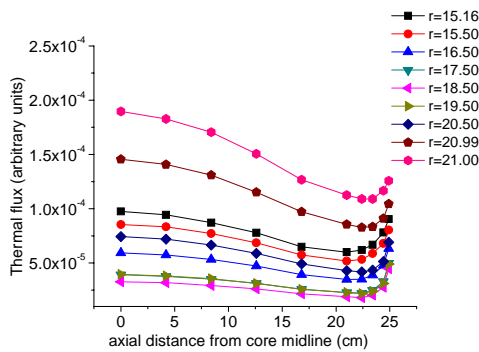


Fig. 4. Axial variation of thermal flux in OFE.

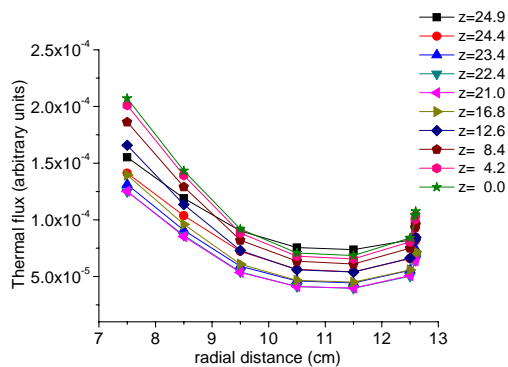


Fig. 5. Radial variation of thermal flux in IFE.

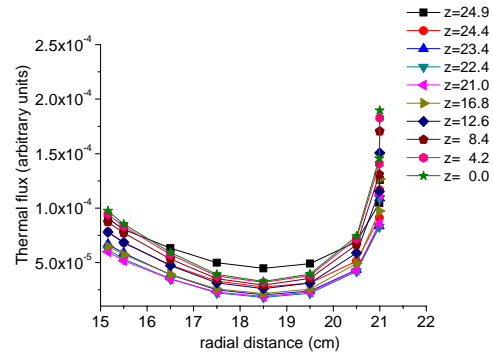


Fig. 6. Radial variation of thermal flux in OFE.

The axial data ( $z$  values) shown in the legends correspond to the lower edge of each axial layer.

An axial and radial zoning identical to that in the 3-D MCNP model was used in a corresponding 2-D NEWT model. The microscopic fission cross sections of  $^{235}\text{U}$  in the thermal energy range for each of the 170 fuel zones were calculated with MCNP by the use of F4 tallies. Corresponding results were obtained with NEWT by collapsing the microscopic fission data from the 238-group library using the problem-dependent neutron flux from the transport calculation. Comparisons of the data are illustrated as a function of the axial distance from the core midline for the first radial region of the IFE (7.14–7.5 cm) in Fig. 7 and for a central radial region of the OFE (17.5–18.5 cm) in Fig. 8.

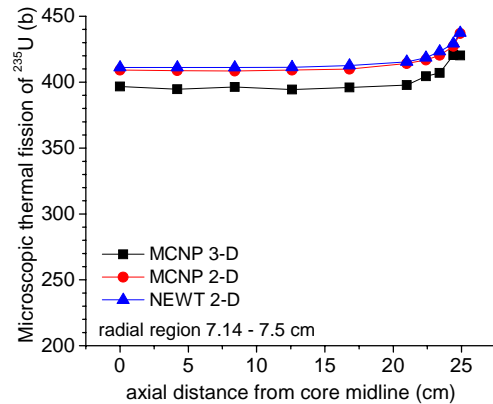


Fig. 7. Microscopic thermal fission cross section of  $^{235}\text{U}$  in IFE radial region 7.14–7.5 cm.

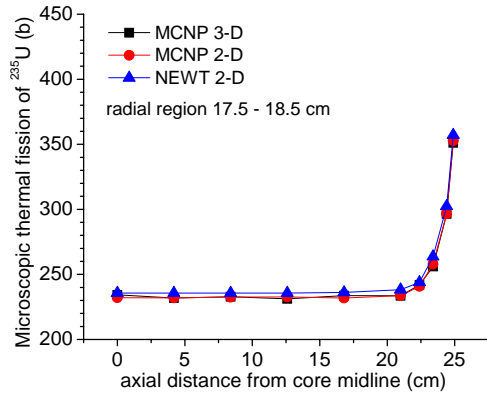


Fig. 8. Microscopic thermal fission cross section of  $^{235}\text{U}$  in OFE radial region 17.5–18.5 cm.

The comparison of the data obtained from the two models showed a good agreement in microscopic fission cross section data, the largest difference, of up to 4.5%, being in the radial region of the IFE interfacing the flux trap region. Good agreement was also observed for the multiplication constant ( $k_{\text{eff}}$ ) value:  $1.0865 \pm 0.0003$  for MCNP and 1.0788 for NEWT, the difference being about 0.7%. Part of the observed difference in the fission cross section was found to be inherent in the 2-D modeling due to the difference in leakage between a 3-D and a 2-D model; the configuration considered involves small radii zones, for which the difference in leakage between the two models would be higher than in a case involving larger radii. As illustrated in Figs. 7 and 8, the thermal fission cross section data obtained with the 2-D NEWT model are similar to the corresponding data obtained with a consistent 2-D MCNP model. A change of the radial dimension for the flux trap region was made in the NEWT model to ensure that the surface-to-volume ratio at the interface of the flux trap and the IFE was more consistent with that of the 3-D model and therefore could better approximate the leakage at the interface between the IFE and the flux trap. The change led to a decrease by about 1% in the difference in the fission cross section data for the inner radial edge of the IFE. As a result, the cross section variation in the radial direction throughout the fuel element showed a level of agreement similar to that for the axial direction.

### 3. Testing of the cross section data using a preliminary LEU fuel design

Preliminary testing of the NEWT-based cross section processing methodology was carried out for a HFIR configuration similar to that described in the previous section, which includes a simplified model, as compared to the real configuration, of the control element and target regions, but models in detail the fuel grading. The radial grading profile for the LEU fuel corresponds to one of the cases described by Ellis et al. (2006). The zoning of the fuel regions is similar to that presented in the previous section, but the widths of the axial layers are a little different in this case, with values of 0.5, 0.5, 1.0, 1.0, 1.4, 4.2, 4.2, 8.2, 3.2, and 1.0 cm from the top of the active fuel region to the core midline. Consistent 3-D MCNP, 2-D NEWT and 3-D BOLD VENTURE models were developed for this simplified HFIR configuration.

Multigroup microscopic cross sections were generated with the NEWT model for all nuclides in the problem for each of the 170 fuel zones. A SCALE 238-group neutron transport cross section library was used in the NEWT calculation. The flux that resulted from the transport calculation was used to collapse the cross section data to a 20-group structure, as shown in Table 1.

The 20-group cross section data were used in diffusion calculations with the BOLD VENTURE model (R-Z geometry). The power density data obtained from BOLD VENTURE were compared with the fission density profile obtained from the MCNP calculation. As expected, differences in power are larger in the fuel zones at the edges of the fuel elements (inner radial edge in IFE and top axial edge in IFE and OFE) that are characterized by large leakage and where the diffusion theory approximation may not be accurate. The differences in power density are illustrated in Figs. 9 and 10 for the IFE and OFE, respectively, as a function of the radial and axial regions. The radial regions are numbered with increasing radius, from 1 to 8 for the IFE and from 1 to 9 for the OFE. The axial regions are numbered from 1 to 10 with increasing axial location from core midline (0 cm) to 25.4 cm, which is the top of the active fuel region.

The largest differences, of about 10%, are observed for the fuel zones at the top left corner of the IFE. For the innermost radial edge of the IFE the difference decreases axially from 10% at the top to

Table 1  
Energy structure for cross section collapsing

| 20-group # | 238-group # | Lower energy (eV)     |
|------------|-------------|-----------------------|
| 1          | 12          | $2.48 \times 10^6$    |
| 2          | 15          | $1.50 \times 10^6$    |
| 3          | 25          | $8.75 \times 10^5$    |
| 4          | 45          | $8.50 \times 10^4$    |
| 5          | 63          | $2.58 \times 10^3$    |
| 6          | 86          | $9.00 \times 10^1$    |
| 7          | 116         | $2.75 \times 10^1$    |
| 8          | 132         | $9.10 \times 10^0$    |
| 9          | 149         | $2.97 \times 10^0$    |
| 10         | 163         | $1.68 \times 10^0$    |
| 11         | 190         | $9.75 \times 10^{-1}$ |
| 12         | 199         | $6.25 \times 10^{-1}$ |
| 13         | 205         | $3.75 \times 10^{-1}$ |
| 14         | 210         | $2.50 \times 10^{-1}$ |
| 15         | 215         | $1.25 \times 10^{-1}$ |
| 16         | 222         | $4.00 \times 10^{-2}$ |
| 17         | 226         | $7.50 \times 10^{-3}$ |
| 18         | 230         | $2.50 \times 10^{-3}$ |
| 19         | 232         | $1.50 \times 10^{-3}$ |
| 20         | 238         | $1.00 \times 10^{-5}$ |

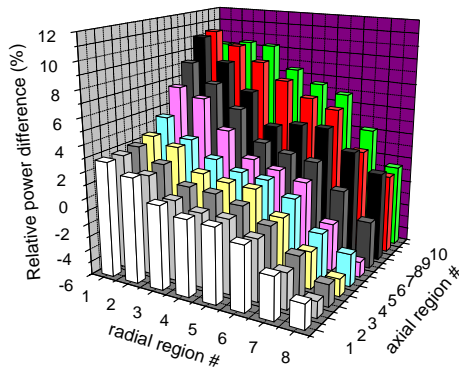


Fig. 9. Difference in relative power for the IFE.

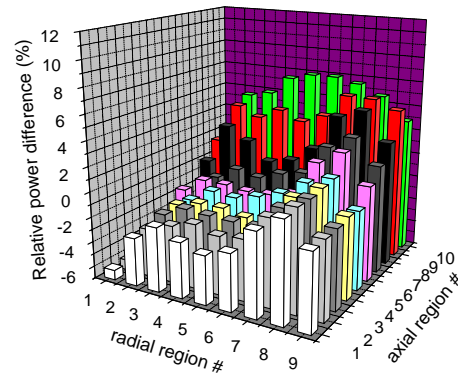


Fig. 10. Difference in relative power for the OFE.

less than 3% at the core midline. In the case of the IFE, the difference generally decreases with increasing radius for a constant axial location, with the exception of the outermost radial regions of the IFE that are close to the core midline. The axial layers (7–10) with larger differences correspond to the top 3 cm of the fuel element.

In the case of the OFE, the largest differences are seen in the top axial layer (up to 7%) and at the innermost radial layer (of up to 6%). The differences in the data for the few top layers in the OFE case are a few percent smaller than the corresponding data for the IFE. The differences in those regions of the OFE in which most of the core power is generated (top axial layers and edge radial layers excluded) are less than 3%.

This level of agreement (maximum error of ~10%) is a significant improvement over the results from previous methods and approaches the level needed for design evaluations. (A value of 5% would correspond to the level of uncertainty in measurements of local reactor physics parameters for the current HEU fuel; i.e., at 5%, the level of agreement among computational methods would correspond to the standard deviation in measured local physics parameters for the HEU fuel).

#### 4. Conclusion

The 2-D cross section processing methodology proves to be promising, as indicated by the results obtained. There is a significant improvement, as compared with a currently used 1-D cross section processing methodology, with respect to the power distribution calculated with BOLD VENTURE,

especially for the fuel regions located at the edges of the fuel elements. This result is of particular importance because a better representation of the power distribution would enable a more accurate thermal-hydraulics analysis of the core where the power data are used and consequently would result in a better estimation of core safety parameters.

The studied configuration is a simplified model of the HFIR. However, it is considered an appropriate model for a proof of principle and for facilitating the estimation of the effect of various uncertainties in the modelling parameters on the results obtained. Going from simpler to complex, more configuration details would need to be included in the current model for a better approximation of the actual core configuration. For example, the control plate region between the two fuel elements will be included in the model.

In addition, the complex BOLD VENTURE depletion model will be verified against results to be obtained with the Monte Carlo-based ALEPH depletion tool (Haeck and Verboomen 2007). Recently, ALEPH was successfully used to simulate the HFIR HEU cycle 400; the model includes detailed zoning of the fuel element regions and explicit simulation of the control element movement during the cycle. A HFIR LEU model for ALEPH is in progress. As for any other Monte Carlo-based tool, the drawback is the computational efficiency, especially when depletion calculations are involved. In those cases, a very fast code such as BOLD VENTURE is preferred for scoping studies because it can be used to perform very quickly numerous fuel grading calculations and to provide estimates of the reactor safety and performance parameters.

## Acknowledgment

The authors would like to thank the U.S. Department of Energy's National Nuclear Security Administration for sponsoring this work through its Global Threat Reduction Initiative program.

## References

- Ellis, R.J., Gehin, J.C., Ilas, G., Primm III, R.T., 2007. Neutronics feasibility study for conversion of the High Flux Isotope Reactor with LEU U-7Mo dispersion fuel. *ANS Transactions* 96, 620-622.
- Ellis, R.J., Gehin, J.C., Primm III, R.T., 2006. Cross section generation and physics modeling in a feasibility study of the conversion of the High Flux Isotope Reactor core to use low-enriched uranium fuel. *Proceedings, PHYSOR 2006* (CD).
- Haeck, W., Verboomen, B., 2007. An optimum approach to Monte Carlo burnup, *Nuclear Science and Engineering* 156, 180196.
- LANL 2003. MCNP—A general Monte Carlo n-particle transport code, version 5, LA-CP-03-0245, Los Alamos National Laboratory.
- ORNL 2006. SCALE: A modular code system for performing standardized computer analyses for licensing evaluations, version 5.1, vols. I–III, ORNL/TM-2005/39. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732.
- Primm, III, R.T., Ellis, R.J., Gehin, J.C., Moses, D.L., Binder, J.L., Xoubi, N., 2006. Assumptions and criteria for performing a feasibility study of the conversion of the High Flux Isotope Reactor core to use low-enriched uranium fuel, *Proceedings, PHYSOR 2006* (CD).
- Vondy, D.R., Fowler, T.B., Cunningham III, G.W., 1981. The BOLD VENTURE computation system for nuclear reactor core analysis, version III, ORNL-5711, Oak Ridge National Laboratory.