May 24, 2000

Paper
Log No: 83

Computational Physics and Engineering Division (10)

Calculational Benchmark Problems for VVER-1000 Mixed Oxide Fuel Cycle

Margaret B. Emmett

Oak Ridge National Laboratory,*
P.O. Box 2008,
Oak Ridge, Tennessee 37831-6370

(865) 574-5276 office number
(865) 576-3513 fax number
mbe@ornl.gov

ANS2000 Radiation Protection and Shielding Division Topical Conference,
Radiation Protection for our National Priorities:
Medicine, the Environment and the Legacy,
September 17–20, 2000,
Spokane, Washington

---

*Managed and operated by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

CALCULATIONAL BENCHMARK PROBLEMS FOR VVER-1000 MIXED OXIDE FUEL CYCLE

Margaret B. Emmett
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, Tennessee 37831-6370
(865) 574-5276

ABSTRACT

The Fissile Materials Disposition Program (FMDP) sponsored the development and solution of a benchmark set to allow comparison of criticality, shielding, and decay heat computations for disposition of plutonium materials in a VVER-1000 assembly. This paper documents the United States contribution to that study.

INTRODUCTION

Specifications for a calculational benchmark problem set for fissile materials disposition with a VVER-type reactor were provided jointly by the Russian and American participants in the Fissile Materials Disposition Program (FMDP). Both fresh and spent fuel storage aspects were required. The study used the following fuels: mixed oxide (MOX) with weapons-grade plutonium, MOX consisting of civil plutonium fuel (reactor-grade) and the traditional uranium dioxide (UOX) low-enriched fuel. Task I was a study of criticality safety in fresh fuel storage for the three types of fuel and will not be discussed in this paper. Task II was a three-part task studying the shielding and radioactive characteristics when the fissile assembly is transported. Task IIa was a study of the radioactive characteristics of a fissile assembly of fresh fuel without a container. Task IIb was a study of a fissile assembly of fresh fuel within a cask. Task IIc was a study of a burned fissile assembly within a spent fuel cask. The cask model is typical of those used to transport fissile assemblies of spent fuel. Modules from the SCALE[1] code system were used for all calculations. The use of the SCALE4.3r version of SCALE was specified because this version had been 'frozen' for use in calculations of these benchmarks.

DESCRIPTION AND RESULTS OF CALCULATIONS

Task IIa

Task IIa was a study of the radioactive characteristics of fresh fuel in a fissile assembly without a container (cask). The geometry model was typical of a VVER-1000: the assembly contained 312 fuel pins with 18 control rod guide tubes and a central instrumentation channel; however, the assembly of fresh fuel was 'dry'. Figure 1 illustrates the geometry. The temperature of the fissile assembly was 300 K. Calculations of dose rates at the surface of the assembly and at 0.5, 1 and 2 m from this surface were made for all three fuel types using the one-dimensional SCALE module SAS1. For convenience, SAS1 was used for fuel assemblies without a cask, while SAS2 was used for fuel assemblies in a cask. SAS1 is a shielding analysis sequence in which the computer codes BONAMI, NITAWL, XSDRN and XSDOSE are executed.

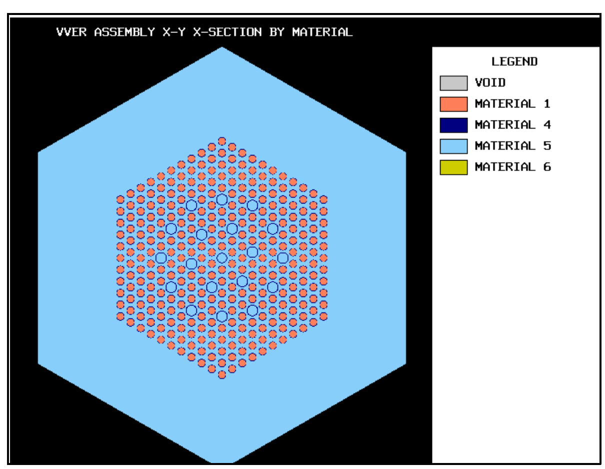

Figure 1. VVER-1000 FA geometry.

The results of the dose-rate calculations for the three types of fuel are given in Table 1. The neutron- and gamma-source strengths were calculated using the SAS2 code sequence. This sequence consists of BONAMI, NITAWL, XSDRN, COUPLE, ORIGEN-S and XSDOSE. The total neutron and gamma sources for the three types of fuel are given in Table 2.

The ORNL Task IIa results were compared with the results generated by several different computer code sequences run by Russian scientists.[2] The neutron source for UOX and MOX-R differ by less than 1%, but the MOX-W difference is slightly higher at 3%. Because the gamma-energy-group structure used by the Russians was completely different from the ORNL structure, the gamma-source results could not be compared directly. In particular, the mean energy of the lowest energy group is quite different, and this results in the source for that group being skewed. In order to try to understand the differences, ORNL ran an ORIGEN-ARP case which has a gamma group structure more like the Russian structure; results agreed to within 5 or 6%.

The neutron dose rate at the surface for UOX is within 1% of the rate calculated by the Russians with the CARE-ANISN code sequence. The gamma results differed by nearly a factor of 9, but investigation revealed that the Russians had included daughter products at equilibrium concentrations which are found in naturally occurring uranium although the benchmark specifications did not include that factor. Applying an estimated equilibrium factor to the ORNL results brings them within a factor of 1.5 of the Russian results. This difference is partially caused by the previously discussed difference in gamma group structure. Because the reported Russian results for the other detector locations are for total dose only (no neutron or gamma results) and the gamma results are influenced by the above factors, a comparison at these locations is inconclusive. The MOX-R and MOX-W total dose rates from the ORNL calculations fall within the range of the three sets of Russian results. For example, the neutron dose rate at the surface for MOX-W is 0.0121 rem/h for one method and 0.0378 rem/h for another; but the ORNL rate is 0.0160 rem/h. For MOX-R the rate is 0.129 rem/h for one method and 0.350 rem/h for another, but the ORNL result is 0.147 rem/h.

Task IIb

Task IIb was a shielding and heat generation study of fresh fuel within a cask model typical of those used to transport fissile assemblies of fresh fuel. The cross-section libraries used were the ENDF/B-IV-based 27-neutron, 18-gamma-group library and the 27-group burnup library, which is also based on ENDF/B-IV data but has ENDF/B-V fission products. Dose rates at the surface of the cask and at 0.5, 1 and 2 m from the surface were calculated using the SAS2 module of SCALE; results are given in Table 3. All three types of fuel were evaluated. Although the total sources for MOX-W and MOX-R are about an order of magnitude different, the gamma dose rates for MOX-R are higher by approximately a factor of 3, and the neutron dose rates are higher by approximately a factor of 9. The neutron dose rate at the surface for all three fuel types differs from the Russian results by 5 to 9%; the ORNL gamma results for MOX-W fall between two sets of Russian results, but the MOX-R is more aligned with the Russian result from the ORIGEN-TWODANT method. For the same reasons as given for Task IIa above, the gamma dose rate for UOX is significantly different from the Russian.

In addition to calculating dose rates, a heat generation study for the fresh fuel cask was made using the ORIGEN module from SCALE. The results for the individual isotopes and the total for each fuel type are either identical to the Russian results or agree to within 2%.

Task IIc

Task IIc was a study of a cask model typical of those used to transport fissile assemblies of spent fuel. The cask contained 12 fissile assemblies. A pin irradiation with a burnup of 60GWd/MTHM at average power of 166 W/cm was done. The fuel temperature was T = 1027 K, and the temperature of the clad and the borated-light-water coolant was T = 579 K. Each of the three types of fuel was analyzed. Dose rates at the surface of the cask and at 0.5, 1 and 2 m from the surface after a 3-year disposition in a pool storage were calculated using the SAS2 module of SCALE. Results of these calculations are given in Table 4. Initially the gamma dose rates were expected to be relatively independent of the fuel type. Thus, the higher gamma dose rates for the MOX fuels were surprising. Investigation of these differences revealed that the relatively higher neutron leakage with the MOX fuels as compared with UOX fuel produced more captured gammas. Because nearly 90% of the gamma dose is due to captured gammas, the resulting dose rates for MOX are higher than for low-enriched uranium.

The neutron dose rate for UOX at the surface is within 5%, and for MOX-R, within 1% of that calculated by the Russians using CARE-ANISN; however, the MOX-W results differ by approximately 15%. The gamma dose rate differences are higher, ranging from about 18% for UOX to 6% for MOX-R to 20% for MOX-W. The MOX-R

Table 1. SAS1 results for fresh fuel single assembly (Task IIa)

	UOX		MOX-W		MOX-R	
	Neutron	Gamma	Neutron	Gamma	Neutron	Gamma
Detector	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)
At surface	4.252×10^{-5}	2.233×10^{-4}	1.602×10^{-2}	1.115×10^{-2}	1.470×10^{-1}	1.304×10^{-1}
0.5 m from surface	6.064×10^{-6}	3.124×10^{-5}	2.286×10^{-3}	1.522×10^{-3}	2.097×10^{-2}	2.106×10^{-2}
1 m from surface	3.008×10^{-6}	1.592×10^{-5}	1.135×10^{-3}	7.725×10^{-4}	1.041×10^{-2}	1.126×10^{-2}
2 m from surface	1.185×10^{-6}	6.533×10^{-6}	4.479×10^{-4}	3.173×10^{-4}	4.109×10^{-3}	4.998×10^{-3}

Table 2. Total neutron and gamma source for fresh fuel from SAS-2

Particle type	UOX	MOX-W	MOX-R
Neutron (n/s)	5.73×10^{3}	2.10×10^{6}	1.90×10^{7}
Gammas (MeV/s)	2.78×10^{8}	5.38×10^{10}	1.59×10^{12}

Table 3. SAS-2 results for fresh fuel calculations (Task IIb)

	UOX		MOX-W		MOX-R	
	Neutron	Gamma	Neutron	Gamma	Neutron	Gamma
Detector	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)
At surface	8.038×10^{-6}	8.162×10^{-6}	2.904×10^{-3}	1.056×10^{-3}	2.635×10^{-2}	3.265×10^{-3}
0.5 m from surface	1.889×10^{-6}	1.985×10^{-6}	6.825×10^{-4}	2.561×10^{-4}	6.192×10^{-3}	7.652×10^{-4}
1 m from surface	1.044×10^{-6}	1.112×10^{-6}	3.774×10^{-4}	1.425×10^{-4}	3.424×10^{-3}	4.199×10^{-4}
2 m from surface	4.695×10^{-7}	5.157×10^{-7}	1.701×10^{-4}	6.467×10^{-5}	1.543×10^{-3}	1.860×10^{-4}

Table 4. SAS-2 results for spent fuel calculations (Task IIc)

	UOX		MOX-W		MOX-R	
	Neutron	Gamma	Neutron	Gamma	Neutron	Gamma
Detector	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)	Dose rate (rem/h)
At surface	5.628×10^{-3}	3.345×10^{-2}	1.497×10^{-2}	6.903×10^{-2}	5.653×10^{-2}	2.241×10^{-1}
0.5 m from surface	3.082×10^{-3}	1.881×10^{-2}	8.197×10^{-3}	3.775×10^{-2}	3.096×10^{-2}	1.202×10^{-1}
1 m from surface	2.142×10^{-3}	1.289×10^{-2}	5.696×10^{-3}	2.536×10^{-2}	2.152×10^{-2}	7.949×10^{-2}
2 m from surface	1.276×10^{-3}	6.941×10^{-3}	3.126×10^{-3}	1.312×10^{-2}	1.181×10^{-2}	3.983×10^{-2}

total dose gives the best comparison for all detectors. The total neutron and gamma sources after a 3-year cooling are given in Table 5. The ORNL neutron source for UOX agrees to within 1% with the Russian and the MOX-W result to within 4%, but the MOX-R result varies the most at 10%.

Table 5. Total neutron and gamma source for spent fuel after a 3-year cooling (from SAS-2)

Particle type	UOX	MOX-W	MOX-R
Neutron (n/s)	6.83×10^8	1.81×10^9	6.37×10^9
Gammas (MeV/s)	6.37×10^{15}	7.29×10^{15}	6.99×10^{15}

In addition to calculating dose rates, a heat generation study for the spent fuel cask at various times of disposition was done using the ORIGEN module from SCALE. The heat generation results vary from being the same to being up to 6% different than the Russian results from a calculation using the CARE-ANISN-CONSYST code sequence.

SUMMARY

ORNL results were compared with the results that were obtained by the Russians using several computer code sequences. The Russian cross-section libraries had different gamma-group structures than the libraries used at ORNL; therefore, direct comparisons of gamma source results were inconclusive. Additional analysis using the same group structures would likely resolve this issue. The use of ENDF/B-IV cross sections for Task IIb was the result of the author not being aware that the 44-neutron-group library, which is based on ENDF/B-V data actually contained burnup data; the 27-group burnup library was thought to be the only option. However, note that the 44-group library could not be used for the shielding part of the calculation because it has no gamma cross sections. Dose rate results for fresh fuel compared favorably with the Russian results, except for UOX cases in which the Russians took into account the daughter products of ^{238}U; ORNL made no equilibrium assumptions. The ORNL dose-rate predictions for spent fuel compared reasonably well with those of the Russians. Complete ORNL results are published in Ref. 2, which also contains the Russian results in the Appendices.

ACKNOWLEDGMENTS

This work was funded by the Office of Fissile Material Disposition, Office of Nuclear Nonproliferation, United States Department of Energy. The Oak Ridge National Laboratory is managed and operated by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

REFERENCES

1. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2/R5), Vols. I, II, and III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

2. M. B. Emmett, *Calculational Benchmark Problems for VVER-1000 Mixed Oxide Fuel Cycle*, ORNL/TM-1999/207, Lockheed Martin Energy Research Corp., Oak Ridge National Laboratory, March 2000.