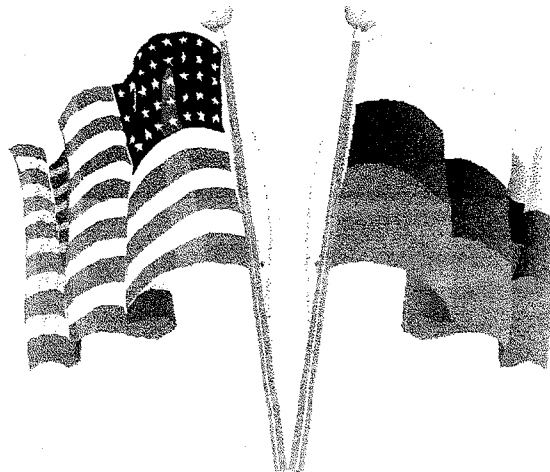


**OAK RIDGE
NATIONAL
LABORATORY**



**Creation of Computational Benchmarks
for LEU and MOX Fuel Assemblies Under
Accident Conditions**

**A. M. Pavlovitchev
A. G. Kalashnikov
M. A. Kalugin
A. P. Lazarenko
L. V. Maiorov
V. D. Sidorenko**



Fissile Materials Disposition Program

MANAGED AND OPERATED BY
LOCKHEED MARTIN ENERGY RESEARCH CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness or any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

**CREATION OF COMPUTATIONAL BENCHMARKS FOR LEU
AND MOX FUEL ASSEMBLIES UNDER
ACCIDENT CONDITIONS**

A. M. Pavlovitchev
A. G. Kalashnikov
M. A. Kalugin
A. P. Lazarenko
L. V. Maiorov
V. D. Sidorenko

Date Published: November 1999

Report Prepared by
LOCKHEED MARTIN ENERGY RESEARCH CORP.
P.O. Box 2008
Oak Ridge, Tennessee 37831-6363
under
Subcontract Number B99398V

Funded by
Office of Fissile Materials Disposition
United States Department of Energy

Prepared for
Computational Physics and Engineering Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
managed by
LOCKHEED MARTIN ENERGY RESEARCH CORP.
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-96OR22464

RUSSIAN RESEARCH CENTER "KURCHATOV INSTITUTE"
INSTITUTE OF NUCLEAR REACTORS
VVER DIVISION

*Joint U.S./Russian Project to Update, Verify and Validate Reactor Design/Safety
Computer Codes Associated With MOX Fuel Usage in Water Reactors.*

**CREATION OF COMPUTATIONAL BENCHMARKS FOR LEU AND MOX FUEL
ASSEMBLIES UNDER ACCIDENT CONDITIONS. CALCULATE KINETIC PARAMETERS,
DOPPLER COEFFICIENT, AND THE EFFECT OF DECREASING THE WATER DENSITY.**

FINAL REPORT

Project manager

A.M. Pavlovitchev

Executors

A.G. Kalashnikov

M.A. Kalugin

A.P. Lazarenko

L.V. Maiorov

V.D. Sidorenko

Moscow 1998

ABSTRACT

The results of VVER-1000 computational benchmarks calculations obtained with the use of various Russian codes (such as MCU-RFFI/A, TVS-M and WIMS-ABBN) are presented. List of benchmarks includes LEU and MOX cells with fresh and spent fuel under various conditions (for calculation of kinetic parameters, Doppler coefficient, reactivity effect of decreasing the water density).

Calculation results are compare with each other and results of this comparison are discussed.

CONTENTS

ABSTRACT	2
CONTENTS	3
1. INTRODUCTION.....	4
2. COMPUTER CODES USED	4
3. CALCULATION RESULTS	5
3.1 MULTIPLICATION FACTOR.....	5
1.2 REACTIVITY EFFECTS.....	5
1.3 KINETIC PARAMETERS	5
4. CONCLUSION	6
TABLES	8

1. INTRODUCTION

Verification and validation of computer codes is the component part of the problem of MOX fuel using in VVER reactors. Within the framework of Joint American-Russian Fissile Materials Disposition Program a set of VVER computational benchmarks was formulated. This set consists of pin cell and multi-assembly geometries with LEU and weapon-grade MOX. The calculations call for a wide range of temperatures, water densities and soluble boron concentrations to estimate an accuracy of prediction of Doppler coefficient, reactivity effect of water density decreasing. The list of parameters to be calculated includes kinetics parameters.

Complete description of mentioned above benchmark is given in [1].

The presented report contains some results of calculations performed with computer codes applying in Russia as well as inter-comparison of these results.

2. COMPUTER CODES USED

Computer codes used in the calculations were the following :

- MCU-RFFI/A [2] - continuous energy Monte Carlo code developed in RRC KI;
- TVS-M [3] - spectral code for VVER lattice and assembly burnup calculations (RRC KI);
- WIMS-ABBN [4] - an updated WIMS-D4 code. The modernization was mainly connected with introducing of minor actinide chains and with library updating (pin cell variants V15-V18);
- TRIANG-PWR [5] code for pin-by-pin computation using constants from WIMS-ABBN (multi-assembly variants V19-V20);

It should be noted that two different options of the code were used to perform the calculations.

The POINTWISE option uses the pointwise cross sections for all the energy region (0 – 20 MeV). Thermalization effects are taken into account if neutron energy is less than 4 eV.

The MULTIGROUP option, intended to verify the design codes, solves the transport equation using the 40-group approximation for thermal region (0 – 1 Ev).

It should be emphasized that MCU-RFFI/A and TVS-M codes are based on the same nuclear data whereas WIMS-ABBN has different constant library.

3. CALCULATION RESULTS

Presented material contains preliminary results of calculations of the following values:

- K_o
- reactivity effects
- kinetic parameters (β , β_{eff} , ℓ)

3.1 MULTIPLICATION FACTOR

Results of K_o calculations obtained with the use of MCU-RFFI/A, TVS-M and WIMS-ABBN codes are presented in Table 1. Concerning the Monte Carlo calculations it should be mentioned that all of them were performed with statistical error less than 0.1% and that two K_o values obtained with both pointwise and multigroup MCU options are given. As it is seen from the Table differences between K_o calculated with these two MCU options can be remarkable (up to 1%) in case of variants with Pu in fuel.

It is observed that multigroup MCU results are in a good agreement with the ones obtained by TVS-M code, which also uses multigroup thermal cross sections library. For all variants discrepancies do not exceed 0.003.

As to WIMS-ABBN code it's results demonstrates rather good agreement with MCU and TVS-M in case of pin cell variants with LEU fuel and spent MOX fuel (differences do not exceed 0.01). However for V17 variant (pin cell with fresh MOX fuel) discrepancies rise running up to 0.015. Partially it can be explained by different nuclear data libraries.

TRIANG-PWR results differs from the ones obtained with other codes approximately by 1 % (TRIANG-PWR underestimates the value of K_o).

3.2 REACTIVITY EFFECTS

From the practical point of view it is especially important to calculate with a good accuracy reactivity effects such as Doppler, effect of water density changing and so on. In Table 3 reactivity effects obtained with various codes are presented. As it is seen from this Table all codes demonstrates very good agreement. The only exception is WIMS-ABBN which slightly overestimates Doppler effect value (approximately by 10%) in comparison with other codes.

The states parameters are given in Table 2.

3.3 KINETIC PARAMETERS

For computing of effective fraction of delayed neutrons and prompt neutrons lifetime different codes used different approaches. In MCU-RFFI/A β_{eff} was defines as follows:

$\beta_{eff} = (K_{eff} - K_{prompt}) / K_{eff}$, where K_{prompt} is multiplication factor with only prompt neutrons taking into account.

In TVS-M and WIMS-ABBN codes β_{eff} and ℓ are calculated with the use of perturbation theory. TRIANG used so called "direct" method.

Results of β_{eff} , β / β_{eff} and ℓ calculations are presented in Table 4-6.

As it is seen from Table 4 values of β_{eff} obtained with different codes are close and maximum deviation does not exceed 5%. Especially good agreement is observed between MCU and WIMS-ABBN results.

The β_{eff}/β values given in Table 5 have better agreement than β_{eff} , because of β_{eff}/β characterizes the computer code algorithms quality, while β_{eff} also depends on the cross section libraries used in a code. This circumstance gives the reason to suppose that delayed neutrons constants used in TVS-M possibly differ from MCU data.

Prompt neutron lifetime ℓ calculated with TVS-M and WIMS-ABBN codes is given in Table 6 (MCU results are not available). Data of this Table demonstrate a good agreement between two codes. Discrepancies do not exceed 5%. The only exception is V16 variant state S9 where results deviation is about 20%.

4. CONCLUSION

In this report the results of several benchmarks calculations performed with MCU-RFFI, TVS-M, WIMS-ABBN and TRIANG-PWR codes are presented.

It was discovered that as a whole all codes have demonstrated a good agreement. For the pin cell variants K_o discrepancies lie within 1% with exception of WIMS-ABBN results for V17 (fresh MOX) variant which differ from others by 1-1.5%. The possible reason of it is differences in nuclear data for Pu isotopes, but more detailed analysis including reaction rates comparison is necessary.

As for kinetics parameters calculations there is rather good agreement between values of β_{eff} , ℓ and especially β_{eff}/β obtained with various codes.

LITERATURE

1. Develop variant 14, including burnup and graded MOX surrounded by LEU configuration. Creation of computational benchmarks for LEU and MOX fuel assemblies under accident conditions. Calculate kinetic parameters, Doppler coefficient, and the effect of decreasing the water density. Draft report, 1998
2. E.Gomin, L.Maierov. The MCU-RFFI Code. In Proceedings of the Int. Conf. on Math., Comp. Reactor Phys. and Envir. Apr.30-May 4, Portland, USA,1995.
3. V.D. Sidorenko et. al. Spectral Code TVS-M for Calculation of Characteristics of Cells, Supercells and Fuel Assemblies of VVER-Type Reactors. 5-th Symposium of the AER, Dobogoko, Hungary, October 15-20, 1995.
4. Neutronics Benchmarks for the Utilization of Mixed-Oxide Fuel: Joint U.S./Russian Progress Report for Fiscal Year 1997, Volume 3

TABLES

Table 1 Calculated value of K_0 obtained with various codes.

Var.	State	MCU-RFFI/A		TVS-M	WIMS-ABBN/ TRIANG
		Pointwise	Multigroup		
V15 fresh LEU	S7	1.3809	1.3805	1.3789	1.3745
	S8	1.3543	1.3547	1.3517	1.3448
	S9	1.0742	1.0729	1.0699	1.0634
	S10	1.2644	1.2633	1.2613	1.2581
	S11	-	-	1.3682	1.3631
	S12	-	-	1.4547	1.4518
V16 spent LEU	S7	1.1032	1.1093	1.1058	1.1068
	S8	-	-	1.0792	1.0788
	S9	-	-	0.7990	0.7956
	S10	1.0173	1.0218	1.0187	1.0209
	S11	-	-	1.1038	1.1044
	S12	-	-	1.1968	1.1994
V17 fresh MOX	S7	1.2610	1.2706	1.2665	1.2544
	S8	1.2311	1.2384	1.2354	1.2194
	S9	0.9700	0.9725	0.9687	0.9563
	S10	1.2024	1.2108	1.2050	1.1957
	S11	-	-	1.2632	1.2507
	S12	-	-	1.3766	1.3708
V18 spent MOX	S7	1.0704	1.0808	1.0782	1.0765
	S8	-	-	1.0497	1.0468
	S9	-	-	0.7844	0.7843
	S10	1.0071	1.0143	1.0119	1.0124
	S11	-	-	1.0773	1.0755
	S12	-	-	1.1718	1.1738
V19 fresh MOX+fresh LEU	S7	1.3639	1.3666	1.3655	1.3520
	S8	-	-	1.3384	1.3264
	S9	-	-	1.0621	1.0948
	S10	-	-	1.2534	1.2456
	S11	-	-	1.3565	1.3468
	S12	-	-	1.4442	1.4361
V20 fresh MOX+spent LEU	S7	1.1614	1.1680	1.1665	1.1581
	S8	-	-	1.1397	1.1318
	S9	-	-	0.8598	0.8959
	S10	-	-	1.0786	1.0776
	S11	-	-	1.1638	1.1583
	S12	-	-	1.2581	1.2529

Table 2 State parameters.

State	Fuel zones temperature, K	Non-fuel zones temperature, K	Moderator density, g/cc	Boron conc., g/kg	B_z^2 , cm ⁻²
S7	1027	579	0.716	0.0	0.0
S8	2000	579	0.716	0.0	0.0
S9	1027	579	0.2	0.0	0.0
S10	1027	579	0.716	1.2	0.0
S11	1027	579	0.716	0.0	critical
S12	300	300	1.000	0.0	critical

Table 3 Calculated values of reactivity effects (such as Doppler, effect of decreasing water density, boron effect) obtained with various codes.

Var.	Effect	Value, %			
		MCU-RFFI/A		TVS-M	WIMS-ABBN/ TRIANG
		POINTWISE	MULTIGROUP		
V15	Doppler	-1.9	-1.9	-2.0	-2.2
	Water dens.	-22.2	-22.3	-22.4	-22.6
	Boron	-8.4	-8.5	-8.5	-8.5
V16	Doppler	-	-	-2.4	-2.5
	Water dens.	-	-	-27.7	-28.1
	Boron	-7.8	-7.9	-7.9	-7.8
V17	Doppler	-2.4	-2.5	-2.5	-2.8
	Water dens.	-23.1	-23.5	-23.5	-23.8
	Boron	-4.6	-4.7	-4.9	-4.7
V18	Doppler	-	-	-2.6	-2.8
	Water dens.	-	-	-27.2	-27.1
	Boron	-5.9	-6.2	-6.1	-6.0

Remark : effect value was defined as follows:

$$EFF_i = 100 \cdot (K_o(S_i) - K_o(S7)) / K_o(S7), \text{ where } i=8 \text{ corresponds to Doppler effect,}$$

$$i=9 \text{ - to effect of decreasing water density,}$$

$$i=10 \text{ - to boron effect.}$$

Table 4 Calculated value of effective fraction of delayed neutrons β_{eff} obtained with various codes.

Var.	State	MCU-RFFI/A	TVS-M	WIMS-ABBN/ TRIANG
V15	S7	0.00713	0.007202	0.007161
	S8	0.00712	0.007203	0.007161
	S9	0.00733	0.007392	0.007369
	S10	0.00712	0.007203	0.007164
	S11	-	0.008218	0.008143
	S12	-	0.008404	0.008312
V16	S7	0.00515	0.005309	0.005211
	S8	-	0.005318	0.005200
	S9	-	0.005949	0.005879
	S10	0.00517	0.005328	0.005232
	S11	-	0.005559	0.005454
	S12	-	0.005853	0.005755
V17	S7	0.00314	0.003170	0.003169
	S8	0.00317	0.003184	0.003184
	S9	0.00389	0.003962	0.003977
	S10	0.00317	0.003200	0.003200
	S11	-	0.003576	0.003550
	S12	-	0.003542	0.003511
V18	S7	0.00373	0.003874	0.003752
	S8	-	0.003890	0.003761
	S9	-	0.004764	0.004642
	S10	0.00375	0.003912	0.003789
	S11	-	0.004023	0.003891
	S12	-	0.004035	0.003901
V19	S7	0.00614	0.006071	0.006326
	S8	-	0.006076	0.006325
	S9	-	0.006333	0.006610
	S10	-	0.006066	0.006286
	S11	-	0.006926	0.007144
	S12	-	0.007093	0.007270
V20	S7	0.00453	0.004603	0.004560
	S8	-	0.004611	0.004334
	S9	-	0.005236	0.005321
	S10	-	0.004620	0.004564
	S11	-	0.004943	0.004934
	S12	-	0.005167	0.005060

Table 5 Calculated value of ratio β/β_{eff} obtained with various codes.

Var.	State	MCU-RFFI/A	TVS-M	WIMS-ABBN/ TRIANG
V15	S7	0.975	0.976	0.975
	S8	0.971	0.974	0.974
	S9	0.927	0.922	0.921
	S10	0.967	0.969	0.969
	S11	-	1.103	1.099
	S12	-	1.147	1.142
V16	S7	0.957	0.959	0.960
	S8	-	0.957	0.958
	S9	-	0.870	0.872
	S10	0.950	0.952	0.954
	S11	-	0.999	0.999
	S12	-	1.050	1.050
V17	S7	0.963	0.965	0.964
	S8	0.964	0.963	0.961
	S9	0.888	0.893	0.889
	S10	0.961	0.961	0.960
	S11	-	1.062	1.057
	S12	-	1.122	1.116
V18	S7	0.954	0.954	0.952
	S8	-	0.952	0.949
	S9	-	0.859	0.854
	S10	0.945	0.948	0.947
	S11	-	0.984	0.981
	S12	-	1.038	1.037
V19	S7	0.978	0.978	0.984
	S8	-	0.977	0.982
	S9	-	0.926	0.924
	S10	-	0.971	0.977
	S11	-	1.105	1.089
	S12	-	1.146	1.130
V20	S7	0.962	0.967	0.953
	S8	-	0.966	0.953
	S9	-	0.893	0.887
	S10	-	0.960	0.949
	S11	-	1.030	1.007
	S12	-	1.076	1.043

Table 6 Calculated value of prompt neutrons lifetime ℓ obtained with various codes.

Var.	State	TVS-M	WIMS-ABBN
V15	S7	2.109e-5	2.11e-5
	S8	2.101e-5	2.11e-5
	S9	1.604e-5	1.60e-5
	S10	1.877e-5	1.88e-5
	S11	2.047e-5	2.04e-5
	S12	2.106e-5	2.12e-5
V16	S7	1.945e-5	1.92e-5
	S8	1.936e-5	1.90e-5
	S9	1.290e-5	1.58e-5
	S10	1.719e-5	1.70e-5
	S11	1.926e-5	1.90e-5
	S12	2.177e-5	2.19e-5
V17	S7	1.118e-5	1.08e-5
	S8	1.109e-5	1.07e-5
	S9	8.639e-6	0.83e-5
	S10	1.034e-5	1.01e-5
	S11	1.098e-5	1.06e-5
	S12	1.321e-5	1.31e-5
V18	S7	1.470e-5	1.43e-5
	S8	1.460e-5	1.41e-5
	S9	9.847e-6	0.94e-5
	S10	1.325e-5	1.29e-5
	S11	1.460e-5	1.42e-5
	S12	1.757e-5	1.75e-5

ORNL staff comments on the Final Report, *Creation of Computational Benchmarks for LEU and MOX Fuel Assemblies Under Accident Conditions. Calculate Kinetic Parameters, Doppler Coefficient, and the Effect of Decreasing the Water Density*

- (1) It is ORNL's understanding that K_0 is the value of the effective multiplication factor computed with the neutron energy spectrum of a system infinite in the dimensions not modeled. A buckling correction has been applied to the computed value of the multiplication factor for the system. The correction is applied after the solution procedure—which can be iterative or stochastic—for the neutron transport equation. This differs from the usual practice in the United States of incorporating the buckling factor as a part of the procedure for determining the values of the neutron fluxes. Both methods are approximations and neither is necessarily preferred.
- (2) In Section 3.3, the statement is made that the effective delayed neutron fraction and the prompt neutron lifetime are calculated with perturbation theory in the TVS-M and WIMS-ABBN codes. Perturbation theory is a familiar mathematical technique but its use in the determination of these two parameters is not familiar. It is ORNL's belief that the solution to the transport equation containing the effective neutron fraction is assumed to be a small perturbation to the unperturbed solution without delayed neutrons so that a solution of the form $y = x(1) + y^*x + \text{other terms}$ is substituted into the transport equation and solved.
- (3) U.S. methods for effective delayed neutron fraction are based on matching reaction rates between an "effective" fission neutron fraction in an energy group and the actual reaction rate due to the delayed neutrons in a given energy group. It is ORNL's belief that the "direct" method used in TRIANG the same as used in the U.S. This same issue is important for the discussion of beta-effective given in Section 3.3, next-to-last paragraph. Future reports should provide additional explanation as to why "beta-effective/beta characterizes the computer code algorithms quality".
- (4) Literature—Reference 1 can now be listed as: J. C. Gehin, C. Dourougie, M. B. Emmett, and R. A. Lillie, "Analysis of Weapons-Grade MOX VVER-1000 Benchmarks with HELIOS and KENO," ORNL/TM-1999/78, July 1999.
- (5) In section 3.1, page 5, first paragraph. The statement is made that "it should be mentioned that all of them were performed with statistical error less than 0.1%." It is ORNL's belief that this statement means that one standard deviation was 0.1%.
- (6) For Table 6, it is ORNL's belief that the unit of measurement for lifetime is seconds.
- (7) This report is the deliverable for Task 1.9 under the US fiscal year 1998 funding for Russia. Results correspond to the U.S. calculations reported in ORNL/TM-1999/78.

INTERNAL DISTRIBUTION

- | | |
|---------------------|---------------------------------------|
| 1-5. B. B. Bevard | 19. G. E. Michaels |
| 6. J. J. Carbajo | 20. D. L. Moses |
| 7. E. D. Collins | 21-25. R. T. Primm III |
| 8. B. S. Cowell | 26. C. C. Southmayd |
| 9. R. J. Ellis | 27. B. S. Yarborough |
| 10-14. J. C. Gehin | 28. G. L. Yoder, Jr. |
| 15. S. R. Greene | 29. Central Research Library |
| 16. T. W. Horning | 30-31. ORNL Laboratory Records (OSTI) |
| 17. D. T. Ingersoll | 32. ORNL Laboratory Records (RC) |
| 18. M. A. Kuliasha | |

EXTERNAL DISTRIBUTION

33. M. L. Adams, Department of Nuclear Engineering, Texas A&M University, Zachry 129, College Station, TX 77843
34. D. Alberstein, Los Alamos National Laboratory, MS-E502, P.O. Box 1663, Los Alamos, NM 87545
35. J. Baker, Office of Fissile Materials Disposition, U.S. Department of Energy, MD-3, 1000 Independence Avenue SW, Washington, DC 20585
36. L. Holgate, Office of Fissile Materials Disposition, U.S. Department of Energy, MD-1/2, 1000 Independence Avenue SW, Washington, DC 20585
37. A. Caponiti, Office of Fissile Materials Disposition, U.S. Department of Energy, MD-3, 1000 Independence Avenue SW, Washington, DC 20585
38. L. Jardine, Lawrence Livermore National Laboratory, P.O. Box 808, MS-L166, Livermore, CA 94551
- 39-44. Dr. Alexander Kalashnikov, Institute of Physics and Power Engineering, 1 Bondarenko Square, Obninsk, Kaluga Region, Russia 249020
- 45-49. Dr. Alexander Pavlovitchev, Russian Research Center "Kurchatov Institute," Institute of Nuclear Reactors, VVER Division, VVER Physics Department, 123182, Kurchatov Square, 1, Moscow, Russia