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MCNP-to-TORT Radiation Transport Calculations in Support of Mixed Oxide Fuels Testing for the Fissile Materials Disposition Program

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Abstract

The United States (US) Department of Energy Fissile Materials Disposition Program has begun studies for disposal of surplus weapons-grade plutonium (WG-Pu) as mixed uranium-plutonium oxide (MOX) fuel for commercial light-water reactors (LWRs). Currently MOX fuel is used commercially in a number of foreign countries, but is not in the US. Most of the experience is with reactor-grade plutonium (RG-Pu) in MOX fuel. Therefore, to use WG-Pu in MOX fuel, one must demonstrate that the experience with RG-Pu is relevant.

As a first step in this program, the utilization of WG-Pu in a LWR environment must be demonstrated. To accomplish this, a test is to be conducted to investigate some of the unresolved issues. The initial tests will be made in an I-hole of the Advanced Test Reactor (ATR) at the Idaho National Engineering and Environmental Laboratory (INEEL).

Initial radiation transport calculations of the test specimens were made at INEEL using the MCNP Monte Carlo radiation transport code. These calculations were made to determine the linear heating rates in the fuel specimens. Unfortunately, the results of the calculations could not show the detailed high and low power-density spots in the specimens. However, a discrete-ordinates radiation transport code could pinpoint these spatial details. Therefore, INEEL was tasked with producing a MCNP source at the boundary of a rectangular parallelepiped enclosing the ATR I-hole, and Oak Ridge National Laboratory was tasked with transforming this boundary source into a discrete-ordinates boundary source for the Three-dimensional Oak Ridge radiation Transport (TORT) code. Thus, the TORT results not only complemented, but also were in agreement with the MCNP results.

1. INTRODUCTION

The United States (US) Department of Energy Fissile Materials Disposition Program has begun studies for disposal of surplus weapons-grade plutonium (WG-Pu) as mixed uranium-plutonium oxide (MOX) fuel for commercial light-water reactors (LWRs). The goal of plutonium disposition is to make surplus plutonium as inaccessible and unattractive for retrieval and weapons use as the residual plutonium in spent fuel from commercial reactors. Most of the experience is with reactor-grade plutonium (RG-Pu) in MOX fuel. Therefore, to use WG-Pu in MOX fuel, one must demonstrate that the experience with RG-Pu is relevant. Initial tests will be made in an I-hole of the Advanced Test Reactor (ATR) at the Idaho National Engineering and Environmental Laboratory (INEEL), to aid in the investigation of some of the unresolved issues. One of these issues is to understand the impact of Gallium on LWR MOX fuel performance, since it is present in small amounts in WG-Pu.

Initial radiation transport calculations of the test specimens have been made at INEEL using the MCNP Monte Carlo radiation transport code[1]. These calculations were made to determine the linear heating rates in the fuel specimens. Due to the nature of Monte Carlo, it is extremely time consuming and inefficient to show detailed hot spots in the specimens. However, results from discrete-ordinates radiation transport calculations could show these spatial details. Therefore, INEEL was tasked with producing a MCNP source at the boundary of a rectangular parallelepiped enclosing the ATR I-hole, and Oak Ridge National Laboratory (ORNL) was tasked with transforming this boundary source into a discrete-ordinates boundary source for the Three-dimensional Oak Ridge radiation Transport (TORT) code[2].

The remainder of the paper will discuss the cross sections used in the calculations, the codes written to produce the TORT geometry, the code used to produce the TORT boundary source, the TORT calculations, and the results as compared to the INEEL MCNP calculations. Additionally, isodose plots will be shown to help in the visualization of the heating as the radiation inundates the test specimens.

DISCLAIMER

2. MCNP CALCULATIONS

Figure 1 shows a plan view of the ATR northwest (NW) quarter core model, with the appropriate I-hole highlighted. Figure 2 shows a plan view of a MOX test assembly in the MCNP parallelepiped.

The MCNP coordinate system was constructed such that the y-axis origin began at the center of the NW quarter core and the axis passed through the center of the I-hole, the x-axis origin began at the center of the I-hole, and the z-axis origin began at 60.96 cm below the midplane of the ATR. The coordinates of the planes of the parallelepiped were x = -3 and +3 cm, y = +58.96 and +63.96 cm, and z = -2.54 and +127.0 cm.

Gray Chang, INEEL, performed an MCNP calculation for the NW quarter core model, which included the MOX test assembly, and saved the following incoming neutron/photon information at the boundary planes of the parallelepiped: weight, energy, x-y-z coordinates, entrant direction cosines (u,v,w), and a value to indicate particle type (1=neutron, 2=photon). This information was then forwarded electronically to ORNL.

3. CROSS SECTIONS

The raw MCNP data entering the x-y planes were transformed to produce a boundary directional source for the SAS2 one-dimensional (1D) XSDRNPM module of the SCALE code system[3]. The SAS2 module was altered by O.W. Hermann, ORNL, to use modified directional data from the MCNP calculation to generate burned MOX isotopics and resulting cross-section libraries. The modified SAS2 coding allowed for generation of neutron cross-section libraries for burned MOX pins. The coding also allows for libraries having an arbitrary group structure and using two separate 1D models of the MOX capsule geometry, one based on a central capsule and the other based on a capsule modeded as a cylindrical annulus near the edge of the test assembly. The final code was used to generate a 7-energy-group neutron (Table 1.) macroscopic cross-section library for the fresh MOX fuel. Macroscopic cross sections were generated for the following mixtures: H_2O, SS316, MOX (5 wt% PuO_2), Inconel 600, Be-H_2O, Zircaloy, Al-6061T, and UO_2 (depleted).

In addition, the neutron kerma factors from the KAOS[4] (ENDF/B-V) library for the elements/isotopes in the above materials were processed into the 7-group structure with the RETRIEVE code[4], and the materials were mixed and the units changed to kW•s/cm with the AXMIX code[5]. Two nuclear responses were used in the study: the recommended prompt neutron kerma factor (RNKF), and the recommended kerma factor plus total decay heat (RNKF+TDH). These two were chosen to help bracket the actual heating, since no photon transport was carried out in the study.

4. TORT GEOMETRY CODES

A utility code, MCTORGOM, was written by the author by expanding a two-dimensional code by C.O. Slater, ORNL, for generating finite difference models in Cartesian geometry for use with the TORT code (variable mesh is not allowed in MCTORGOM). The model MCTORGOM generates is based on a combinatorial geometry representation of the three-dimensional problem to be analyzed. MCTORGOM uses routines from the SCALE MARS module, which allows for free-form input. Once the combinatorial geometry has been completed, the SCALE PICTURE module is used to determine if the MARS input correctly depicts the geometry. A set of x-y-z mesh boundaries are input by the user (not generated) to MCTORGOM, which then determines what MARS zone the mid-point of each x-y-z cell is located. It will then output either or both an ISOPL3D[6] zone map file (from XTORID[6]) and a TORT VARMAP file. Once the MCTORGOM code has been run for the problem, the ISOPL3D code is run to determine if the chosen TORT x-y-z mesh is sufficient.

5. MCNP-TO-TORT BOUNDARY SOURCE CODE

Another utility code, MCTORBDY, was written to create a TORT boundary-source file (VARBND) using the MCNP-generated incoming neutron/photon information at the boundary planes of the parallelepiped. MCTORBDY reads the discrete-ordinates energy-group boundaries, the x-y-z cell boundaries, and the directional quadrature. From this input it calculates all the quadrature directional boundary information required for each of the six sides of the parallelepiped. Spatial information containing the fine-mesh areas is then determined for each of the six sides. It reads the MCNP output of weight, energy, x-y-z coordinates, entrant direction cosines (u,v,w), and the particle type (1=neutron, 2=photon). From this information it determines what type particle is being examined, the discrete-ordinates energy group in which to place the particle, the particular discrete direction in which to place the particle, the spatial side of the pallellepiped, and the particular fine-mesh cell in which it is to be placed. The weight of the particle is then converted to flux, and the information is written to the TORT VARBND file.

6. TORT CALCULATIONS

TORT models of the problem are shown in Figures 3 - 4. Figure 3 is an x-z slice at the y=61.9 cm position. A fuel capsule contains 15 MOX fuel pellets. There is sufficient volume in the final assembly to hold 9 fuel capsules for irradiation in the I-hole. All fuel capsules in the current design contained WG-MOX except the top and middle fuel capsules in Figure 3; these contained only depleted UO_2. Figure 4 is an x-y slice at the z=39.5 cm position. The total number of mesh cells for the problem was 4,551,000 (205 in the x-direction, 200 in the y-direction, and 111 in the z-direction). The quadrature was a standard S4, and the 7-neutron group cross-section Legendre expansion was P_1. CPU running time on a RISC 6000, model 590, was approximately 22 hours.

7. POST-PROCESSOR CODES

Flux output from the TORT calculation was processed through the TORTACT utility code. This utility reads a TORT ntscl (varscl format) file and produces activities from response factors input, then outputs to a TORT ntrso (flxmom format) file. The activities are defined as the integral of the fluxes and response factors over energy group and zone space. Different response factors may be used and are numbered in the order they are input. These response factors for the different responses can be input by energy group and response number. The response number can be entered by zone number to provide a different activity for each zone. The activities in the ntrso file were processed with the ISOPL3D code to produce iso-activity plots at the desired planes.

8. RESULTS

Fluences from the calculations were folded with the RNKF and RNKF+TDH values; however, only plots using RNKF+TDH are shown. Figure 5 shows a y-z grey-shaded plot at a x-plane which cuts through the midplane of the test capsules furthest from the core. This plot shows that increased capsule heating is occuring on the outside edges. It is also seen how ragged the heating is outside the capsules. This is a result of the MCNP source; the source does not contain sufficient particles to provide nonzero entries in all the TORT source angles, i.e. many TORT discrete angles have zero entries.

Figure 6 shows a x-y grey-shaded plot at a z-plane which intersects the midplane of the top three capsules. Likewise, this plot shows the increased heating occuring on the edges of fuel capsules closest to the ATR core. Again, the MCNP-induced ragged heating is seen near the edges of the system.

Table 2 shows a comparison of the MCNP and TORT linear heating results in the MOX fuel. These results were obtained by integrating the heat densities over the volumes of the MOX fuel capsules, then dividing by the lenghts of the fuel capsules. The TORT results clearly bracket the MCNP results. Also, Table 2 shows the average, maximumn, and minimum RNKF heating densities in the fuel capsules. The TORT maximum values are approximately a factor of 2 greater than the minimum values. Thus, TORT is capable of producing the heating densities on a fine grid and can show detailed hot spots.

9. CONCLUSIONS

Codes written to provide three-dimensional geometry translations from MORSE combinatorial geometry to TORT geometry, convert MCNP boundary sources to TORT boundary sources, and provide TORT activity analyses have been shown to work properly and provide heating rates which are in agreement with MCNP. Additional improvements to the boundary source code include providing both a spatial and angle averaging option which will decrease the number of zero-source values in the discrete angles. These improvements should mitigate the irregular or uneven outline in the TORT results near the external boundaries. With the currently available communication between MCNP and TORT, tremendous detail can be obtained for very complicated geometries.

Table 1. 7-Group neutron energy boundaries (eV)

Group	Energies
1	2.00E+7
2	1.00E+5
3	1.00E+2
4	6.25E-1
5	3.33E-1
6	1.62E-1
7	3.00E-2
	1.00E-5*

*Note: Bottom energy of group 7.

Table 2. Comparisons of TORT and MCNP calculations

Target Location		TORT(RNKF) (kW/m)	MCNP(K) (kW/m)	TORT(RNKF+TDH) (kW/m)	TORT RNKF (kW/cm^3) average	maximum	minimum
TOP	1 UO2	23.39	23.75	30.09	.433	.613	.357
	2 (WG-MOX)	25.10	29.04	32.64	.463	.740	.362
	3 (WG-MOX)	25.00	28.41	32.51	.461	.783	.360
MID	1 UO2	24.64	25.23	31.73	.456	.691	.379
	2 (WG-MOX)	26.38	28.67	34.28	.487	.781	.379
	3 (WG-MOX)	26.28	29.95	34.32	.485	.766	.374
BOT	1 (WG-MOX)	18.34	22.15	23.65	.339	.521	.280
	2 (WG-MOX)	24.84	28.58	32.28	.458	.741	.354
	3 (WG-MOX)	24.84	28.41	32.35	.458	.793	.354

Note: RNKF = KAOS recommended neutron heating kerma only,
K = heating kerma from the MCNP run, which includes heating from both neutrons and photons,
RNKF+TDH = neutron and total decay photon heating kerma; only neutrons were run in the TORT calculation; any photons produced were assumed absorbed in the materials in which they were produced.

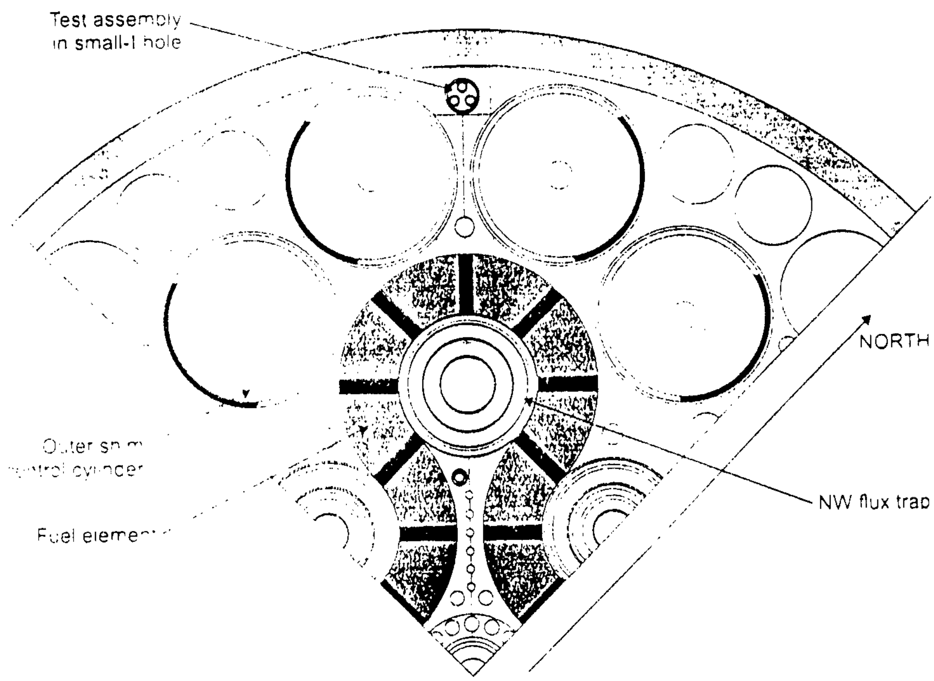

Fig. 1. Plan view of the NW quarter core MCNP model.

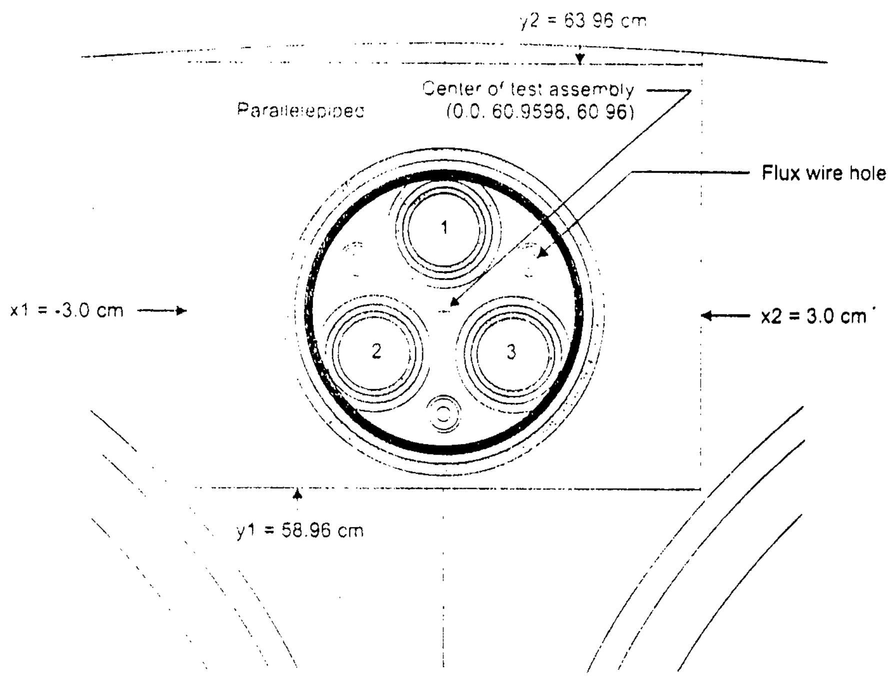

Fig. 2. Plan view of MCNP MOX test assembly model.

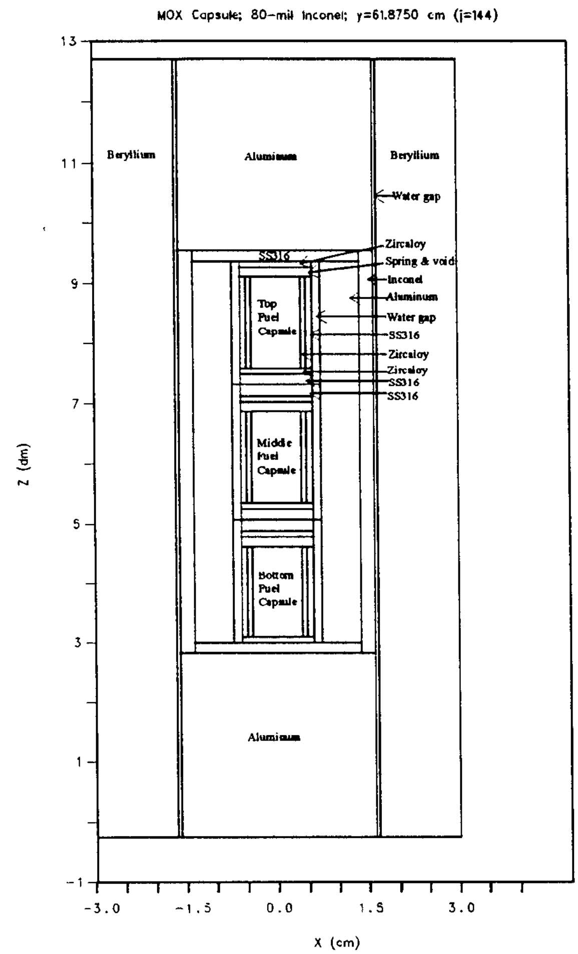

Fig. 3. TORT two-dimensional slice in y-plane showing the axial fuel capsule 1 arrangement for the capsule farthest from the core.

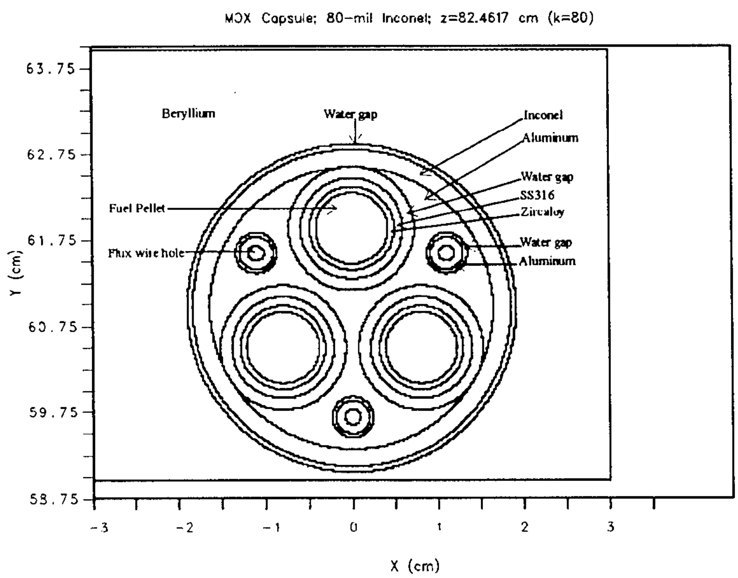

Fig. 4. TORT two-dimensional slice in z-plane through MOX irradiation experiment in NW small I hole I-24.

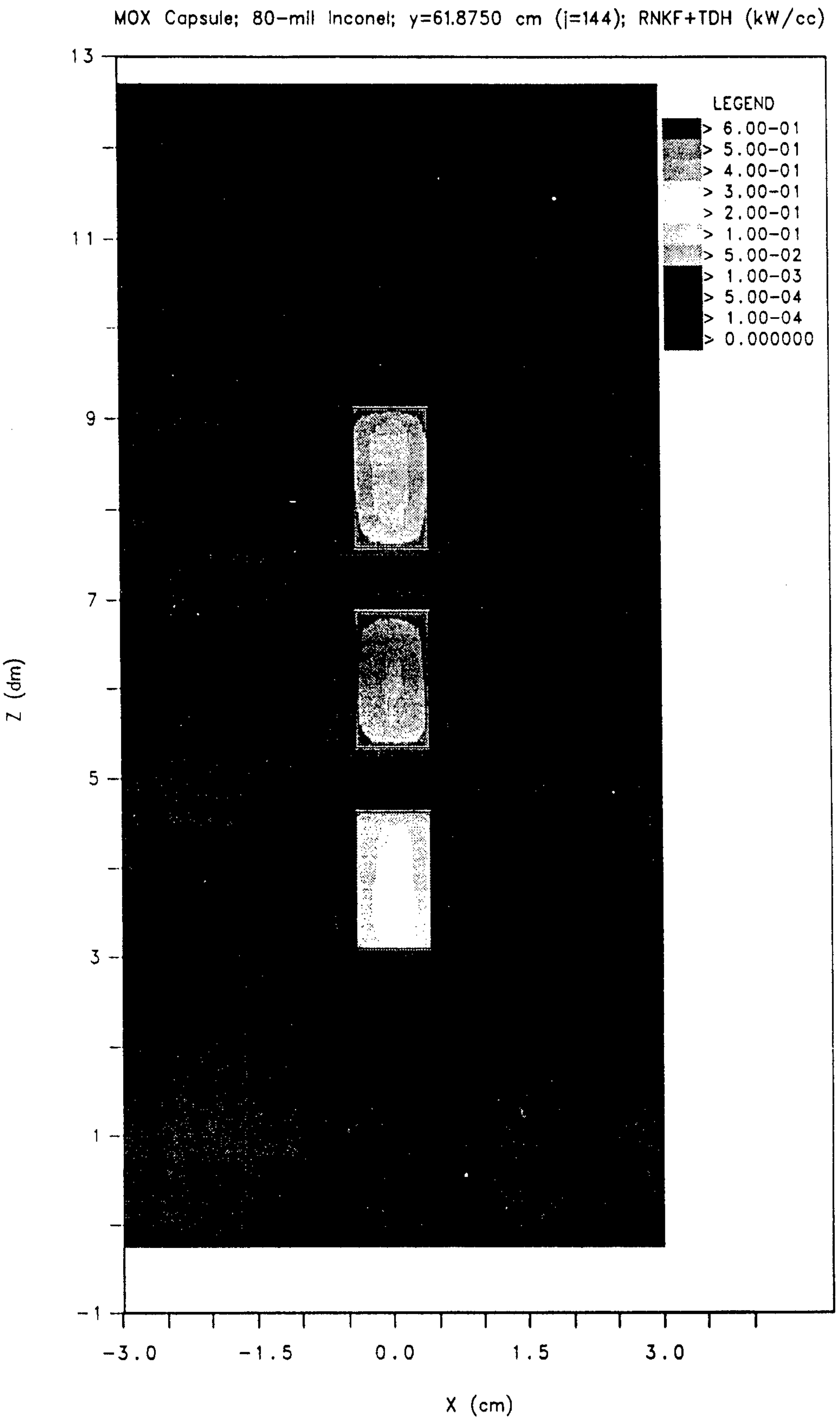

Fig. 5. Heating density (kW/cm³) for MOX capsule geometry shown in Fig. 3.

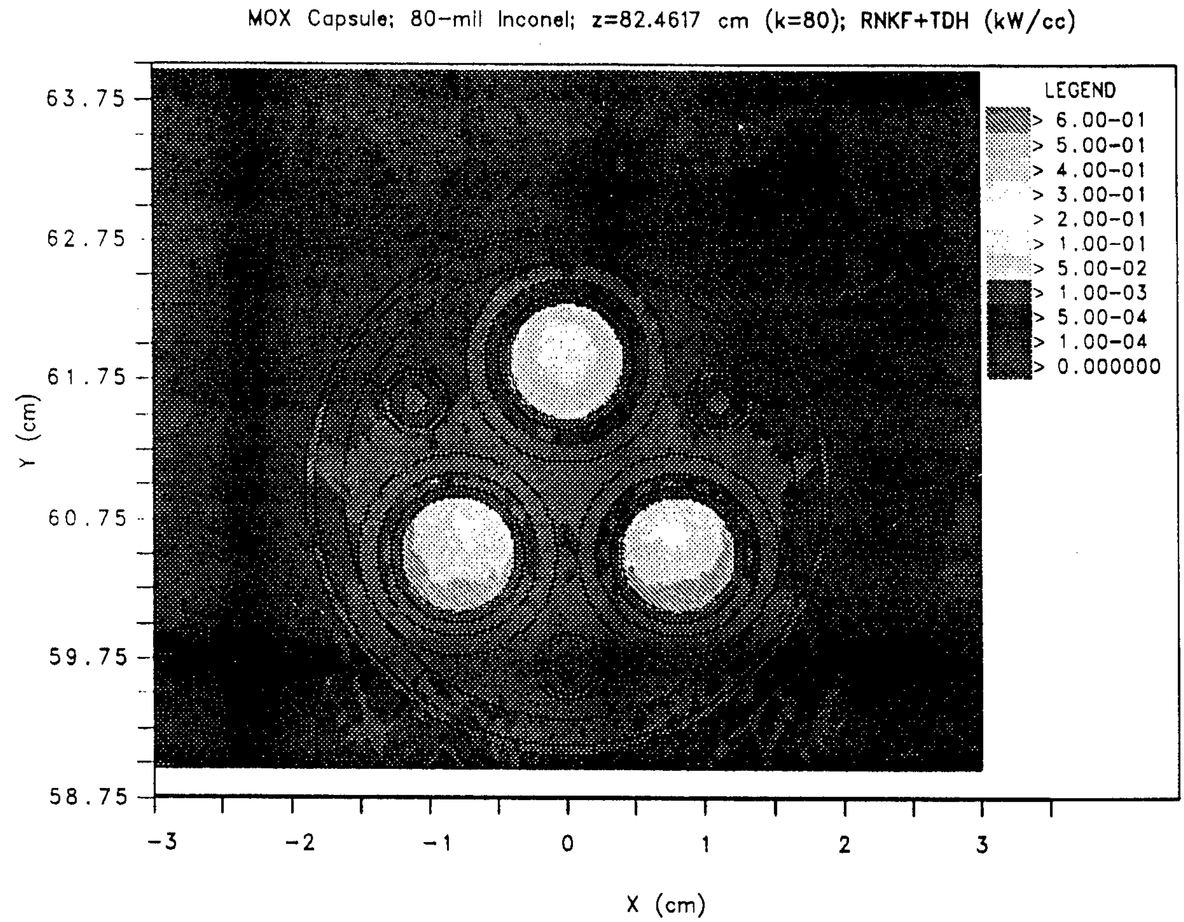

Fig. 6. Heating density (kW/cm^3) for MOX capsule geometry shown in Fig. 4.

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