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NUCLEAR CRITICALITY SAFETY STUDY OF LOSS OF MODERATION CONTROL IN 10-TON AND 2 1/2-TON UF_6 CYLINDERS BY KENO V.a COMPUTER CODE ANALYSES

by

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TABLE OF CONTENTS

LIST OF TABLES

TABLE OF CONTENTS
(Continued)

LIST OF FIGURES

NUCLEAR CRITICALITY SAFETY STUDY OF LOSS OF MODERATION CONTROL IN 10-TON AND 2 1/2-TON UF_6 CYLINDERS BY KENO V.a COMPUTER CODE ANALYSES

INTRODUCTION

Large cylinders with up to 48-inch diameters are routinely used at the Portsmouth Gaseous Diffusion Plant and other DOE-ORO sites for handling, storing, and shipping low enriched uranium hexafluoride (UF_6). For criticality control, the filled cylinders must conform to moderation limits and maximum uranium-235 (U-235) enrichment limits. Moderation control in a filled UF_6 cylinder can be compromised if a cylinder valve is broken off, or the cylinder wall is punctured or split. The expected conditions within a breached cylinder after exposure to wet air or water has previously been a matter of speculation in the case of these large UF_6 cylinders. Thus, a DOE investigating team(1) recommended that an assessment be performed of potential cylinder breach accidents where moderation control may be disturbed. The PAI Corporation at Oak Ridge, Tennessee, performed this assessment regarding the loss of moderation control in large UF_6 cylinders. The nuclear criticality safety (NCS) study presented in this report was performed in support of the NCS assessment(2) by PAI Corporation.

SUMMARY

The purpose of this study was to estimate the required amounts of water entering these large UF_6 cylinders to react with, and to moderate the uranium compounds sufficiently to cause criticality. Hypothetical accident situations were modeled as a uranyl fluoride (UO_2F_2) slab above a UF_6 hemicylinder, or a UO_2F_2 sphere centered within a UF_6 hemicylinder, and were investigated by computational analyses utilizing the KENO V.a(3) Monte Carlo Computer Code. Assumptions, descriptions, and results of the KENO computer code calculations are presented and discussed. The 2 1/2-ton cylinder was evaluated at 5.0 % U-235, and the 10-ton cylinder was evaluated at both 4.5 % and 5.0 % U-235 enrichments. The minimum estimated amounts of water required for criticality were five gallons of water for a spherical geometry, and 129 gallons of water for a slab geometry in a 10-ton cylinder containing UF_6 at 5.0 % enrichment. For the 2 1/2-ton cylinder at 5.0 % U-235 enrichment, the minimum estimated amounts were six gallons of water for a spherical geometry, and 57.5 gallons of water for a slab geometry.

RESULTS

The results of this study are tabulated in Table 1. The estimated minimum amounts of water required for criticality within the large UF_6 cylinders are presented both as pounds and as gallons of water. Also shown are the maximum amounts of water that could enter a cylinder and be considered safe for the given conditions. The six situations represented are the following:

TABLE 1

ESTIMATED CRITICAL AND SAFE PARAMETERS
IN STUDY OF
LOSS OF MODERATION CONTROL IN 10-TON AND 2 1/2-TON CYLINDERS

			Estimated Critical		Estimated Safe	
Cylinder Size	U-235 Assay	Geometry	Pounds Water	Gallons Water	Pounds Water	Gallons Water
10-ton	4.5%	Slab	1,133.8	136.0	992.1	119.0
10-ton	5.0%	Slab	1,075.5	129.0	933.7	112.0
2 1/2-ton	5.0%	Slab	479.4	57.5	429.4	51.5
10-ton	4.5%	Sphere	45.8	5.5	35.8	4.3
10-ton	5.0%	Sphere	41.7	5.0	32.9	3.95
2 1/2-ton	5.0%	Sphere	50.0	6.0	39.2	4.7

1) a moderated UO_2F_2 slab above a UF_6 hemicylinder in a 10-ton cylinder at 4.5 % U-235 enrichment,

2) a moderated UO_2F_2 slab above a UF_6 hemicylinder in a 10-ton cylinder at 5.0 % U-235 enrichment,

3) a moderated UO_2F_2 slab above a UF_6 hemicylinder in a 2 1/2-ton cylinder at 5.0 % U-235 enrichment,

4) a moderated UO_2F_2 sphere centered within a UF_6 hemicylinder in a 10-ton cylinder at 4.5 % U-235 enrichment,

5) a moderated UO_2F_2 sphere centered within a UF_6 hemicylinder in a 10-ton cylinder at 5.0 % U-235 enrichment, and

6) a moderated UO_2F_2 sphere centered within a UF_6 hemicylinder in a 2 1/2-ton cylinder at 5.0 % U-235 enrichment.

In Table 1, six gallons is the estimated amount of water required for criticality in a spherical geometry in a 2 1/2-ton cylinder at 5.0 % U-235 enrichment. It is interesting to note that this is approximately equal to the amount of water required to convert from UF_6, and optimumly moderate, the minimum critical mass of UO_2F_2 at 5.0 % U-235 enrichment when full water reflection is also provided. Also note that the smallest estimated amount of 5 gallons of water in Table 1 is for criticality in the spherical geometry in a 10-ton cylinder at 5.0 % U-235. It appears that a smaller optimumly moderated UO_2F_2 mass is critical since more reactivity is furnished by the thicker UF_6 surrounding the sphere in the larger 10-ton cylinder than in the 2 1/2-ton cylinder, or the water reflection for the minimum critical mass at 5.0 % U-235.

The estimates for the 10-ton cylinder using 4.5 % U-235 enrichment can also be conservatively applied to the 14-ton cylinder.

BACKGROUND

Large 2 1/2-ton, 10-ton, and 14-ton cylinders are routinely used at the Portsmouth Gaseous Diffusion Plant and other DOE-ORO sites for handling, storing, and shipping low enriched UF_6. These large cylinders are not geometrically safe, and the contained uranium mass may greatly exceed the minimum critical mass for the U-235 enrichment involved. Thus, when these large cylinders are used for enriched UF_6, both moderation control limits and maximum U-235 enrichment limits must be met. Moderation control for this purpose is defined as UF_6 having a purity of 99.5 percent or greater. This is equivalent to a hydrogen to uranium (H/U) atomic ratio of 0.088, or less. With moderation control, the U-235 enrichment limits approved by DOE-ORO[4] are 5.0% U-235 for the 2 1/2-ton cylinders, and 4.5% U-235 for the 10-ton cylinders and the Model 48Y 14-ton cylinders.

In this study, the 10-ton cylinder was also investigated at the 5.0% U-235 enrichment level. This was done because the Portsmouth Plant has requested DOE-ORO approval to withdrawal UF_6 up to 5.0% U-235 enrichment into 10-ton cylinders for on-site usage at the Portsmouth Plant.

The Model 48Y 14-ton UF_6 cylinder was not modeled nor investigated during this study because the results for the 10-ton cylinder could conservatively be applied to the 14-ton cylinders.

An H/U atomic ratio of 0.088 is the maximum moderation allowable by DOE-ORO for shipment of enriched UF_6. To assume that this amount of moderation is initially in the UF_6 is a reasonable and conservative assumption for the calculations. Thus, the UF_6 was considered to be moderated by HF to an atomic ratio of H/U = 0.088, which is equivalent to a density of 4.958 $gmUF_6$/cc.

The UO_2F_2 material was considered to be moderated with water, and optimum moderation of the UO_2F_2 would give conservative results in the calculations. Consequently, two series of K-infinity computer problems were run at various H/U values for both 4.5 % U-235 and 5.0 % U-235 enrichments using the CSAS1X control module in the KENO V.a computer code. The results are tabulated in Table 2 and plotted in Figure 1. The maximum K-infinity values are at an H/U of 11 for 4.5 % U-235, and an H/U of 11.65 for 5.0 % U-235 enrichments. Thus, these are the moderation values that were used for the KENO K-effective calculations. The equivalent densities were 2.327 $gmUO_2F_2$/cc and 2.214 $gmUO_2F_2$/cc, respectively.

During all operations, these large cylinders are filled, handled, stored, and transported with their longitudinal axis horizontal. After the cylinder has been filled with liquid UF_6, a cool down period of 5 days is required to allow the UF_6 to solidify. After solidification, a vacuum exists in the cylinder and the normal expected conditions for the UF_6 would be a dense solid mass located in the bottom of the cylinder.

This study considers loss of moderation control only for cylinders containing UF_6 in the solid state. In the case of a cylinder containing liquid UF_6, the internal pressure would force the contents out of the cylinder, thereby preventing moisture or water from entering. The resulting criticality safety problems would be influenced by the conditions outside the cylinder. Many of these situations have been considered in other NCS evaluations and are outside the scope of this study.

ANALYTICAL TECHNIQUE

In contemplating the loss of moderation control, one quickly realizes that there are many possible situations that could occur within a large cylinder containing solid UF_6 when the valve is broken off, or the cylinder wall is breached, and then the cylinder is exposed to moisture or water. Both chemical reactions and the physical conditions must be considered.

The stoichiometry for the reaction between uranium hexafluoride and water is represented by:

$$UF_6 + 2H_2O \rightarrow UO_2F_2 + 4HF\uparrow .$$

TABLE 2

K-INFINITY KENO V.a COMPUTER PROBLEMS
IN STUDY OF
LOSS OF MODERATION CONTROL IN 10-TON AND 2 1/2-TON CYLINDERS

H/U	K-Infinity	
	4.5 % U-235	5.0 % U-235
5.0	1.36671	1.38327
7.5	1.40770	1.42730
9.0	1.41736	1.43878
10.0	1.42021	1.44277
11.0	1.42097	1.44470
12.5	1.41918	1.44454
15.0	1.41068	1.43853
25.0	1.34729	1.38313

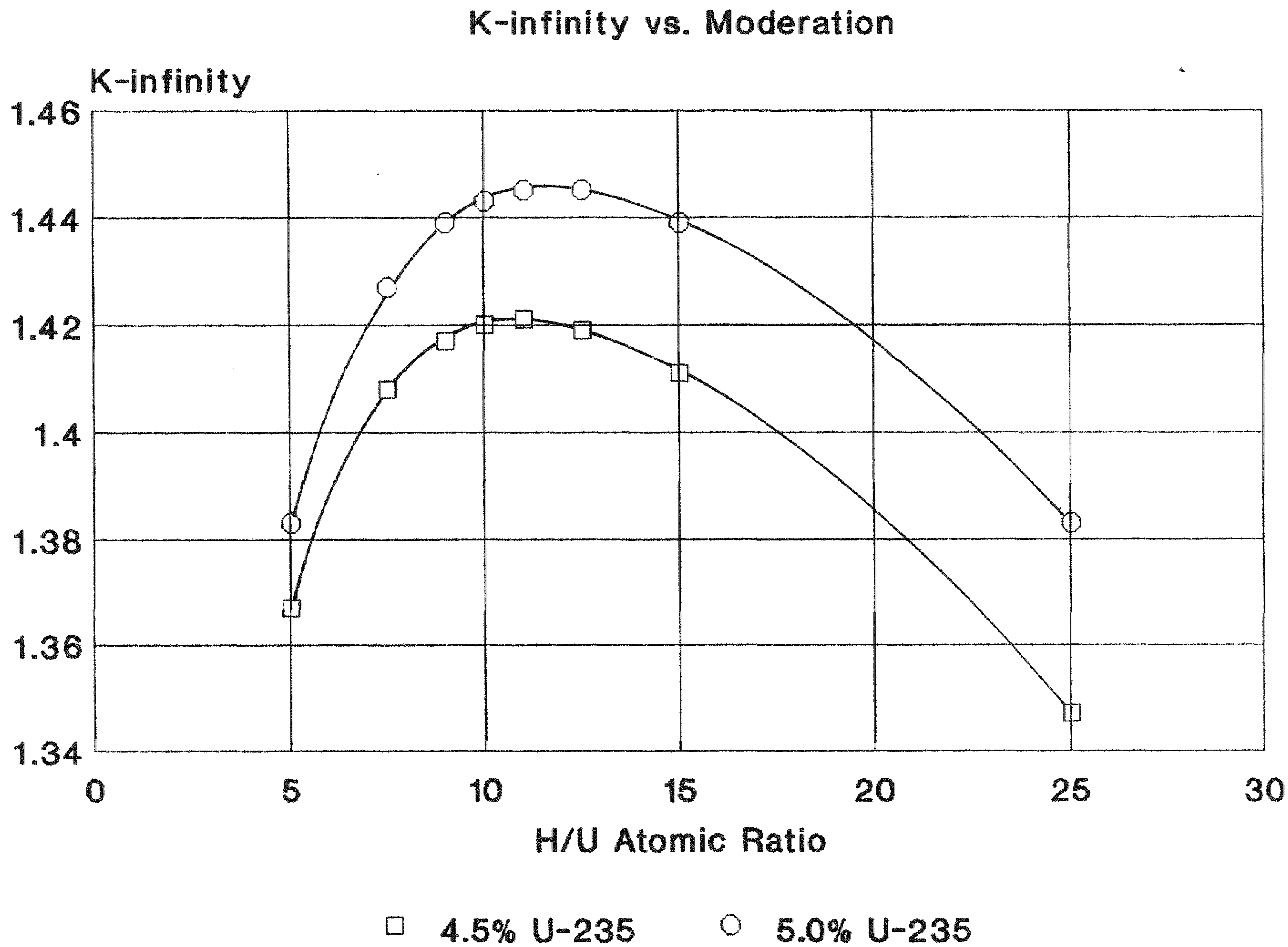

FIGURE 1 - INFINITE UO2F2 SYSTEM

The uranyl fluoride (UO_2F_2) normally exists as a solid and the hydrogen fluoride (HF) normally exists as a gas. However, if excess water is available, both the uranyl fluoride and the hydrogen fluoride are very soluble in the water.

The physical conditions would depend upon several factors such as the location and size of the puncture or opening, source and flow rate of the water into the cylinder, crystalline form and geometry of the solid UF_6 inside the cylinder, lapsed time since water entered the cylinder, etc. However, these conditions and situations fall into two categories. Namely, a breach in the cylinder wall below the upper surface of the solid UF_6 and a breach above the upper surface of the solid UF_6.

In the first category, the moisture or water would contact the solid UF_6 and might possibly seal the hole by forming a solid plug of UO_2F_2 over the opening, at least temporarily. It is the author's opinion that continued exposure of the solid UO_2F_2 plug to water would eventually result in an enlargement or growth of the UO_2F_2 material, possibly forming a spherical, hemispherical, or conical configuration of UO_2F_2 within the UF_6 inside the cylinder.

In the second category, the water entering a cylinder breached above the surface of the solid UF_6 could possibly form UO_2F_2 in the configurations mentioned above if the inleakage was at a slow rate; or, if the inleakage was at a relatively faster rate, into a layer or slab type configuration at the upper surface of the solid UF_6.

Thus, calculations to investigate the spherical geometry would provide estimates for the minimum amounts of water for criticality, and the slab type geometry might be more realistic in particular situations. These two situations would span the other possible geometries. The estimates for the 10-ton cylinder using 4.5 % U-235 enrichment can also be conservatively applied to the 14-ton cylinder.

KENO computer code problems were run to investigate masses of moderated uranium material in slab and spherical geometries in both the 10-ton and 2 1/2-ton cylinders. The 2 1/2-ton cylinder was evaluated at 5.0 % U-235, and the 10-ton cylinder was evaluated at both 4.5 % and 5.0 % U-235 enrichments. At least three problems were run for each situation.

The slab geometry model was an optimumly moderated UO_2F_2 layer above a UF_6 hemicylinder inside a carbon steel cylinder, which was reflected at the bottom by 12-inch thick concrete. The spherical geometry model was an optimumly moderated UO_2F_2 sphere located at the center of the UF_6 hemicylinder inside a carbon steel cylinder, similarly reflected. A representation of the KENO 10-ton cylinder model with a UO_2F_2 slab is shown in Figure 1, and a representation of the KENO 2 1/2-ton cylinder model with a UO_2F_2 sphere is shown in Figure 2.

Please note that the cylinders were modeled lengthwise as three equal units. This allowed the "cosine" neutron start type to be used in the KENO calculations and ensured that most of the 300 neutron per generation would be started in the middle unit. This was considered especially important in the problems for the spherical geometry.

Model 48X 10-ton Cylinder

Inside diameter	48.125"
Outside diameter	49.355"
Wall thickness	0.615"
Inside length	115.52"
Outside length	116.75"

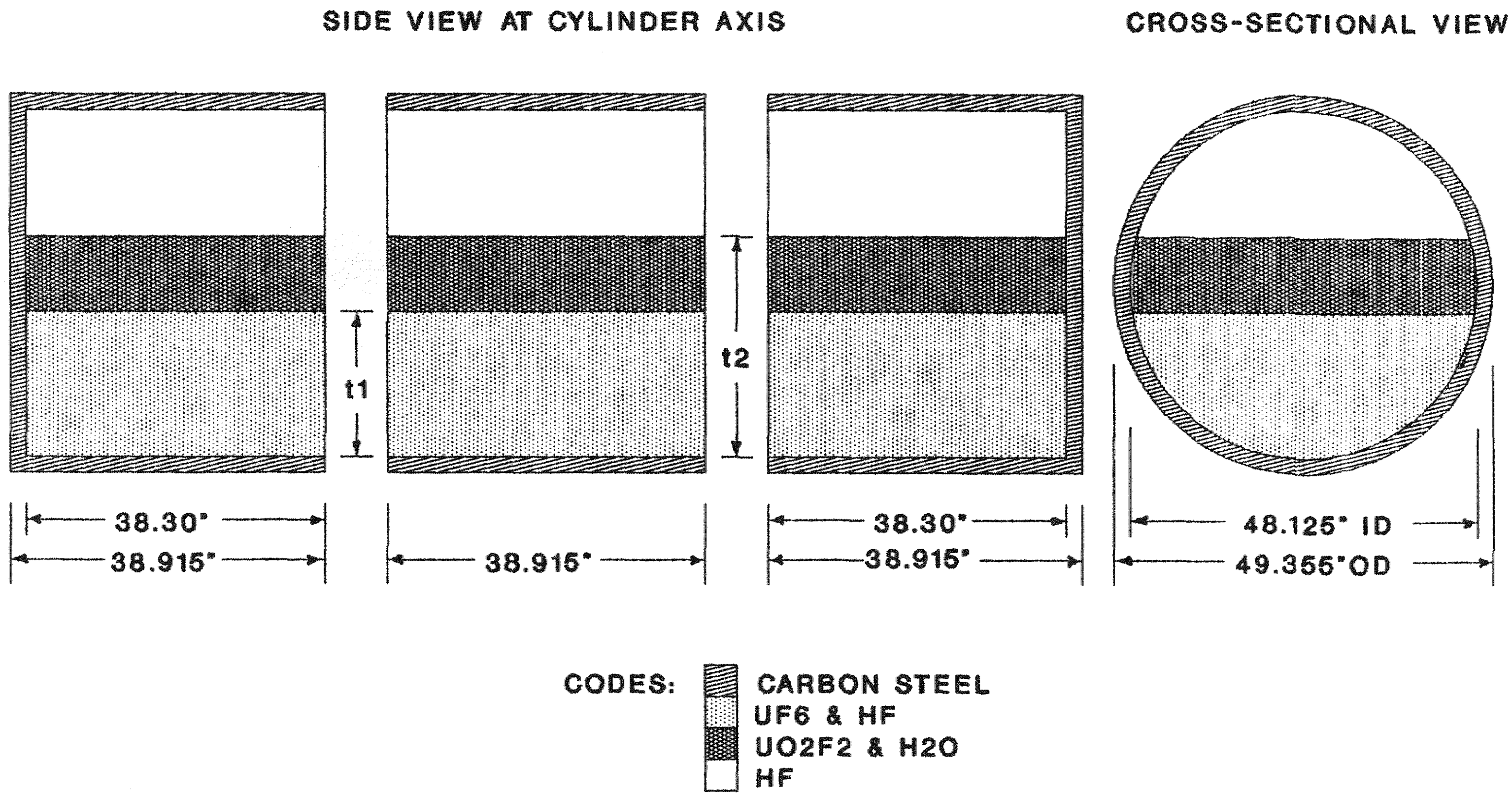

FIGURE 2 - KENO 10-TON CYLINDER MODEL WITH UO2F2 SLAB

MODEL 30B 2 1/2-TON CYLINDER

Inside diameter	29.25"
Outside diameter	30.25"
Wall thickness	0.50"
Inside length	75.50"
Outside length	76.50"

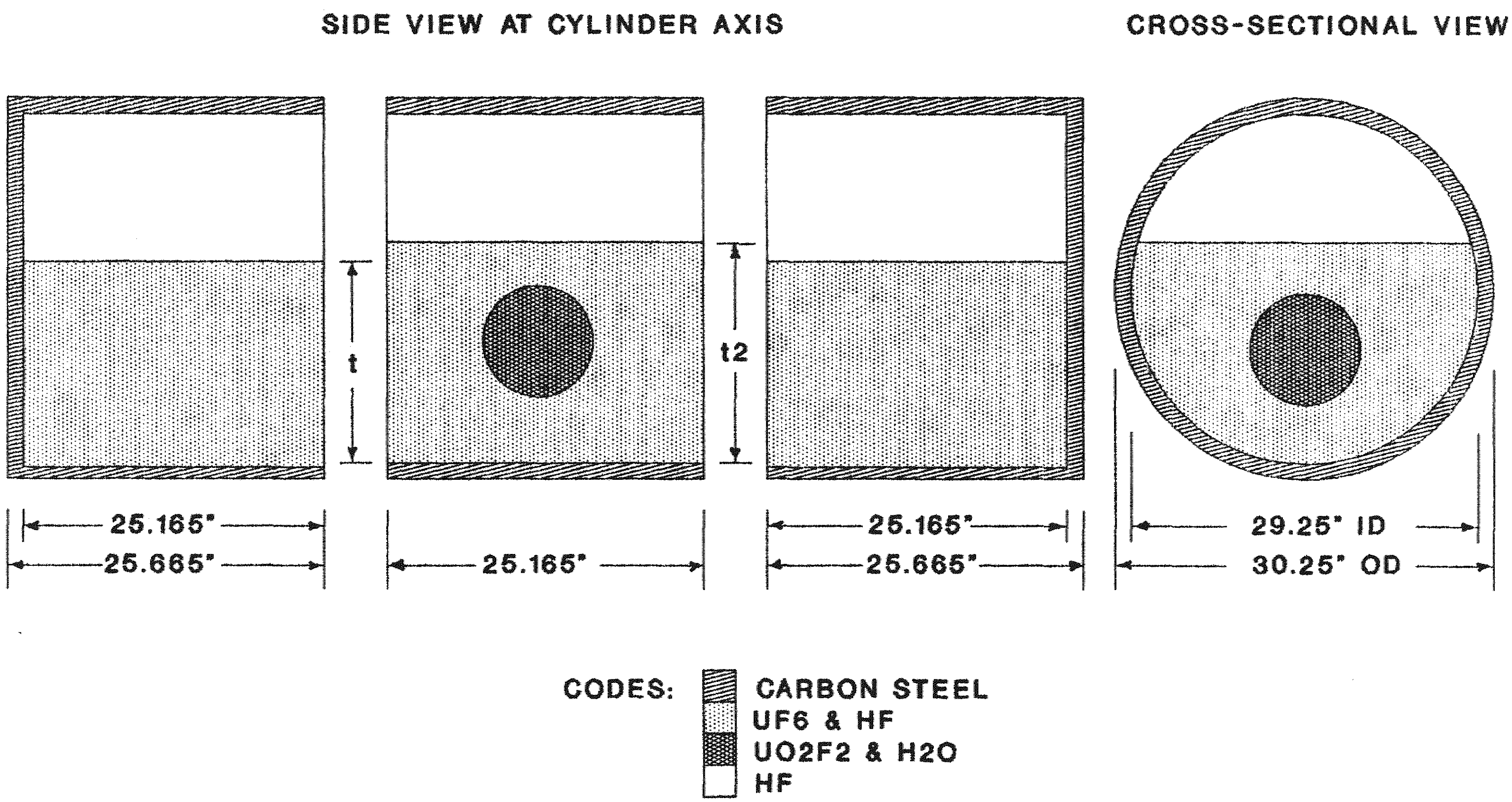

FIGURE 3 - KENO 2 1/2-TON CYLINDER MODEL WITH UO2F2 SPHERE

To create different KENO problems, the thickness of the UO_2F_2 slab or sphere diameter was varied for a particular geometry type and U-235 enrichment. As the volume of UO_2F_2 was varied, the volume of UF_6 was changed by an equivalent amount to simulate the UF_6 being converted to UO_2F_2 by reacting with water. Thus, the upper surface of the UF_6 hemicylinder, and the upper surface of the UO_2F_2 slab, as appropriate, were adjusted in each problem so that the total uranium mass remained constant within the round-off error of the calculations.

In the problems for the spherical geometry, only the UF_6 surface in the middle unit was changed. This was a choice in geometry modeling technique, and is not considered significant in these particular problems.

Fortran programs for an IBM personal computer were written and utilized to calculate these changes for the KENO input data. Examples of the Fortran input and output data and the KENO input data for Problems 2 and 19 are presented in Appendix 1.

The Fortran programs also calculated KENO nuclide number densities for the total mass of HF both liberated and produced during the chemical reaction between UF_6 and water for each particular problem. The total HF mass was first considered as remaining in the cylinder and occupying the otherwise void volume above the UF_6 and UO_2F_2 materials. The HF is mixture 3 in the KENO input data.

In the slab type geometries, the nuclide number densities were relatively high and were equivalent to several atmospheres of pressure inside the cylinder. This increased the K-eff value approximately 7 to 8 percent compared to problems with void or HF at atmospheric pressure in this volume. It was judged that this high pressure was unrealistic, since the HF could get out if water could get into the cylinder. Especially, since the slab geometries represented a cylinder breached above the surface of the solid UF_6. Consequently, for the problems listed in Table 3, the HF was considered to be at atmospheric pressure for the slab geometry problems, and were the actual number densities calculated by the Fortran program for the spherical geometry problems.

At least three KENO computer problems were run for each of the six situations so that the calculated K-effective values spanned the range of interest. The final list of KENO problems used in this study is presented in Table 3.

These K-effective values plotted as a function of gallons of water for each particular geometry type and U-235 enrichment are shown in Figures 4 through 7. The estimated critical and safe amounts of water for each situation were taken where the curves intersect the K-effective values of 1.0 and 0.95, respectively, in Figures 4 through 7. These interpolated data were used as the estimated critical and safe amounts of water presented in Table 1.

Keno V.a problems[5] used in this study to validate the KENO V.a SCALE package on the unclassified 3081 computer at the K-25 Computer Facility are discussed in Appendix 1.

TABLE 3

K-EFFECTIVE KENO V.a COMPUTER PROBLEMS
IN STUDY OF
LOSS OF MODERATION CONTROL IN 10-TON AND 2 1/2-TON CYLINDERS

Problem No.	U-235 Assay	Thickness S/D*	Thickness Total	Pounds H2O	Gallons H2O	K-eff	Standard Deviation
			10-Ton Cylinder with Slab				
1	4.5%	4.490"	28.271"	916.566	109.94	0.91785	+/- 0.00440
2	4.5%	5.050"	28.531"	1,031.248	123.70	0.96526	+/- 0.00465
3	4.5%	5.800"	28.881"	1,184.102	142.03	1.01170	+/- 0.00452
4	5.0%	3.931"	28.111"	796.767	95.57	0.89423	+/- 0.00416
5	5.0%	4.501"	28.391"	912.465	109.45	0.94220	+/- 0.00440
6	5.0%	5.121"	28.701"	1,036.122	124.28	0.98674	+/- 0.00417
7	5.0%	5.495"	28.881"	1,113.493	133.56	1.01308	+/- 0.00446
8	5.0%	5.900"	28.931"	1,203.196	144.32	1.03348	+/- 0.00450
			2 1/2-Ton Cylinder with Slab				
9	5.0%	5.000"	18.231"	401.517	48.16	0.91345	+/- 0.00487
10	5.0%	5.758"	18.611"	461.065	55.09	0.98169	+/- 0.00471
11	5.0%	6.249"	18.851"	500.504	60.03	1.01488	+/- 0.00421
			10-Ton Cylinder with Sphere				
12	4.5%	10.0"	26.465"	19.315	2.32	0.83373	+/- 0.00354
13	4.5%	12.0"	26.672"	33.377	4.00	0.93384	+/- 0.00389
14	4.5%	14.0"	26.961"	53.002	6.36	1.02190	+/- 0.00418
15	5.0%	10.0"	26.464"	19.167	2.30	0.85638	+/- 0.00393
16	5.0%	12.0"	26.671"	33.121	3.97	0.95276	+/- 0.00420
17	5.0%	14.0"	26.960"	52.595	6.31	1.03622	+/- 0.00434
			2 1/2-Ton Cylinder with Sphere				
18	5.0%	11.0"	16.721"	25.512	3.06	0.87297	+/- 0.00357
19	5.0%	13.0"	17.346"	42.111	5.05	0.96544	+/- 0.00454
20	5.0%	15.0"	18.204"	64.690	7.76	1.03314	+/- 0.00394

* Slab thickness or sphere diameter of UO2F2.

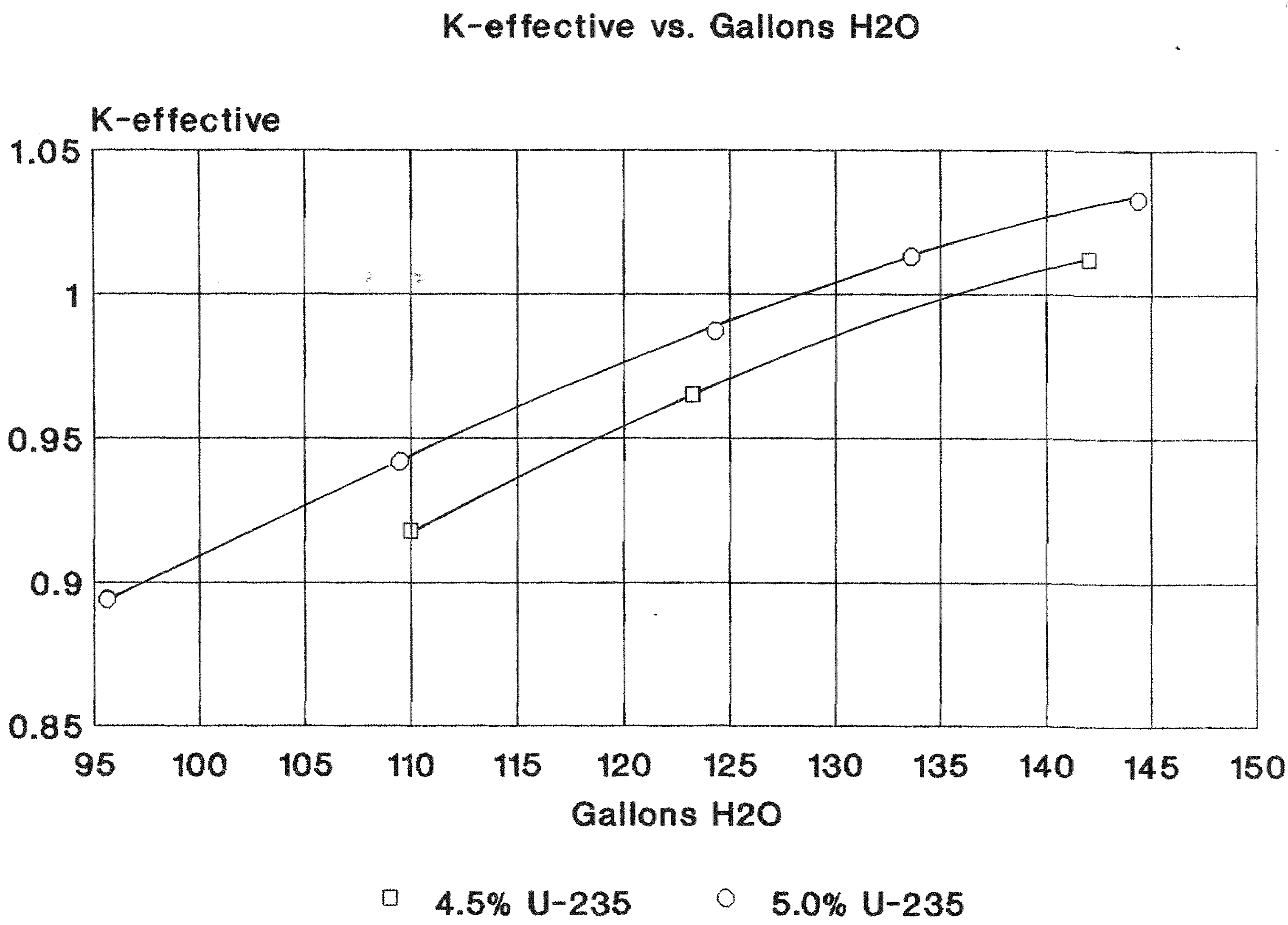

FIGURE 4 - UO2F2 SLAB IN MODEL 48X 10-TON CYLINDER

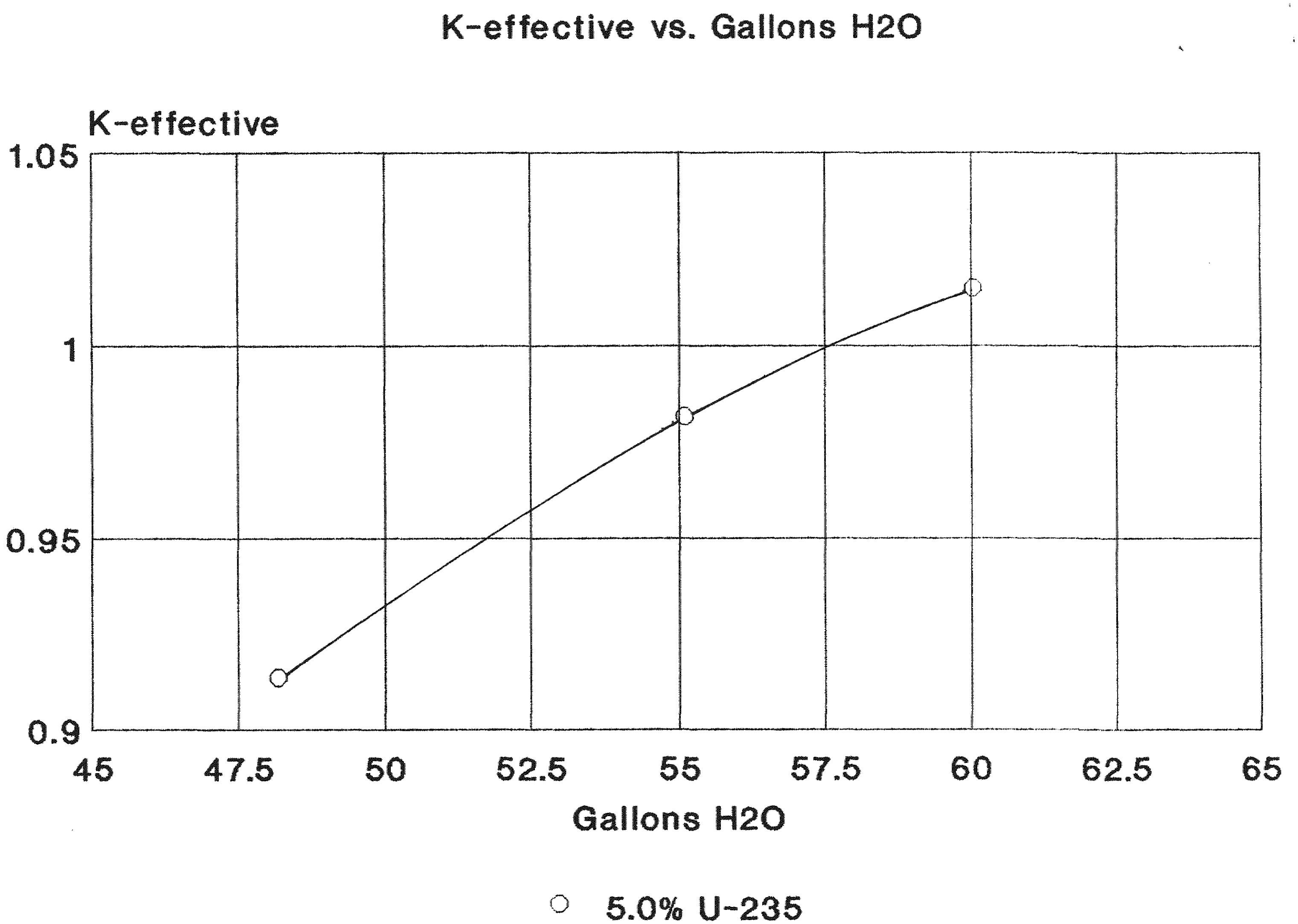

FIGURE 5 - UO2F2 SLAB IN MODEL 30B 2 1/2-TON CYLINDER

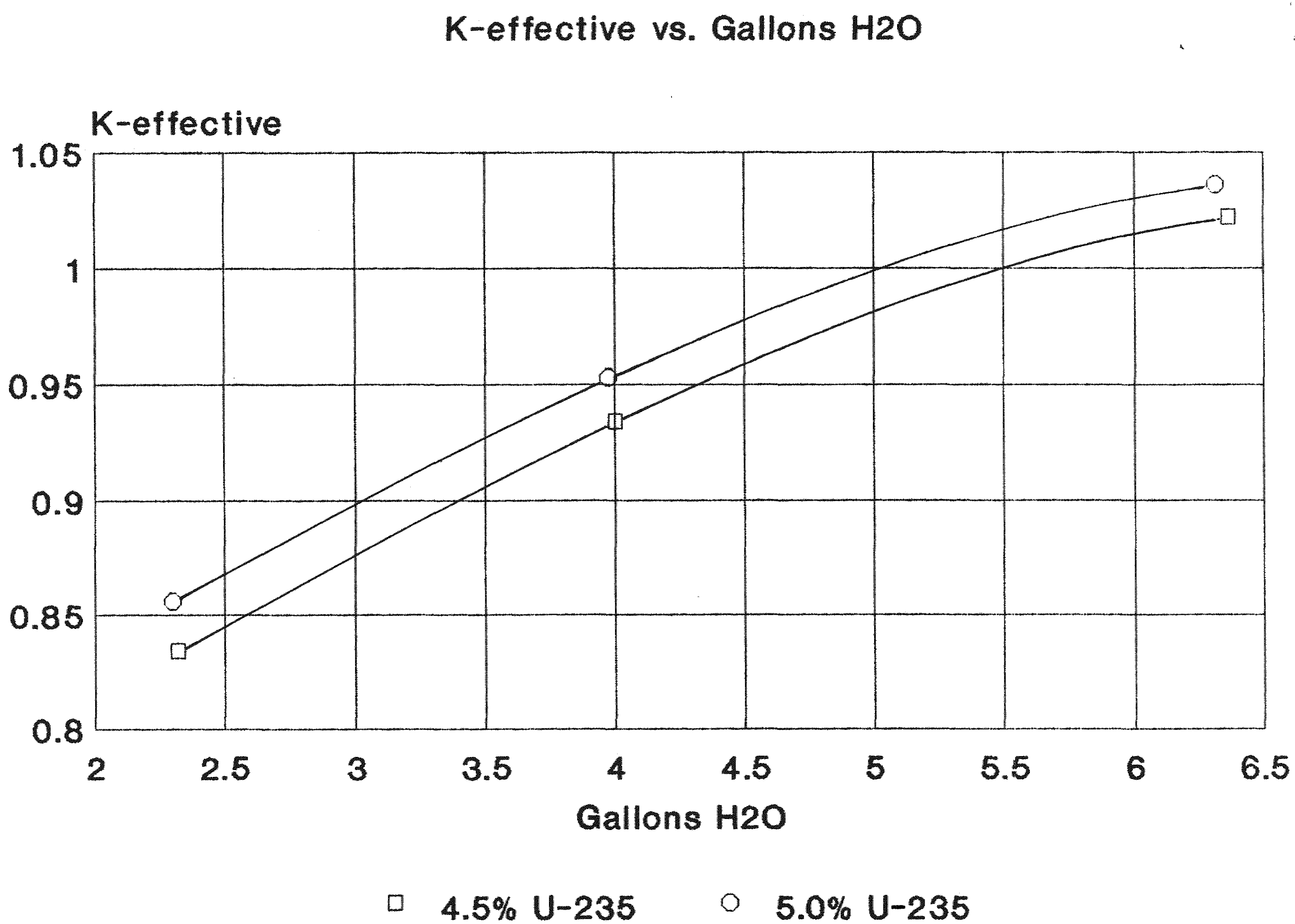

FIGURE 6 - UO2F2 SHPERE IN MODEL 48X 10-TON CYLINDER

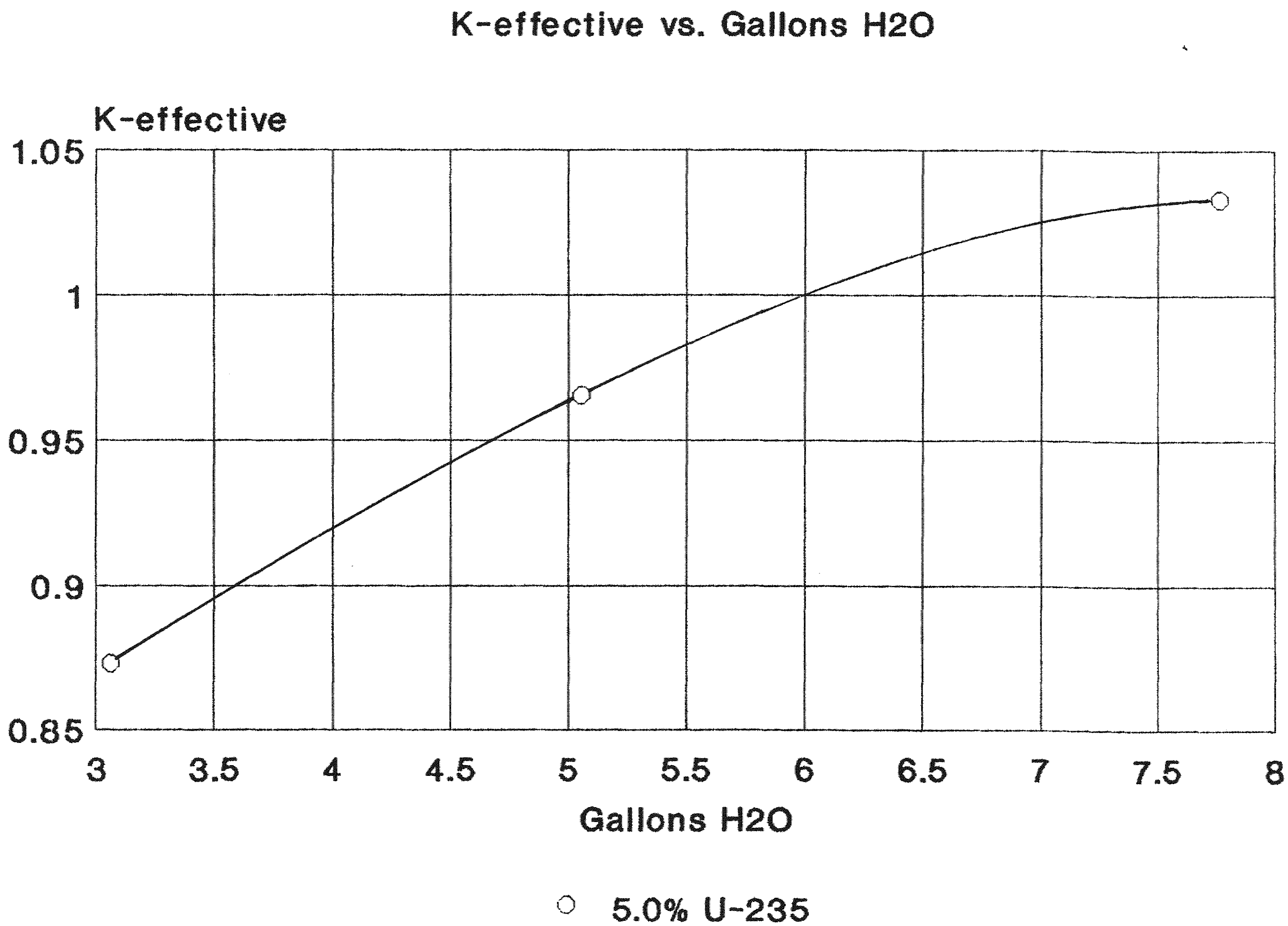

FIGURE 7 - UO2F2 SPHERE IN MODEL 30B 2 1/2-TON CYLINDER

REFERENCES

1. UF_6 Cylinder Drop Investigation and Cylinder Lifting Program, DOE/ORO-888, March 1, 1988.

2. W. A. Pryor, *Proposed Scope of Study to Implement Nuclear Criticality Safety in Response to Report DOE/ORO-888 Entitled "UF_6 Cylinder Drop Investigation and Cylinder Lifting Program Review" of March 1, 1988,* Unclassified, PAI Corporation, Oak Ridge, Tennessee, June 20, 1988.

3. L. M. Petrie and N. F. Landers, "KENO V.a An Improved Monte Carlo Criticality Program With Supergrouping," *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation,* Section F11, NUREG/CR-200, Volume 2, U.S. Nuclear Regulatory Commission, Published December 1984.

4. Uranium Hexafluoride: Handling Procedures and Container Criteria, ORO-651, Revision 5, Oak Ridge Operations, United States Department of Energy, Oak Ridge, Tennessee, November, 1986.

5. W. C. Jordan, N. F. Landers, and L. M. Petrie, *Validation of KENO V.a Comparison with Critical Experiments,* ORNL/CSD/TM-238, Unclassified, Martin Marietta Energy Systems, Computing and Telecommunications Division, Oak Ridge National Laboratory, December 1986.

KENO Validation Problems

Case CAS25 in Table 3 of the Reference 5 report was the best experimental data located that simulated the uranium materials and the KENO geometry models for the problems being contemplated for this study. Thus, this case was chosen to provide validation data that the KENO V.a Computer Code Module being used for the problems presented in this report was working properly, and had not been altered during the period these problems had been run.

The experimental description given on page 11 of the Reference 5 report is as follows:

Case	Experimental description	Reference	K-eff +/-
CAS25	A reflected rectangular parallelepiped of homogeneous $U(3)F_4$ and paraffin with an H/U-235 atomic ratio of 133.4; 61.36 cm x 61.36 cm x 38.67 cm, reflected with 15.2 cm of paraffin on top and sides and 15.2 cm of Plexiglas on the bottom	18*	1.0201 +/- 0.0032

* S. J. Raffety and J. T. Mihalczo, *Homogenized Critical Assemblies of 2 and 3% Enriched Uranium in Paraffin,* Y-DR-14, Union Carbide Corporation, Nuclear Division, Oak Ridge Y-12 Plant, 1969.

The problem input is given in Table A.3 on Page A-44 of the Reference 5 report. This input is actually two problems back-to-back, one using the 27 group NDF4 cross-section library, and the other using the 16 group Hansen-Roach cross-section library. The reference problem was originally run on the 3033 computer at ORNL using KENO V.a in the Y12CSG package.

This input data for the 27 group NDF4 cross-section library was run at 1008 hours on February 23, 1989, using KENO V.a in the SCALE package on the unclassified IBM 3081 computer at the K-25 Computer Facility. This same input was run at 1013 hours on December 8, 1989. The K-effective values and standard deviations were 1.01490 +/- 0.00395 in both cases.

Attempts on February 23, and December 8, 1989, to run the input data for the 16 group Hansen-Roach library was unsuccessful using KENO V.a in the SCALE package on the unclassified IBM 3081 computer. However, at 0233 hours on December 9, 1989, the 16 group input was executed successfully using the KENO V.a Y12CSG77 package on the unclassified IBM 3081 computer. The K-effective value and standard deviation were 1.01820 +/- 0.00345. The input data for the 16 group Hansen-Roach library was also successfully executed at 1822 hours, December 12, 1989, using the KENO V.a SCALE77 package on the unclassified IBM 3081 computer. The K-effective value and standard deviation were also 1.01820 +/- 0.00345.

All of these values agree within two standard deviations of the K-effective value listed above for the case CAS25 problem in the Reference 5 report, and the largest difference is approximately 0.5 percent.

Considering that different computers and KENO V.a packages and modules were used, that the random starting numbers were probably different, and that I was uncertain for a time that the reference K-effective value was obtained using the 27GROUPNDF4 27-group, or the HANSEN-ROACH 16-group cross-section libraries, it appears that the KENO V.a SCALE package on the 3081 computer that was used to run the problem presented in this report was performing satisfactorily, and had not been modified by program changes that effected the type of problems being run.

A positive bias of greater than 1.5 percent in cases CAS21 through CAS32 in Table 3 of Reference 5 is discussed on page 49 of the referenced report. For case CAS25, for example, the K-effective value was 1.0201 using the standard NITAWL treatment, and this value was reduced to 1.0066 by using a modified treatment of the cross-section data.

Thus, it appears that the problems presented in this report also have a positive bias. Since the bias is conservative for the situations investigated, no attempt was made to quantify this bias, nor to modify the calculated K-effective values presented in Table 3.

Summary of Assumptions for KENO Problems

1. In mixture 1, the uranium materials were considered to be UF_6 moderated by HF to an atomic ratio of H/U = 0.088. This is equivalent to a density of 4.958 gmUF_6/cc.

2. In mixture 2, the uranium materials were considered to be UO_2F_2 optimumly moderated by H_2O. From the data presented in Table 2 and the curves shown in Figure 1, the optimum moderation is at an H/U atomic ratio of 11 for 4.5 percent U-235 enrichment, and an H/U of 11.65 for 5.0% U-235 enrichment. The equivalent densities were 2.327 gmUO_2F_2/cc and 2.214 gmUO_2F_2/cc, respectively.

3. The assays in both mixtures 1 and 2 were either 4.5 % U-235, 0.039 % U-234, and 95.461 % U-238 or 5.0 % U-235, 0.043 % U-234, and 94.957 % U-238.

4. In mixture 3, the hydrogen and fluorine nuclide number densities were equivalent to HF at atmospheric pressure in the slab geometry problems. The actual calculated number densities equivalent to the HF liberated and produced in the chemical reaction between the UF_6 and water were used in the spherical geometry problems.

5. The 2 1/2-ton and 10-ton UF_6 cylinders were modeled from the data presented in Report ORO-651, Revision 5[4] for the Model 30B and 48X cylinders, respectively. The maximum inside dimensions and the minimum wall thicknesses were used. The dimensions used were as follows:

Parameter	Model 30B 2 1/2-ton Cylinder	Model 48X 10-ton Cylinder
Inside diameter	29.25"	48.125"
Outside diameter	30.25"	49.355"
Wall thickness	0.50"	0.615"
Inside length	75.50"	115.52"
Outside length	76.50"	116.75"

6. The longitudinal axis of the cylinder was in the horizontal plane.

7. The mass of solid UF_6 was considered to have a uniform density throughout, and to be in a hemicylinder occupying the lower portion of the steel cylinder.

8. The layer, or slab, of UO_2F_2 was located above the mass of UF_6, and its edges conformed to the steel cylinder walls.

9. The sphere of UO_2F_2 was located at the center of the cylinder lengthwise, and was vertically centered midway between the inside bottom of the cylinder and the surface of the solid UF_6.

10. The surface of the UF_6 was adjusted from problem to problem to maintain a constant uranium mass equivalent to the cylinder fill limit. Thus, the total mass of UF_6 and UO_2F_2 in a cylinder changed from problem to problem, but the mass of uranium remained constant, within the round-off error of the calculations.

11. The cylinder was modeled in three equal units lengthwise for the KENO calculations and a cosine neutron start type was used. Thus, a large majority of the neutrons were started in the middle one-third of the cylinder in the vicinity of most interest.

12. The default values of 300 neutrons per generation, 103 generations, and 3 generations skipped were used in these problems.

13. The cylinder was reflected only at the bottom with 12-inch thick concrete. The replicate option with biasing was used.

TABLE 4

FORTRAN INPUT AND OUTPUT DATA
FOR KENO INPUT TO
PROBLEM 2

```
C1SLAB.30B
4.5% U-235 UO2F2 slab in 10-ton cylinder

The input and output data are the following:

wt4         0.039  weight percent U-234
wt5         4.500  weight percent U-235
wt8        95.461  weight percent U-238
d          48.125  inside cylinder diameter
l         115.520  inside cylinder length
r          24.063  inside cylinder radius.
mnet    21030.0    net weight UF6/HF in cylinder before reaction
mhfi      104.688  pounds HF in UF6 before reaction
massu   14147.1    net weight U in cylinder before reaction
h1          0.088  H/U atomic ratio of UF6/HF
h2         11.000  H/U atomic ratio of UO2F2/H2O
du1         3.352  gmU/cc density of UF6
duf6        4.958  gmUF6/cc density of UF6
du2         1.798  gmU/cc in UO2F2
duo2f2      2.327  gmUO2F2/cc in UO2F2
                t       massu         atest         dif
           26.181     14147.1       14147.6        -0.5
chord       2.118  initial chord position for UF6
dec         2.700  inches UF6 surface is decreased
mh2oc     275.000  mass H2O consumed in the reaction
mh2om     756.249  mass H2O to moderate UO2F2 layer
mh2ot    1031.248  mass H2O total, both consumed and for moderation
mhfv3     624.223  mass HF total, both liberated and produced
               t2      mu2tot         btest        diff
           28.531      8430.6        8432.3        -1.7
t1         23.481  inches thickness for new UF6 surface
t2         28.531  total thickness of v1 (UF6) and v2 (UO2F2)
tuo2f2      5.050  thickness of UO2F2 slab
chord1     -0.582  inches UF6 chord after reaction - (  -1.477  cm)
chord2      4.469  inches UO2F2 chord after reaction - (  11.350  cm)
ndhfv3 .647240E-02 HF number density in V3 for KENO input
```

TABLE 5

KENO INPUT FOR PROBLEM 2

```
=CSAS25
TENTON.30B - UF6 (H/U=.088) WITH UO2F2 (H/U = 11.0) SLAB IN 10-TON CYLINDER
27GROUPNDF4     INFHOMMEDIUM
H              1  0.0  7.46667-4    END
F              1  0.0  5.16558-2    END
U-234          1  0.0  3.36383-6    END
U-235          1  0.0  3.86478-4    END
U-238          1  0.0  8.09501-3    END
H              2  0.0  5.00612-2    END
O              2  0.0  3.41326-2    END
F              2  0.0  9.10203-3    END
U-234          2  0.0  1.80425-6    END
U-235          2  0.0  2.07295-4    END
U-238          2  0.0  4.34192-3    END
H              3  0.0  2.68880-5    END
F              3  0.0  2.68880-5    END
CARBONSTEEL    4  1.0               END
REG-CONCRETE   5  1.0               END       END COMP
CASE - 4.5 % U-235, .039 % U-234, 4.958 GMUF6/CC, 2.327 GMUO2F2/CC
READ PARAMETERS    TME=16    NUB=YES    FLX=YES    FDN=YES    END PARAMETERS
READ GEOMETRY
UNIT 1
COM=' UF6 T = 23.481", UO2F2 T = 28.531" - LEFT THIRD OF 10-TON CYLINDER '
YHEMICYL-Z     1  1  61.12               98.85    1.562   CHORD    -1.477
YHEMICYL-Z     2  1  61.12               98.85    1.562   CHORD    11.350
YCYLINDER      3  1  61.12               98.85    1.562
YCYLINDER      4  1  62.68               98.85    0.0
CUBOID         0  1  62.68    -62.68     98.85    0.0     62.68    -62.68
UNIT 2
COM=' 5.050" UO2F2 SLAB - MIDDLE THIRD OF 10-TON CYLINDER '
YHEMICYL-Z     1  1  61.12               49.425 -49.425   CHORD    -1.477
YHEMICYL-Z     2  1  61.12               49.425 -49.425   CHORD    11.350
YCYLINDER      3  1  61.12               49.425 -49.425
YCYLINDER      4  1  62.68               49.425 -49.425
CUBOID         0  1  62.68    -62.68     49.425 -49.425   62.68    -62.68
UNIT 3
COM=' RIGHT THIRD OF 10-TON CYLINDER '
YHEMICYL-Z     1  1  61.12               97.288   0.0     CHORD    -1.477
YHEMICYL-Z     2  1  61.12               97.288   0.0     CHORD    11.350
YCYLINDER      3  1  61.12               97.288   0.0
YCYLINDER      4  1  62.68               98.85    0.0
CUBOID         0  1  62.68    -62.68     98.85    0.0     62.68    -62.68
CORE           0  1   0.0       0.0       0.0
REPLICATE      5  2   0.0       0.0       0.0     0.0      0.0       5.0   5
REPLICATE      5  7   0.0       0.0       0.0     0.0      0.0       5.48  1
END GEOMETRY
READ BIAS      ID=301   2   7    END BIAS
READ ARRAY     ARA=1   NUX=1    NUY=3   NUZ=1
               FILL  1  2  3     END FILL        END ARRAY
READ PLOT      TTL='  VERTICAL SLICE ALONG THE CYLINDER AXIS'
               XUL=     62.68  YUL=     -5.0     ZUL=    130.0
               XLR=     62.68  YLR=   300.0      ZLR=     -5.0
               VAX=      1     WDN=     -1       NAX=    130
               NCH=' *+.#@'    RUN=  YES         PLT=    YES      END
               TTL='  VERTICAL SLICE ACROSS CYLINDER AT THE MIDDLE'
               XUL=     -5.0   YUL=  148.275     ZUL=    130.0
               XLR=    130.0   YLR=  148.275     ZLR=     -5.0
               UAX=      1     WDN=    -1        NAX=    130
               NCH=' *+.#@'    RUN=  YES         PLT=    YES      END
END PLOT
READ START     NST=1    END START
END DATA
END
```

TABLE 6

FORTRAN INPUT AND OUTPUT DATA FOR KENO INPUT TO PROBLEM 19

```
C3SPH.07B
5.0% U-235 UO2F2 sphere in 2 1/2-ton cylinder

The input and output data are the following:

wt4           .043  weight percent U-234
wt5          5.000  weight percent U-235
wt8         94.957  weight percent U-238
id          29.250  inside cylinder diameter
l           75.500  inside cylinder length
r           14.625  inside cylinder radius (  37.147 cm)
mnet      5020.0    net weight UF6/HF in cylinder before reaction
mhfi        24.991  pounds HF in UF6 before reaction
massu     3376.9    net weight U in cylinder before reaction
h1            .088  H/U atomic ratio of UF6/HF
h2          11.650  H/U atomic ratio of UO2F2/H2O
du1          3.352  gmU/cc density of UF6
duf6         4.958  gmUF6/cc density of UF6
du2          1.710  gmU/cc in UO2F2
duo2f2       2.214  gmUO2F2/cc in UO2F2
                 t       massu         atest         dif
            15.768       3376.9        3377.2         -.3
chord        1.143  initial chord position for UF6 (   2.903 cm)
r2           6.500  radius of the UO2F2 sphere (  16.510 cm)
d2          13.000  diameter of the UO2F2 sphere
volsph    1150.347  cuin volume of UO2F2 sphere
mu1sph     139.305  mass U as UF6 in sphere
mu2sph      71.066  mass U as UO2F2 in sphere
mh2oc       10.763  mass H2O consumed in the reaction
mh2om       31.348  mass H2O to moderate UO2F2 sphere
mh2ot       42.111  mass H2O total, both consumed and for moderation
mhfl          .526  mass HF liberated from UF6 in the reaction
mhfp        23.905  mass HF produced in the reaction
mhfv3       24.431  mass HF total, both liberated and produced
                t2       mu2tot        btest         diff
            17.346       1265.0        1265.1         -.1
t2          17.346  inches new UF6 surface in middle 1/3 of cylinder
chord2       2.721  inches UF6 chord after reaction (   6.911 cm)
ndhfv3 .988767D-03 HF number density in V3 for KENO input
y2          -5.952  Z inches value for sphere origin ( -15.118 cm)
```

TABLE 7

KENO INPUT FOR PROBLEM 19

```
=CSAS25
TWOTON.07B - UF6 (H/U=.088) WITH UO2F2 (H/U=11.65) SPHERE IN 2 1/2-TON CYLINDER
27GROUPNDF4     INFHOMMEDIUM
H               1  0.0  7.46699-4     END
F               1  0.0  5.16580-2     END
U-234           1  0.0  3.70876-6     END
U-235           1  0.0  4.29410-4     END
U-238           1  0.0  8.05210-3     END
H               2  0.0  5.04449-2     END
O               2  0.0  3.38825-2     END
F               2  0.0  8.66007-3     END
U-234           2  0.0  1.89259-6     END
U-235           2  0.0  2.19130-4     END
U-238           2  0.0  4.10901-3     END
H               3  0.0  9.88767-4     END
F               3  0.0  9.88767-4     END
CARBONSTEEL     4  1.0                END
REG-CONCRETE    5  1.0                END
END COMP
CASE - 5.0 % U-235, .043 % U-234, 4.958 GMUF6/CC, 2.214 GMUO2F2/CC
READ PARAMETERS   TME=16    NUB=YES    FLX=YES    FDN=YES    END PARAMETERS
READ GEOMETRY
UNIT 1
COM=' UF6: T = 15.768" - LEFT THIRD OF 2 1/2-TON CYLINDER '
YHEMICYL-Z     1  1  37.1475          65.19    1.27    CHORD      2.903
YCYLINDER      3  1  37.1475          65.19    1.27
YCYLINDER      4  1  38.4175          65.19    0.0
CUBOID         0  1  38.4175 -38.4175 65.19    0.0    38.4175   -38.4175
UNIT 2
COM=' UF6: T = 17.346" - MIDDLE THIRD OF 2 1/2-TON CYLINDER '
YHEMICYL-Z     1  1  37.1475          31.96   -31.96   CHORD      6.911
HOLE 4                0.0              0.0   -15.118
YCYLINDER      3  1  37.1475          31.96   -31.96
YCYLINDER      4  1  38.4175          31.96   -31.96
CUBOID         0  1  38.4175 -38.4175 31.96   -31.96  38.4175   -38.4175
UNIT 3
COM=' UF6: T = 15.768" - RIGHT THIRD OF 2 1/2-TON CYLINDER '
YHEMICYL-Z     1  1  37.1475          63.92    0.0     CHORD      2.903
YCYLINDER      3  1  37.1475          63.92    0.0
YCYLINDER      4  1  38.4175          65.19    0.0
CUBOID         0  1  38.4175 -38.4175 65.19    0.0     38.4175 -38.4175
UNIT 4
COM='  13-INCH DIAMETER SPHERE OF UO2F2 AT H/U = 11.65 '
SPHERE         2  1  16.510
CORE           0  1   0.0      0.0      0.0
REPLICATE      5  2   0.0      0.0      0.0      0.0      0.0      5.0   5
REPLICATE      5  7   0.0      0.0      0.0      0.0      0.0      5.48  1
END GEOMETRY
READ BIAS      ID=301  2   7    END BIAS
READ ARRAY     ARA=1   NUX=1    NUY=3   NUZ=1
               FILL  1  2  3    END FILL         END ARRAY
READ PLOT      TTL='  PLOT 1 - VERTICAL SLICE ALONG THE CYLINDER AXIS'
               XUL=     38.4175 YUL=     -5.0     ZUL=     80.0
               XLR=     38.4175 YLR=    197.0     ZLR=     -5.0
               VAX=       1     WDN=    -1        NAX=    130
               NCH=' *O.#@'     RUN=  YES         PLT=    YES      END
               TTL='  PLOT 2 - VERTICAL SLICE ACROSS CYLINDER AT THE MIDDLE'
               XUL=     -5.0    YUL=    97.15     ZUL=     80.0
               XLR=     80.0    YLR=    97.15     ZLR=     -5.0
               UAX=       1     WDN=    -1        NAX=    130
               NCH=' *O.#@'     RUN=  YES         PLT=    YES      END
END PLOT
READ START     NST=1    END START
END DATA
END
```