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Minimum Mass of Moderator Required for Criticality of Homogeneous Low-Enriched Uranium Systems

W. C. Jordan
J. C. Turner

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MINIMUM MASS OF MODERATOR REQUIRED FOR CRITICALITY OF HOMOGENEOUS LOW-ENRICHED URANIUM SYSTEMS

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CONTENTS

Page

ABSTRACT ix
1. INTRODUCTION 1
2. MINIMUM MASS OF MODERATOR REQUIRED FOR CRITICALITY OF HOMOGENEOUS LOW-ENRICHED URANIUM SYSTEMS 3
   2.1 CALCULATIONAL RESULTS 3
   2.2 PROCEDURES FOR EXTENDING THE CALCULATED RESULTS 11
3. INVESTIGATION OF A CALCULATIONAL DISCREPANCY 14
   3.1 COMPARISON WITH OTHER CROSS-SECTION LIBRARIES 14
   3.2 ROLAIDS CALCULATIONS 27
   3.3 THE PCTR ANALYSIS 28
4. EFFECTS OF MODERATION LEVEL ON THE NEUTRON SPECTRUM 32
REFERENCES 47
APPENDIX A. DENSITY RELATIONSHIPS 51
APPENDIX B. TABLES OF CALCULATED VALUES FOR SECTION 2 59
APPENDIX C. RESULTS OF THE 1983 MINIMUM MODERATOR MASS STUDY 63
APPENDIX D. TABLES OF CALCULATED VALUES FOR SECTION 3.1 67

LIST OF FIGURES

Figure	Page
1. k_∞ vs H/X for UO_2F_2–H_2O	4
2. k_∞ vs H/X for UF_6–HF	4
3. Critical radius vs H/X for UO_2F_2–H_2O	5
4. Critical volume vs H/X for UO_2F_2–H_2O	5
5. Critical mass of U vs H/X for UO_2F_2–H_2O	6
6. Mass of water required for criticality vs H/X for UO_2F_2–H_2O	6
7. Critical radius vs H/X for UF_6–HF	7
8. Critical volume vs H/X for UF_6–HF	7
9. Critical mass of U vs H/X for UF_6–HF	8
10. Mass of HF for criticality vs H/X for UF_6–HF	8
11. Estimated minimum conditions for criticality UO_2F_2–H_2O	10
12. Estimated minimum conditions for criticality UF_6–HF @ 20°C	10
13. k_∞ vs H/X for 1.4% enriched UO_2F_2–H_2O	16
14. k_∞ vs H/X for 1.7% enriched UO_2F_2–H_2O	16
15. k_∞ vs H/X for 2% enriched UO_2F_2–H_2O	17
16. k_∞ vs H/X for 3% enriched UO_2F_2–H_2O	17
17. k_∞ vs H/X for 5% enriched UO_2F_2–H_2O	18
18. k_∞ vs H/X for 1.4% enriched UF_6–HF	19
19. k_∞ vs H/X for 1.7% enriched UF_6–HF	19
20. k_∞ vs H/X for 2% enriched UF_6–HF	20
21. k_∞ vs H/X for 3% enriched UF_6–HF	20
22. k_∞ vs H/X for 5% enriched UF_6–HF	21
23. Knight-modified Hansen-Roach to SCALE 27-group library comparison, UO_2F_2–H_2O	23
24. Knight-modified Hansen-Roach to SCALE 27-group library comparison, UO_2F_2–H_2O	23
25. Knight-modified Hansen-Roach to SCALE 27-group library comparison, UF_6–HF	24
26. Knight-modified Hansen-Roach to SCALE 27-group library comparison, UO_2F_2–H_2O	24
27. SCALE 16-group to SCALE 27-group library comparison, UO_2F_2–H_2O	25
28. SCALE 16-group to SCALE 27-group library comparison, UO_2F_2–H_2O	25
29. LAW 238-group to SCALE 27-group library comparison, UO_2F_2–H_2O	26
30. LAW 238-group to SCALE 27-group library comparison, UO_2F_2–H_2O	26
31. UO_2F_2–H_2O 5.0% enriched H/X = 5	38

32. UO_2F_2-H_2O 5.0% enriched H/X = 10 38
33. UO_2F_2-H_2O 5.0% enriched H/X = 20 39
34. UO_2F_2-H_2O 5.0% enriched H/X = 50 39
35. UO_2F_2-H_2O 5.0% enriched H/X = 100 40
36. UO_2F_2-H_2O 5.0% enriched H/X = 200 40
37. UO_2F_2-H_2O 5.0% enriched H/X = 500 41
38. UO_2F_2-H_2O 5.0% enriched H/X = 1500 41
39. UF_6-HF 5.0% enriched H/X = 10 42
40. UF_6-HF 5.0% enriched H/X = 50 42
41. UF_6-HF 5.0% enriched H/X = 200 43
42. UO_2F_2-H_2O 1.4% Enriched H/X = 100 44
43. UO_2F_2-H_2O 1.4% Enriched H/X = 500 44
44. UO_2F_2-H_2O 1.4% Enriched H/X = 1500 45

LIST OF TABLES

Table — Page

1. Estimated minimum critical parameters for UO_2F_2–H_2O 9
2. Estimated minimum critical parameters for UF_6–HF 9
3. ROLAIDS comparison 27
4. PCTR results 29
5. H-R replacement calculations for $U(5)O_2F_2$ and water at H/X = 5 31
6. Intercomparison of XSDRNPM and KENO V.a results 34
7. Selected spectral information for $U(5)O_2F_2$–H_2O systems 35
8. Selected spectral information for $U(1.4)O_2F_2$–H_2O systems 36
9. Selected spectral information for $U(5)F_6$–HF 36
10. AEG for several calculated critical spheres 46

A.1. Properties of uranium and moderating compounds 53
A.2. Temperature variation of several compounds 53
A.3. Physical properties of UO_2F_2–H_2O mixtures 55
A.4. Physical properties of UF_6–HF systems 57
B.1. k_∞ for UO_2F_2–H_2O systems using the SCALE 27-group library 60
B.2. k_∞ for UF_6–HF systems using the SCALE 27-group library 60
B.3. Critical parameters for UO_2F_2–H_2O using the SCALE 27-group library 61
B.4. Critical parameters for UF_6–HF using the SCALE 27-group library 62
C.1. k_∞ for UO_2F_2–H_2O systems using the Knight-modified Hansen-Roach cross sections 64
C.2. k_∞ UF_6–HF systems using the Knight-modified Hansen-Roach cross sections 64
C.3. Critical parameters for UO_2F_2–H_2O using the Knight-modified Hansen-Roach cross sections 65
C.4. Critical parameters for UF_6–HF systems using the Knight-modified Hansen-Roach cross sections 66
D.1. k_∞ for UO_2F_2–H_2O systems using the SCALE 16-group library 68
D.2. k_∞ for UF_6–HF systems using the SCALE 16-group library 68
D.3. k_∞ for UO_2F_2–H_2O systems using the LAW-238 ENDF/B-V library 69
D.4. k_∞ for UF_6–HF systems using the LAW-238 ENDF/B-V library 69

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ABSTRACT

A parametric calculational analysis has been performed in order to estimate the minimum mass of moderator required for criticality of homogeneous low-enriched uranium systems. The analysis was performed using a version of the SCALE-4.0 code system and the 27-group ENDF/B-IV cross-section library. Water-moderated uranyl fluoride (UO_2F_2 and H_2O) and hydrofluoric-acid-moderated uranium hexaflouride (UF_6 and HF) systems were considered in the analysis over enrichments of 1.4 to 5 wt % ^{235}U. Estimates of the minimum critical volume, minimum critical mass of uranium, and the minimum mass of moderator required for criticality are presented.

There was significant disagreement between the values generated in this study when compared with a similar undocumented study performed in 1983 using ANISN and the Knight-modified Hansen-Roach cross sections. An investigation into the cause of the disagreement was made, and the results are presented.

1. INTRODUCTION

Where practicable, the nuclear criticality safety of equipment or operations that involve fissile material should be based on single-parameter limits, such as safe mass or geometry, for a specified enrichment.[1] These single-parameter limits are easily controlled and verifiable, and require a minimum of administrative control. The limits are well established and are usually based on optimum moderation and full reflection for the fissile material form under consideration.

There are, however, instances in which single-parameter limits are extremely conservative and unnecessarily limit the size of equipment or mass of uranium. In these cases, multiple parameter limits that control additional variables in conjunction with the mass or geometry may be safely imposed. A common second variable used in industry is the moderation level of the uranium in the process.

An example of a "moderation-limited" fissile material control is the subcritical mass limit for highly enriched uranium metal.[1,2] The single-parameter mass limit for ^{235}U metal is 20.1 kg. This limit is applicable only to a unit that has no reentrant space that can be occupied by water or another moderator. In the absence of any moderation control, the single-parameter subcritical mass limit is 760 g.

Another example of moderation-limited fissile material control may be seen in the use of the 48-in.-diam 10-ton UF_6 cylinder used for storage and transport of up to 4.5% enriched uranium.[3] The cylinder is safe due to moderation control. The cylinder wall isolates the fissile material from any moderators. The integrity of the wall can be checked through monitoring of the cylinder pressure (a vacuum condition). UF_6 reacts with water to form UO_2F_2 and HF. The presence of HF in the cylinder is easily detected by measuring the pressure of the cylinder at a specified temperature. In the absence of moderation control, the subcritical mass limit for 4.5% enriched UF_6 would be on the order of 43.5 kg of uranium; the subcritical infinite cylindrical geometry limit would be a diameter of about 11.0 in.

In each of these examples, the mass of the fissile material significantly exceeds the minimum critical values based on optimum moderation.

A characteristic of low-enriched uranium is that uranium enriched to less than about 5.6 wt % ^{235}U cannot be made critical in the absence of a moderator. Thus, moderation control is of special interest in operations involving low-enriched uranium. It also suggests that a single-parameter limit based on the mass of moderator could be established for low-enriched uranium.

The single-parameter limit on moderator mass has similar characteristics to other single-parameter limits because, by controlling this parameter, a system is safely subcritical independent of the geometry, the manner in which the moderator is intermixed, and the reflective conditions of the material.

The purpose of this report is to establish estimates of the minimum moderator mass required for criticality for H_2O-moderated UO_2F_2 and HF-moderated UF_6 systems involving enrichments ranging from 1.4 to 5 wt % ^{235}U. A similar undocumented study was performed at

the Oak Ridge Gaseous Diffusion Plant (ORGDP) in Oak Ridge in 1983. The original intent of this analysis was to reconfirm the 1983 calculations using current codes and cross sections and to more formally document the results. The results of this study did not agree well with the values determined in 1983. The disagreement was significant enough to warrant investigation to determine the cause of the disagreement. Subsequently, the scope of this report was expanded into additional parts (Sects. 3 and 4).

In Sect. 2, the methodology for estimating the minimum mass of moderator is presented. Included are the techniques used to estimate the physical characteristics, such as uranium density, as a function of moderation level for the two mixtures considered. The results of infinite media multiplication calculations are given, along with the calculational results used to estimate the minimum mass of moderator required for criticality. Procedures for extending the results and estimating the critical spherical radius for systems of the same composition, but with different material densities, reflection conditions, or infinite media multiplication factors, are given.

In Sect. 3, the differences between the 1983 calculations and the current calculations performed with SCALE-4.0 (ref. 4) are investigated. In this investigation five cross-section sets were examined: (1) the SCALE 27-group ENDFB/IV library,[5] (2) the LAW 238-group ENDF/B-V library,[6] and (3) three variations of the Hansen-Roach 16-group cross-section set — the Knight-modified Hansen-Roach cross sections as distributed with KENO-IV,[7,8] the SCALE 16-group library, and the original Hansen-Roach cross sections.[9]

The minimum critical radius, volume, and mass predicted using SCALE-4.0 and the 27-group ENDF/B-IV library are greater than those estimated in 1983 using ANISN[10] and the Knight-modified Hansen-Roach cross sections. There are also large differences in the calculated infinite media multiplication factors. An investigation was conducted to determine the possible causes of these differences. The investigation consists primarily of a comparison of cross-section performance on infinite media calculations. A comparison between the SCALE-4.0 results and the 1983 results are presented. The infinite media calculations presented in Sect. 2 are repeated using the SCALE 16-group library. These calculations were also performed again using the LAW 238-group ENDF/B-V library as an independent reference. Results of calculations using ENDF/B-IV, ENDF/B-V, and Knight-modified Hansen-Roach cross sections are presented. The ROLAIDS[11] code is used to determine the adequacy of the NITAWL[12] resonance region cross-section processing. The performance of each cross-section library on several low-enriched, low-moderated systems that have experimentally measured infinite media multiplication factors, referred to here as the PCTR experiments,[13-15] is presented. A final comparison is then made using the original Hansen-Roach 16-group cross sections.

In Sect. 4, a brief discussion is presented on the effects of moderation level and enrichment on the neutron spectrum. An attempt is made to determine the adequacy of various parameters in establishing the area and range of applicability of a validation.

2. MINIMUM MASS OF MODERATOR REQUIRED FOR CRITICALITY OF HOMOGENEOUS LOW-ENRICHED URANIUM SYSTEMS

2.1 CALCULATIONAL RESULTS

As a first step in determining the minimum mass of moderator required for criticality, the physical characteristics of the fissile mixtures used in the analysis must be accurately described over the specified range of parameters. In this case, the uranium density as a function of the moderation level specified as an H/X (hydrogen-to-fissile uranium atomic ratio) for H_2O-moderated UO_2F_2 and HF-moderated UF_6. The density formulations given in Appendix A were used to estimate the densities at a temperature of 20°C. The temperature used for the determination of the theoretical densities is important because both of these systems have components whose density is a function of temperature.

Uranium-235 enrichments of 5%, 4%, 3%, 2%, 1.7%, and 1.4% were considered. The uranium densities were predicted using the equations given in Appendix A and then used to obtain the compound and moderator densities for the corresponding H/U (hydrogen-to-uranium atomic ratio) value (also tabulated in Appendix A). Tables A.3 and A.4 give the values of uranium, uranium compound, and moderator densities in the mixture as a function of H/X for UO_2F_2–H_2O and UF_6–HF systems, respectively.

Criticality Safety Analysis Sequence No. 1X (CSAS1X) of the CSAS4 module[16] in SCALE-4.0 was used to perform infinite media multiplication (k_∞) calculations for each system described in Tables A.3 and A.4. This control sequence prepares input data and executes BONAMI,[17] NITAWL, and XSDRNPM.[18] The results of these calculations using the 27-group ENDF/B-IV cross-section library are given in Tables B.1 and B.2 and plotted in Figs. 1 and 2.

The infinite media calculations were used to determine the H/X range where peak reactivity occurs for each enrichment. The minimum volume system will occur in the H/X region of peak reactivity. The minimum-mass system will occur in the region of H/X = 500 nearly independent of enrichment.

Critical spherical radius searches were performed with XSDRNPM over the range of H/X from about 100 to 700. The critical radius, volume, mass of uranium, and mass of moderator for each system were calculated. The results are presented in Tables B.3 and B.4 and in Figs. 3 through 10. A minimum occurs for radius, volume, uranium mass, and moderator mass for each enrichment considered. The minimum values were inferred from Figs. 3 through 10 and are tabulated in Tables 1 and 2 and plotted in Figs. 11 and 12.

The estimated values for the infinite media multiplication, critical radius, volume, and mass presented in Tables 1 and 2 do not agree well with values previously calculated. The results of the previous calculations have been included in Appendix C. The results are in best agreement at 5% enrichment and large H/X values and get progressively worse as the enrichment and H/X get smaller. A detailed review of both sets of data is presented in Sect. 3 of this report.

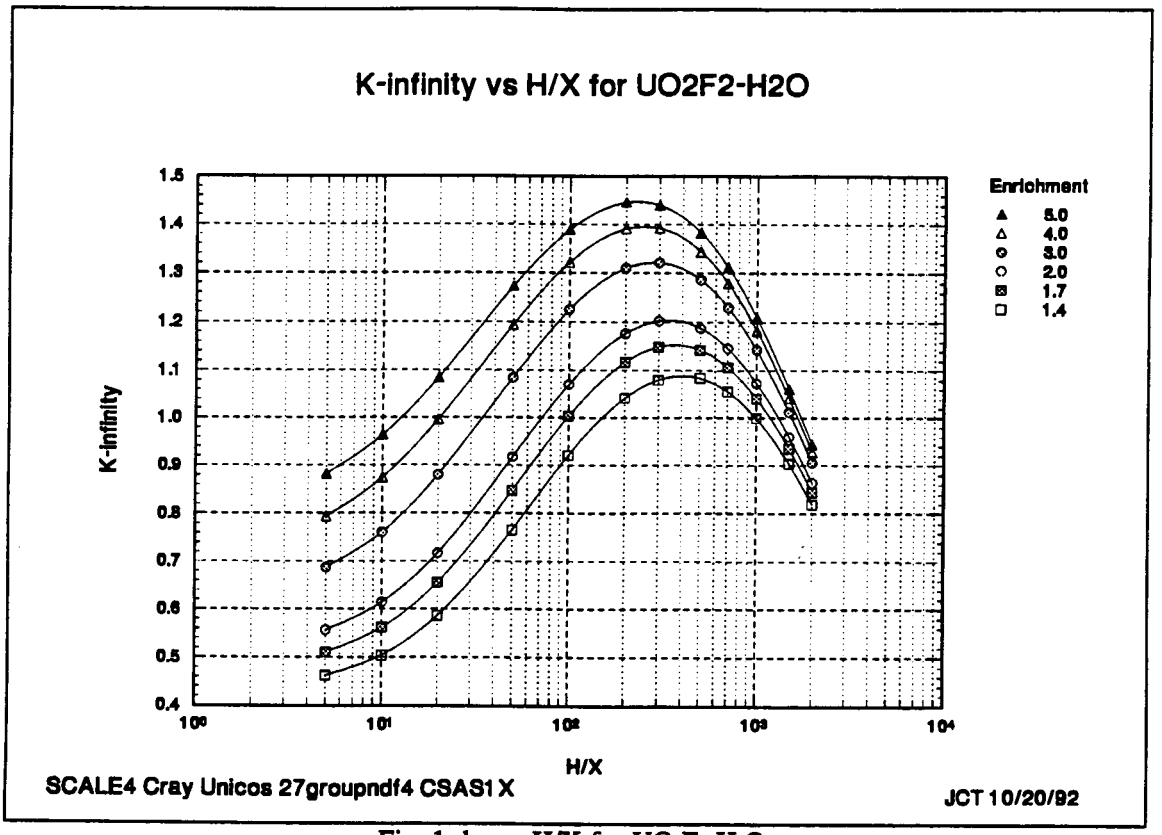

Fig. 1. k_∞ vs H/X for UO_2F_2-H_2O.

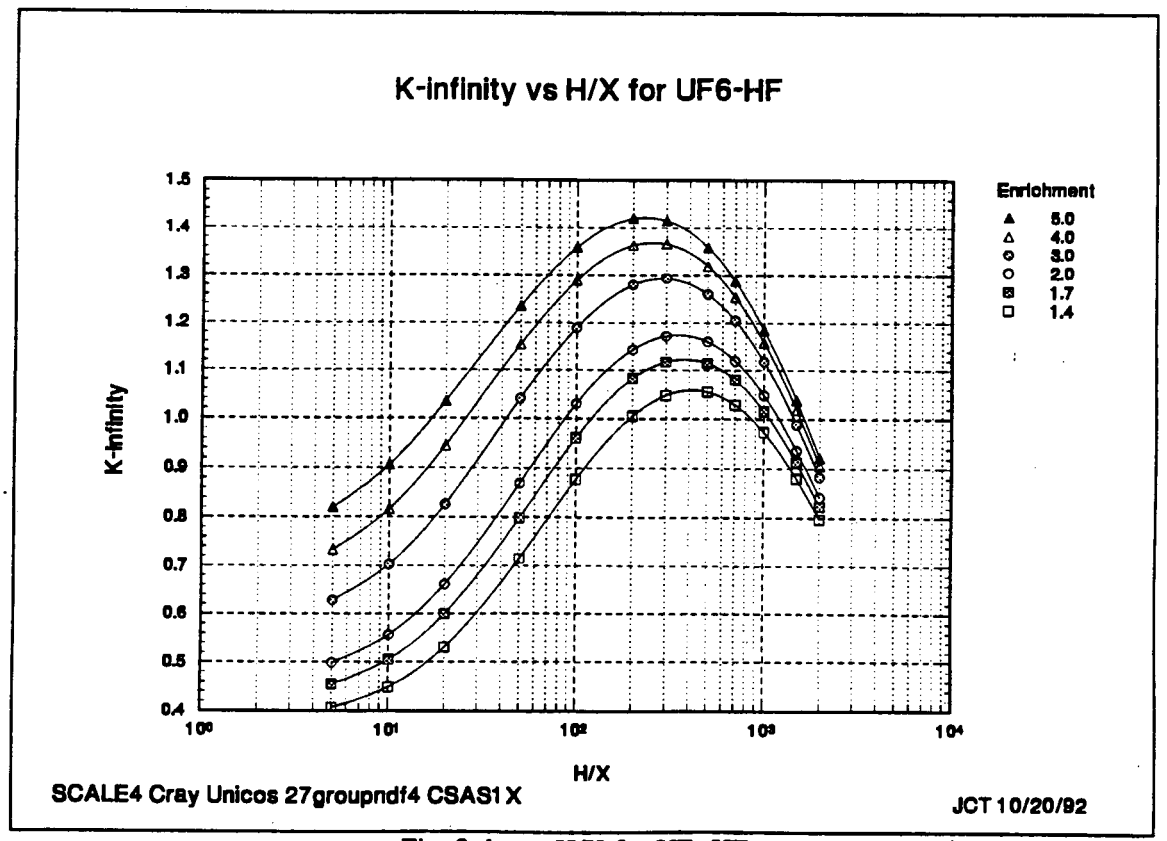

Fig. 2. k_∞ vs H/X for UF_6-HF.

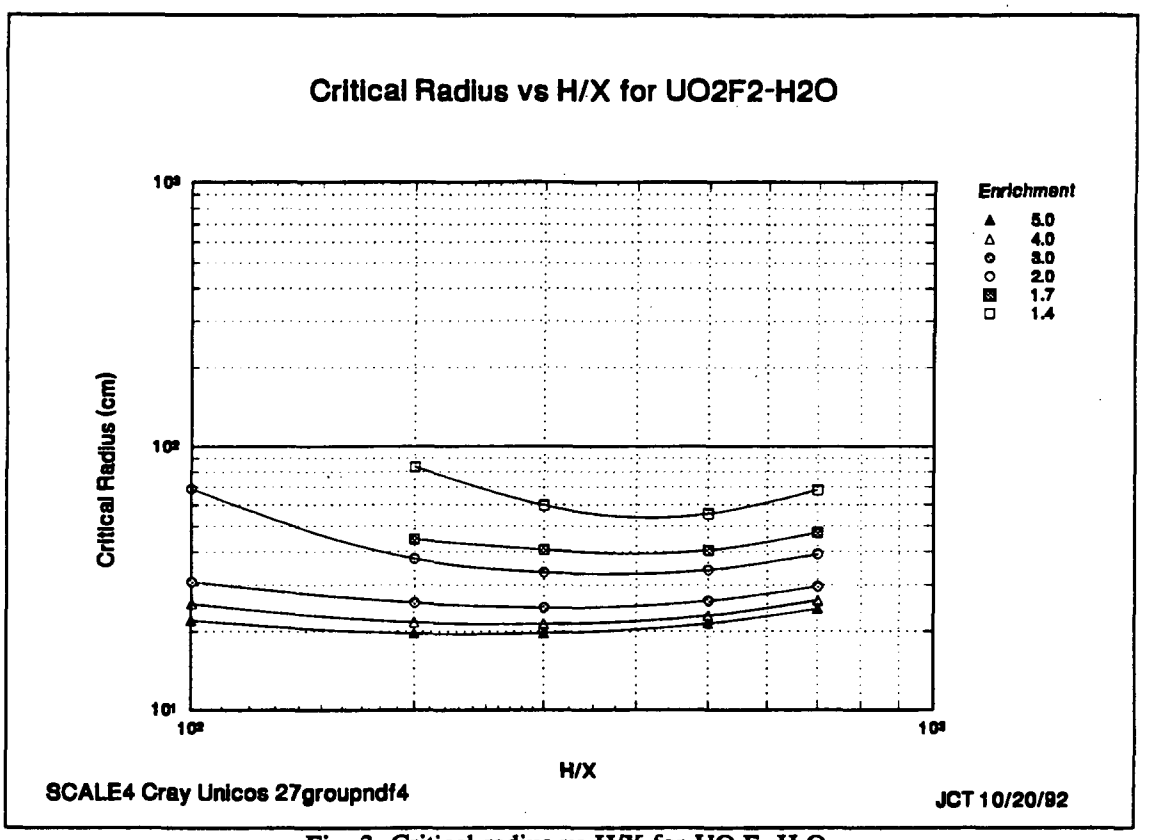

Fig. 3. Critical radius vs H/X for UO_2F_2-H_2O.

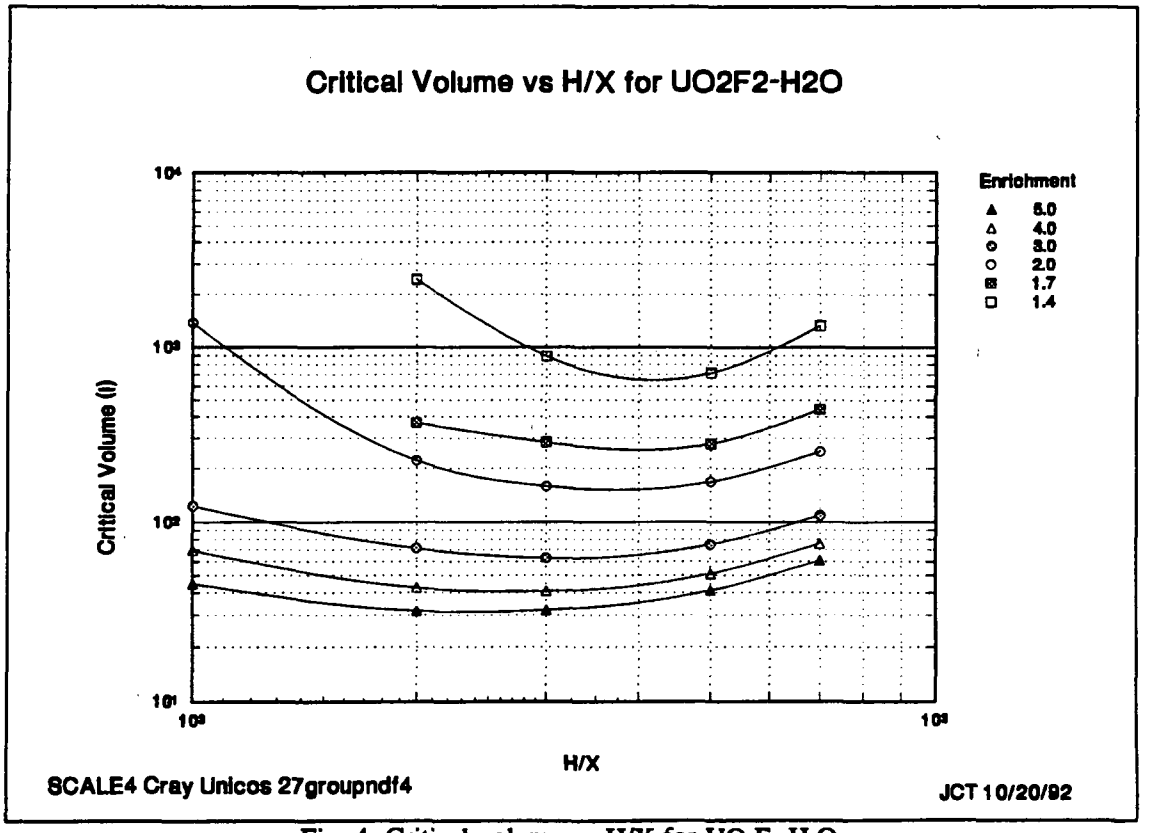

Fig. 4. Critical volume vs H/X for UO_2F_2-H_2O.

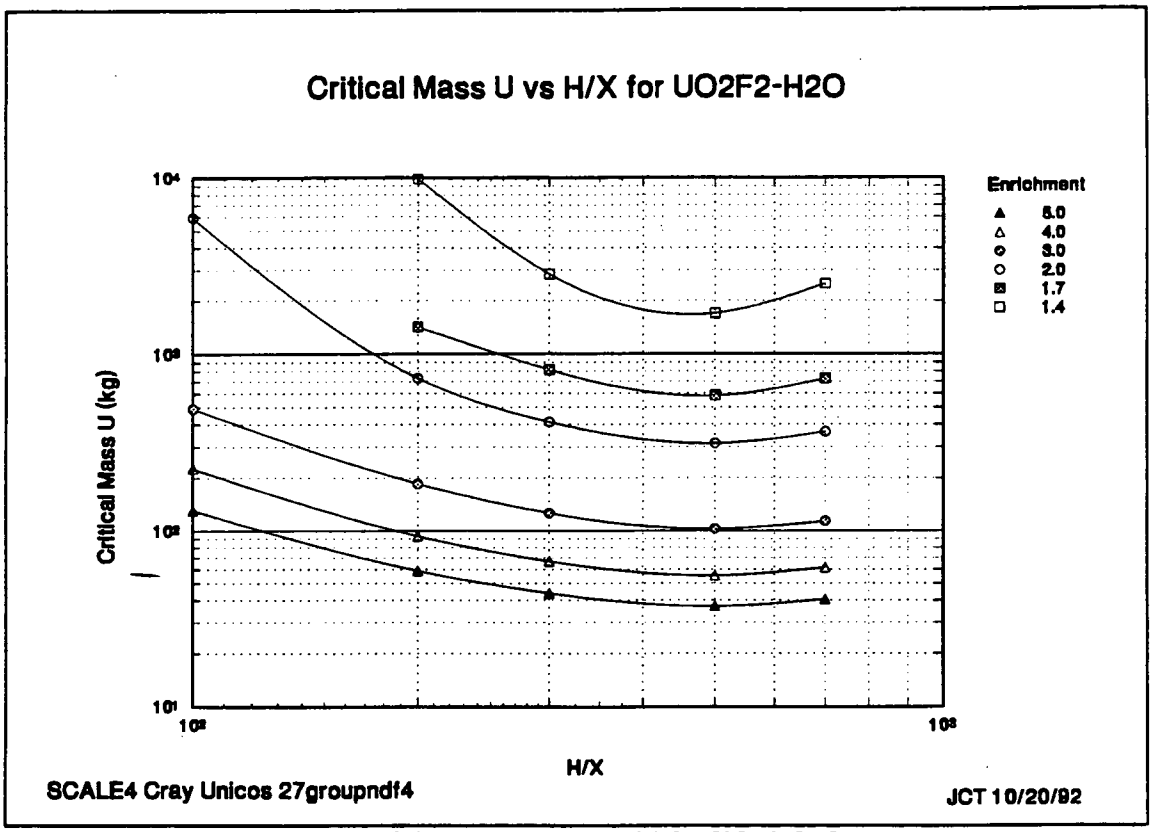

Fig. 5. Critical mass U vs H/X for UO_2F_2-H_2O.

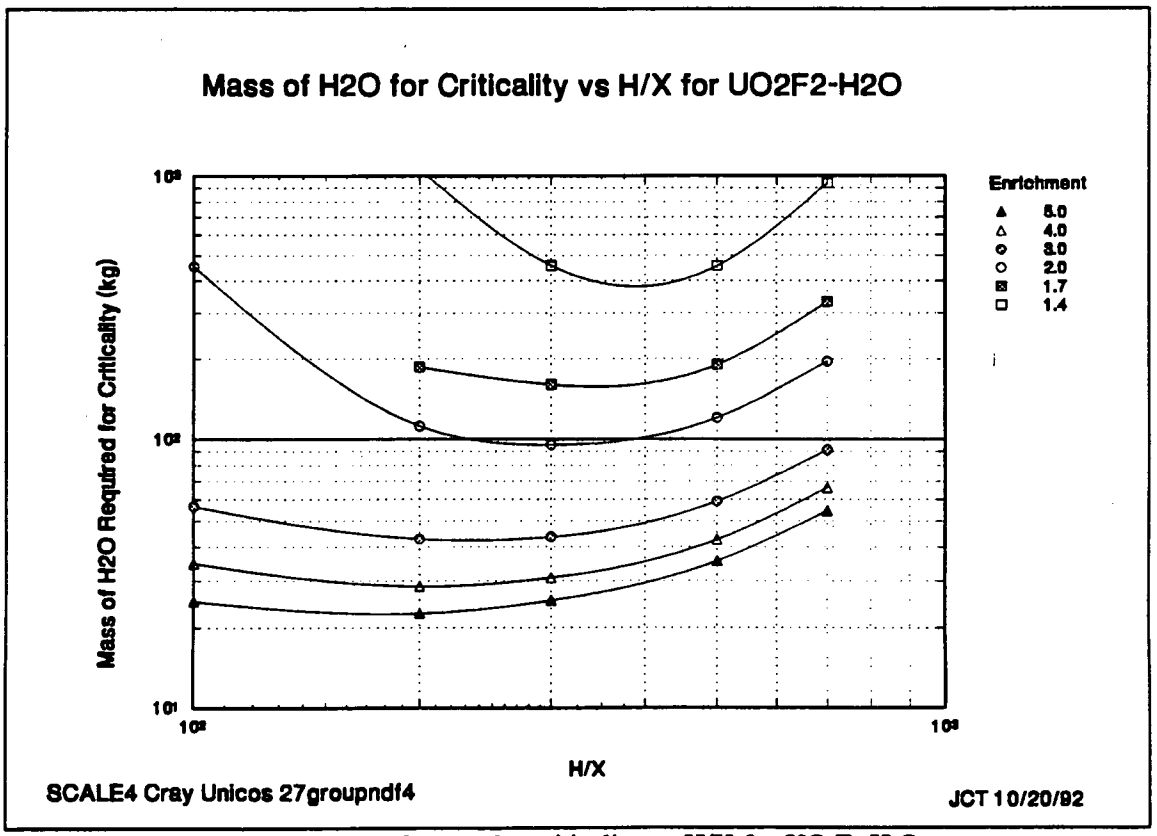

Fig. 6. Mass of water for criticality vs H/X for UO_2F_2-H_2O.

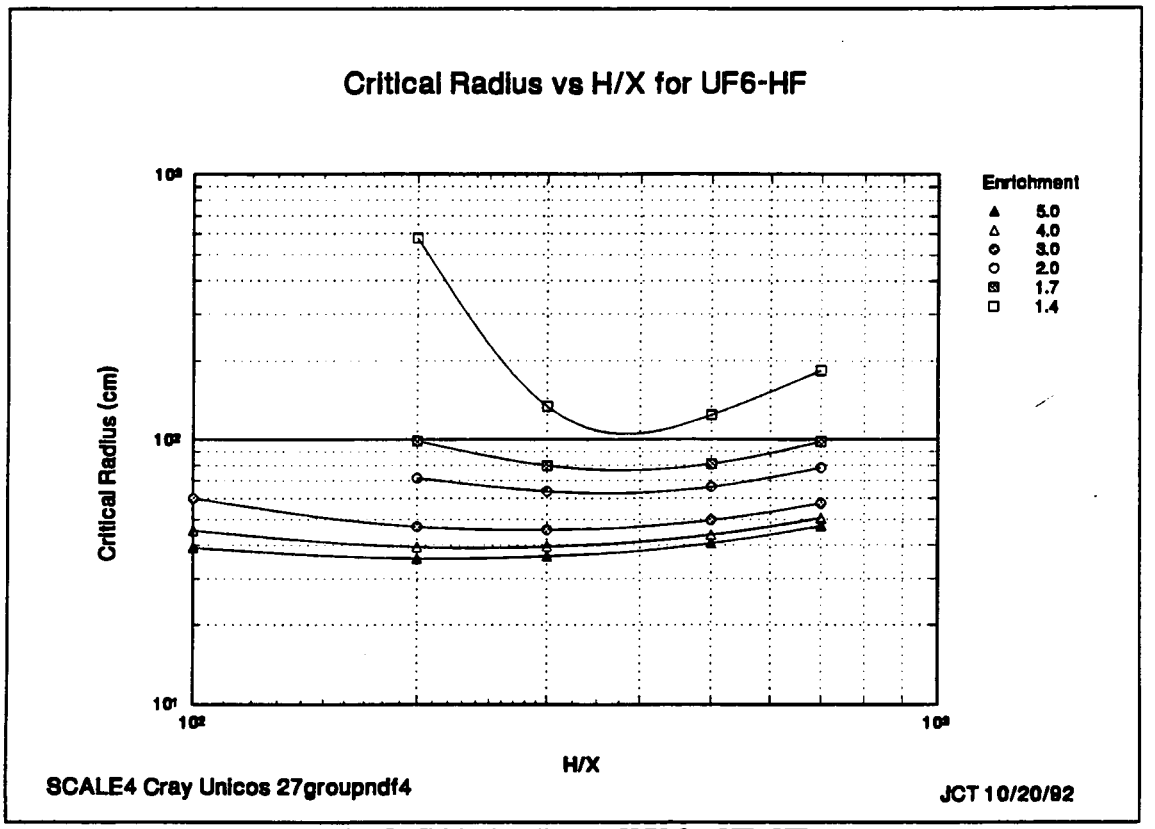

Fig. 7. Critical radius vs H/X for UF_6-HF.

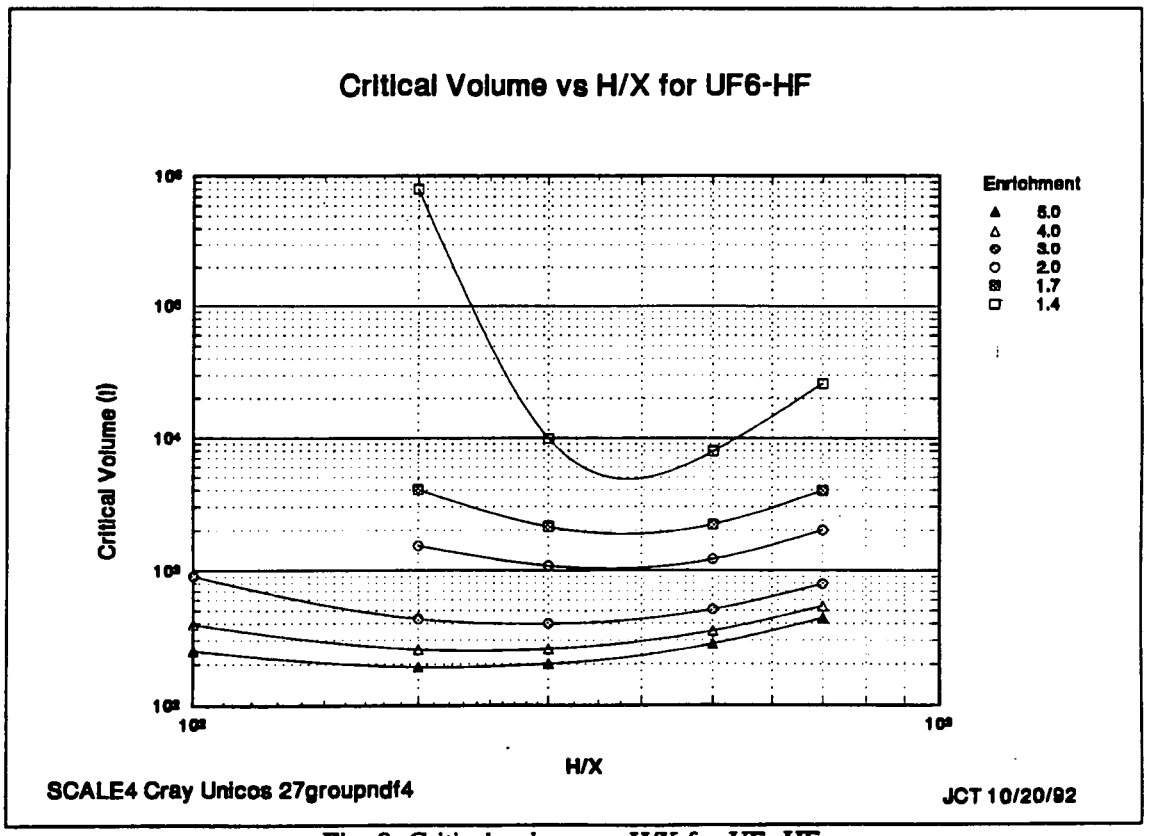

Fig. 8. Critical volume vs H/X for UF_6-HF.

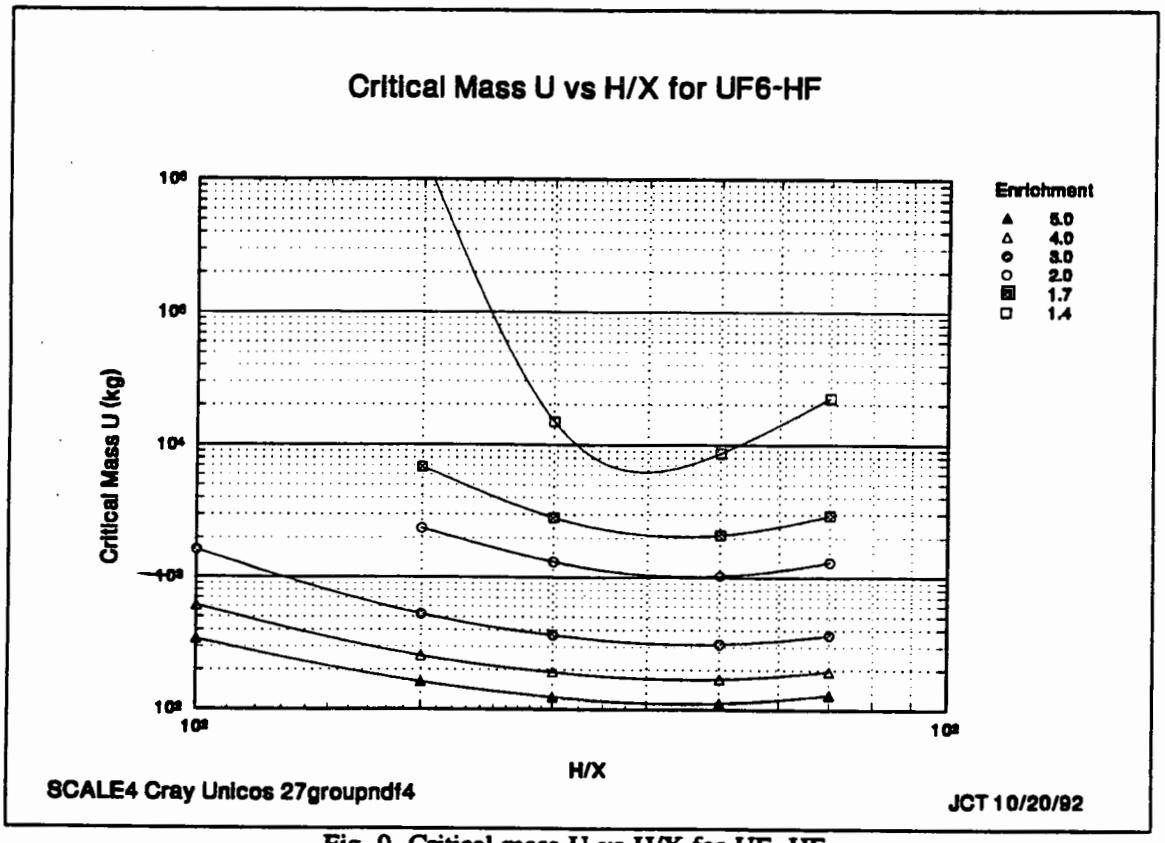

Fig. 9. Critical mass U vs H/X for UF_6-HF.

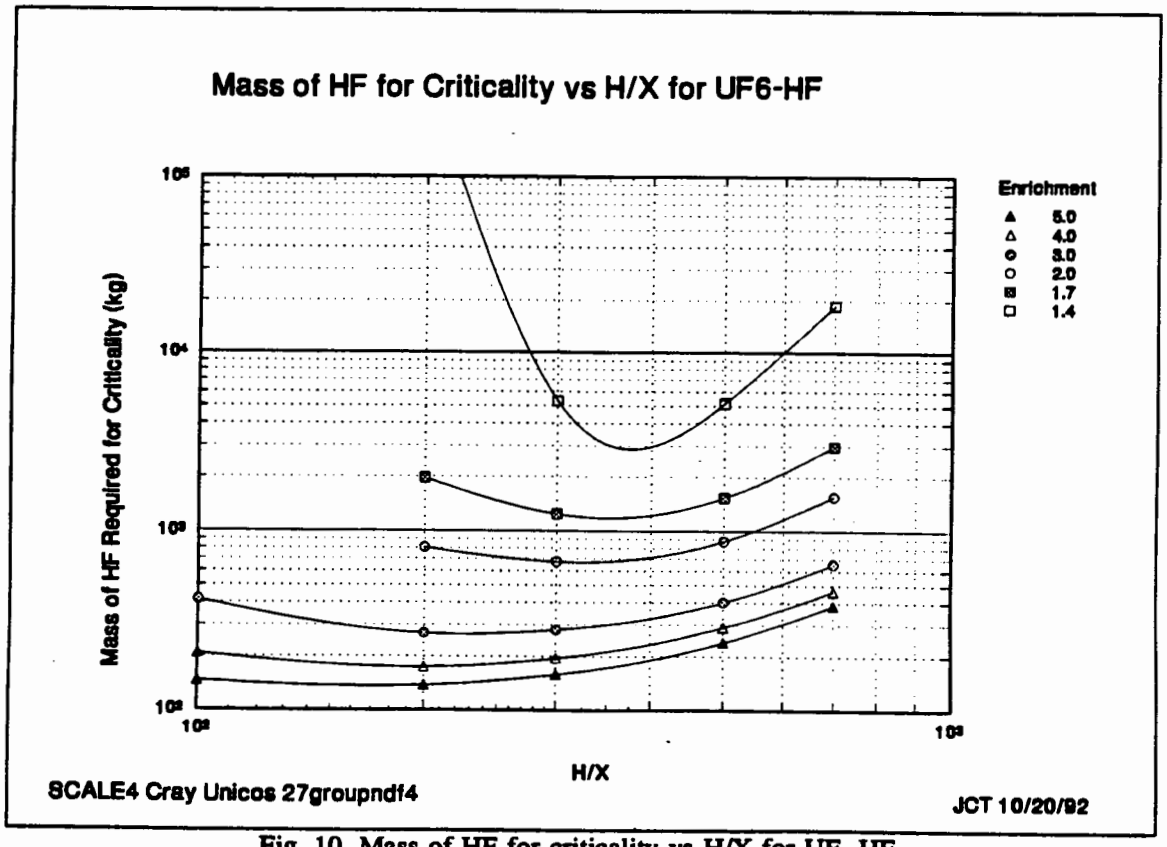

Fig. 10. Mass of HF for criticality vs H/X for UF_6-HF.

Table 1. Estimated minimum critical parameters for UO_2F_2-H_2O

Enrichment	Minimum critical radius (cm)	Minimum critical volume (l)	Minimum critical U mass (kg)	Minimum critical H_2O (kg)
5.0	19.6	31.5	37.0	22
4.0	21.3	40.4	55.5	28
3.0	24.6	62.3	102.0	42
2.0	33.0	150.0	313.0	95
1.7	40.0	268.0	581.0	157
1.4	54.0	659.0	1698.0	405

Table 2. Estimated minimum critical parameters for UF_6-HF

Enrichment	Minimum critical radius (cm)	Minimum critical volume (l)	Minimum critical U mass (kg)	Minimum critical HF (kg)
5.0	35.6	188	105	135
4.0	39.0	248	165	170
3.0	45.0	381	310	265
2.0	62.0	998	1000	670
1.7	75.0	1760	2000	1200
1.4	110.0	5570	7500	3600

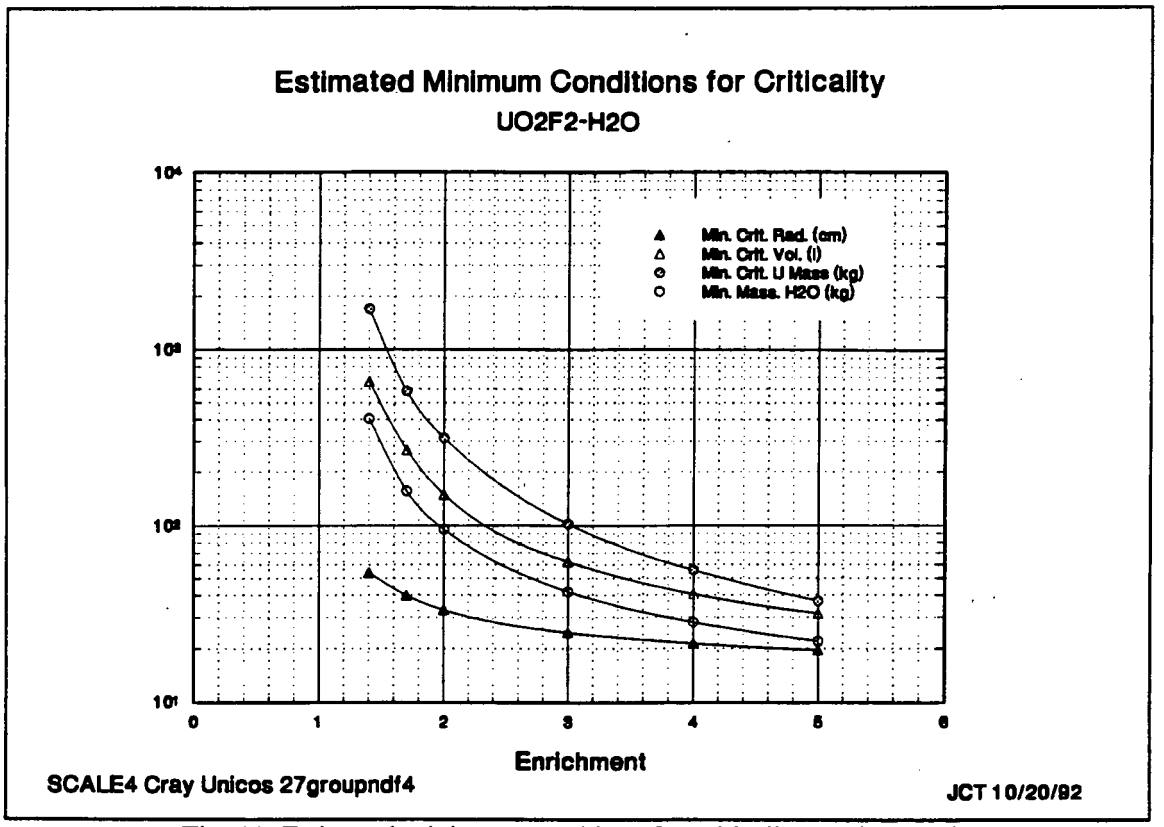

Fig. 11. Estimated minimum conditions for criticality - UO_2F_2-H_2O.

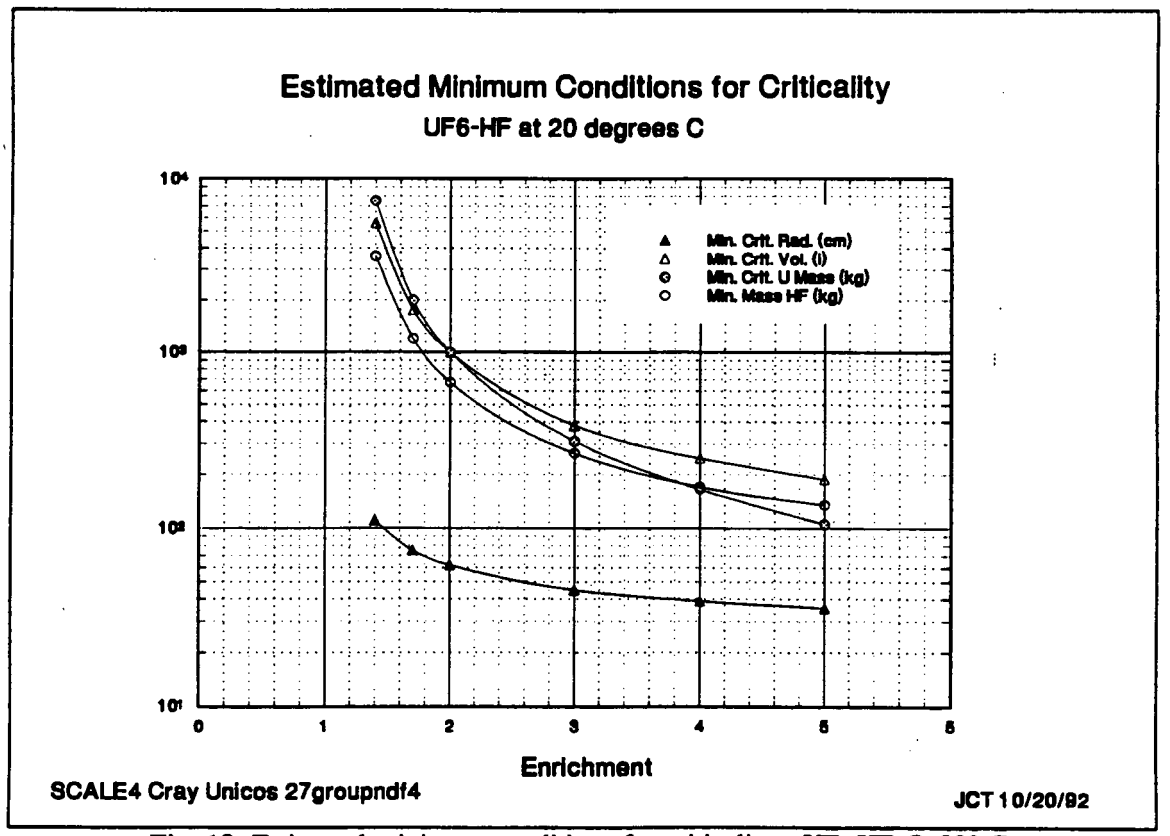

Fig. 12. Estimated minimum conditions for criticality - UF_6-HF @ 20° C.

2.2 PROCEDURES FOR EXTENDING THE CALCULATED RESULTS

The calculated minimum critical values presented in Tables 1 and 2 have a number of assumptions associated with them. These assumptions include the calculation of the physical properties of the system, the implied adequacy of the cross-section library used, and the fact that they were derived from critical systems (calculated $k_{eff} = 1.0$). The ability to predict the effects of slight variations in these assumptions is useful. For example, a temperature of 20°C was used in this analysis. Estimates of the critical parameters for UF_6-HF systems at a temperature of 0°C might be desired. Since the theoretical density of a system is a function of the temperature, estimates of k_{eff} at a different temperature may be made by using the correspondent change in density. Another example might relate to the adequacy of the cross-section library. If one determines that there is a bias in the infinite media calculations, estimates of the effects on the critical parameters could be established by examining the relative change in k_{eff} as a function of changes in k_∞. As a final example, one may determine that they desire limits based on safely subcritical systems as opposed to critical systems. Estimates of a system that would yield a k_{eff} of, for example, 0.95 may be made from calculational results of systems with a $k_{eff} = 1.0$. The purpose of this sub-section is to briefly review the use of simple buckling theory in performing these estimates.

The effective multiplication of a fissile system may be estimated using the simple buckling relationship:[19]

$$k_{eff} = \frac{k_\infty}{1 + M^2 B^2}, \tag{1}$$

where

k_{eff} is the effective multiplication factor,
k_∞ is the infinite media multiplication factor,
M^2 is the neutron migration area,
B^2 is the geometric buckling.

The infinite media multiplication factor and the neutron migration area are neutronic characteristics of the system under consideration. The geometric buckling is a function of the geometry and reflective conditions of the system. Equation (2) gives the geometric buckling for spherical geometry:

$$B^2 = \left(\frac{\pi}{R + \lambda}\right)^2, \tag{2}$$

where

R is the radius of the sphere,
λ is the reflector extrapolation distance.

The extrapolation distance is an artificial quantity that is intended to account for the effects of a reflector. The extrapolation distance is a function of the physical form of the fissile material (fissile material compound, moderation ratio, enrichment, density, etc.) and the reflector material.

The effects of a change in the density of a system from ρ_0 to ρ (where all of the constituents remain in the same relative ratios) may be estimated from the buckling relationship using the following assumptions:

1. k_∞ does not change as a function of density,
2. M^2 is proportional to $(\rho_0/\rho)^2$ [i.e., $M^2 = (\rho_0/\rho)^2 * M_0^2$],
3. λ is constant (i.e., $\lambda = \lambda_0$).

Under these assumptions the radius of the system at the new density is given by Eq. (3):

$$R = \frac{\rho_0(R_0 + \lambda_0)}{\rho} - \lambda \ . \tag{3}$$

The zero-scripted values are those of the original system, and nonscripted values are those at the new conditions. Approximations such as Eq. (3) should be used with caution. This is particularly true because the assumptions may not be valid if the effects of large changes are being estimated. For example, the extrapolation distance, λ, cannot be treated as constant for estimations involving large density changes. Physically, this is related to the change in leakage of the system and to the effectiveness of the reflector in returning neutrons to more important regions of the system. As the density of the fissile material becomes smaller, leakage becomes larger. Reflected neutrons penetrate deeper before interacting. The effectiveness of the reflector increases because of these effects. The extrapolation distance for the new system which yields correct results is a function of the change in density similar to the migration area [i.e., $\lambda = \lambda_0 * (\rho_0/\rho)^c$], where c could be on the order of 1.3.

In some cases it may be desirable to estimate the effect of a change in k_∞ on the critical radius or volume of a system. For example, one could estimate the change in critical geometry between two cross-section libraries which give slightly different values of k_∞ for the same system. Similarly, if a cross-section set is known or suspected to have a bias for a particular type of system, the impact of this bias on the predicted critical parameters may be estimated. The effects of a change in k_∞ may be approximated using the following assumptions:

1. M^2 does not change, and
2. λ is not a function of system size.

Under these assumptions the radius of the system with the modified infinite media multiplication factor may be estimated using Eq. (4):

$$R = \left(\frac{k_\infty^0 - 1}{k_\infty - 1}\right)^{\frac{1}{2}} (R_0 + \lambda) - \lambda \ . \tag{4}$$

It may also be desirable to estimate the critical parameters of a system that has an effective multiplication different than that calculated. For example, critical parameters (values for $k_{eff} = 1.0$) may have been calculated, and the parameters that correspond to a $k_{eff} = 0.95$ or 0.90 may be desired. The radius of a system for a different value of the effective multiplication factor may be estimated using Eq. (5):

$$R = (R_0 + \lambda)\left(\frac{k_{eff}(k_\infty - k_{eff}^0)}{k_{eff}^0(k_\infty - k_{eff})}\right)^{\frac{1}{2}} - \lambda \ . \tag{5}$$

The relationships given in Eqs. (3) through (5) are approximate, but they are useful in estimating the effects of small perturbations on a particular system. An estimate of the extrapolation distance of about 6.5 cm may be used over the H/X range of 100 to 700 for the low-enriched systems considered in this report.[19]

An interesting observation may be made if Eq. (5) is used to evaluate the change in the radius for a decrease in k_{eff} from 1.0 to 0.95. The magnitude of the change in the radius is sensitive to the infinite media multiplication of the system under consideration. For example, if the infinite media multiplication factor is 1.01, the new radius would be only 40% of the radius, which gave a $k_{eff} = 1.0$. If $k_\infty = 1.1$, the new radius would be about 80% of the original radius. If $k_\infty = 2.0$, the new radius would be about 95% of the original. Basing the criticality safety of a system on a calculated k_{eff} of 0.95 (or any other arbitrary value), independent of the characteristics of the system, places a tremendous conservatism on the systems with an already low reactivity. The use of a safety factor on the critical geometry (a 5 or 10% reduction) would seem a reasonable alternative to using a margin of subcriticality on calculated k_{eff}.

Equation (4) indicates that the critical radius is also more sensitive to a change in the infinite media multiplication factor for systems with smaller values of k_∞ than for systems that have a large infinite media multiplication. A 1% uncertainty in the infinite media multiplication around a value of $k_\infty = 1.01$ would yield a change in radius of $0.25R_0 < R < \infty$. A similar uncertainty for $k_\infty = 1.1$ yields a change in radius of $0.81R_0 < R < 1.26R_0$; a value of $k_\infty = 2.0$ yields a change of $0.96R_0 < R < 1.04R_0$. The smaller the infinite media multiplication, the more precise the cross sections, computational techniques, and experimental benchmarks have to be to reasonably predict values for critical radius, volume, and mass.

3. INVESTIGATION OF A CALCULATIONAL DISCREPANCY

The results presented in Sect. 2 did not agree well with those of a similar analysis performed in 1983 using the ANISN code and the Knight-modified Hansen-Roach 16-group cross sections. For reference purposes, the results of the 1983 analysis are presented in Appendix C. There are significant differences in the predicted infinite media multiplication, critical radius, volume, and mass which appear to be a function of enrichment and moderation ratio. The disagreement is of considerable interest for several reasons.

The results of the 1983 analysis were checked against published data available at the time they were performed. Both the critical data for low-enriched uranium presented in TID-7028[20] and the subcritical data presented in TID-7016[21] and "safe" values presented in K-1019[22] tend to support the original calculations. Differences of as large as 10% in the infinite media multiplication factor were observed between the 1983 calculations and those presented in Sect. 2. If the 1983 calculations are taken as correct, then one must conclude that the results from the SCALE-4.0 calculations using the 27-group ENDF/B-IV library are substantially nonconservative.

Both the ANISN code with the Knight-modified Hansen-Roach cross sections and the XSDRNPM code with the SCALE 27-group library have been used extensively and validated against the same set of critical experiments. Even though each of the cross-section libraries have shown indications of bias, there has been no evidence to suggest that there should be a significant inadequacy in either code or cross-section library. It was not expected that there would be as large as a 10% difference in the calculated infinite media multiplication factors for the type of system analyzed here. Since previous validations against the same experiments have not indicated such large differences between the codes and libraries, the discrepancy strongly suggests that there has been inadequate validation and that the codes and cross sections are being used outside the range of validation in this analysis.

The determination as to which calculations are more reliable is not easy in the absence of directly related critical experiment benchmarks. The purpose of this section is to identify which calculations appear to be inadequate. Three separate comparisons were performed toward this end. Each is discussed separately below.

3.1 COMPARISON WITH OTHER CROSS-SECTION LIBRARIES

The input data and calculational methodology used in the 1983 analysis were reviewed to determine if there were any errors or significant differences in the problem being solved. It was determined that there were differences in the formulations used to specify mixture densities.

The calculated densities for the UO_2F_2-H_2O systems were similar except at H/U values less than 4. The density formulation given for UO_2F_2 in Appendix A is discontinuous at an H/U = 4 in order to conservatively account for mixtures of hydrates that may exist below this

moderation level. The formulation used in 1983 is potentially nonconservative for systems below an H/U = 4.

The calculated densities for UF_6–HF systems were considerably different. It was determined that the calculations performed in 1983 were based on a temperature of -100°F (-73.3°C). The theoretical density for UF_6 and HF are 9.5% and 23.6% larger, respectively, at -73.3°C when compared with the theoretical densities at 20°C used in Sect. 2.

In addition, the 1983 calculations were set up using the KENO-IV σ_p methodology. No interpolation was performed between σ_p values for the ^{235}U and ^{238}U cross sections; the nearest σ_p cross-section set below the calculated value was chosen for ^{238}U, and the nearest set above was chosen for ^{235}U. This methodology yields a conservative result with respect to actually interpolating between sets. The 1983 analysis was performed with ANISN as opposed to XSDRNPM.

The differences in the density help explain some of the observed difference in the estimated critical parameters between the current calculations and those performed in 1983, particularly for the UF_6-HF systems. However, this does not explain the large differences in the calculated infinite media multiplication. The infinite media multiplication is a function of the relative ratios of the materials in the fissile system and is independent of the density of the system. Since the infinite media multiplication calculations revealed the largest differences, infinite UO_2F_2-H_2O systems were chosen for further analysis.

All the infinite media systems in Sect. 2 were recalculated using SCALE-4.0 and the SCALE 16-group library. This eliminated the differences in density, built-in conservatism, and codes used. In addition, all the infinite media systems were recalculated using SCALE-4.0, and a preliminary version of the LAW-238 ENDF/B-V fine-group cross-section library was generated at ORNL. The results of these calculations are given in Tables D.1 through D.4. The results of each series of calculations is also presented as k_∞ versus H/X at each enrichment in Figs. 13 through 22.

The differences in calculated k_∞ between the 1983 calculations using the Knight-modified Hansen-Roach cross sections and the current calculations using the SCALE 16-group library are relatively minor (on the order of 1%), as can be seen in Figs. 13 through 22. The 1983 calculations (labeled as KMHR) appear to be slightly conservative with respect to the SCALE 16-group calculations for both the UO_2F_2–H_2O and UF_6–HF systems. This indicates that there is not a significant difference between the two versions of the Knight-modified Hansen-Roach cross sections. It also indicates that there are not significant differences between the ANISN and XSDRNPM codes.

Both the Knight-modified Hansen-Roach and the SCALE 16-group cross sections overpredict the infinite media multiplication factor compared with the SCALE 27-group library. There appears to be a trend between the Knight-modified Hansen-Roach cross sections and the 27-group library which is a function of both the enrichment and H/X. The calculations performed with the LAW 238-group library tend to consistently fall 0.5 to 1% higher than the SCALE 27-group calculations. (These differences appear to be consistent with the changes

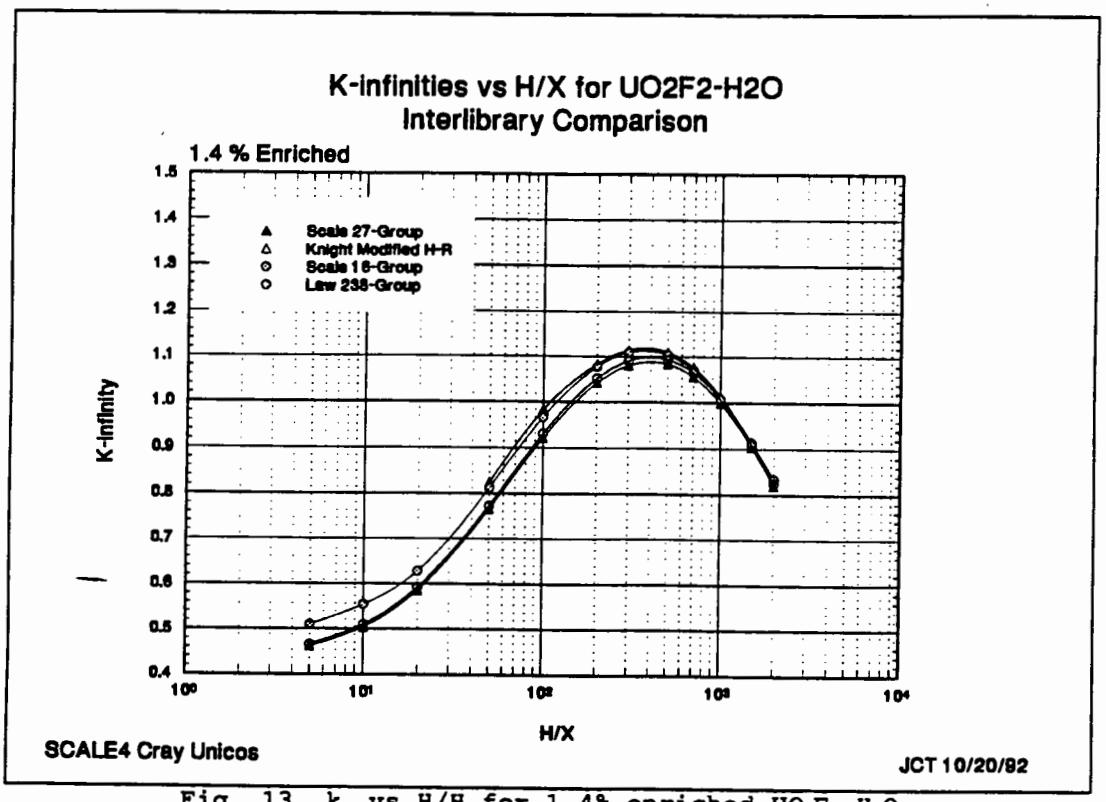

Fig. 13. k_∞ vs H/H for 1.4% enriched UO_2F_2–H_2O.

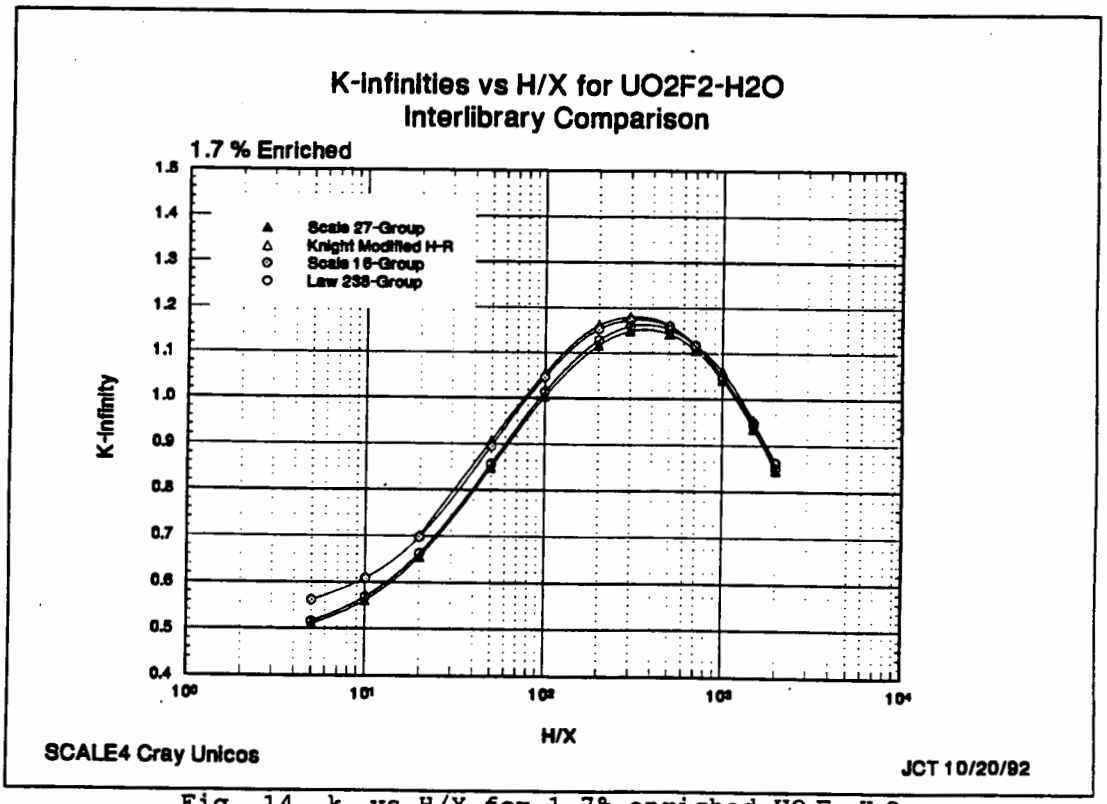

Fig. 14. k_∞ vs H/X for 1.7% enriched UO_2F_2–H_2O.

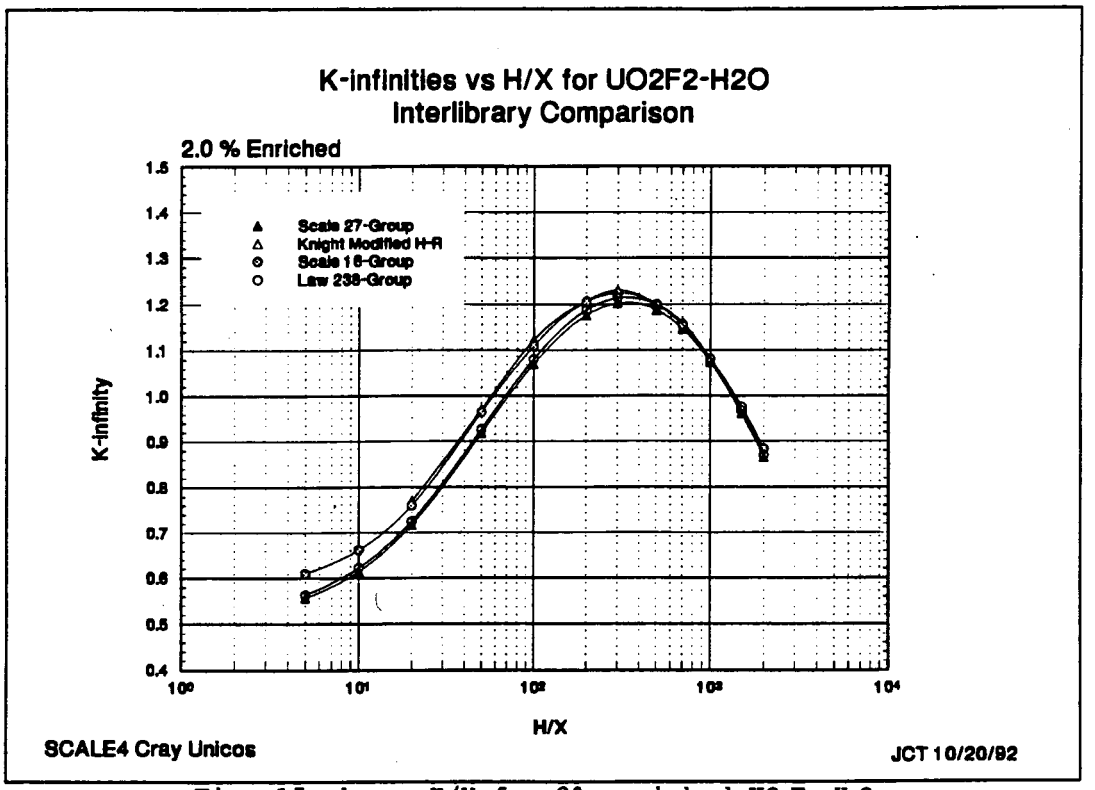

Fig. 15. k_∞ vs H/X for 2% enriched UO_2F_2–H_2O.

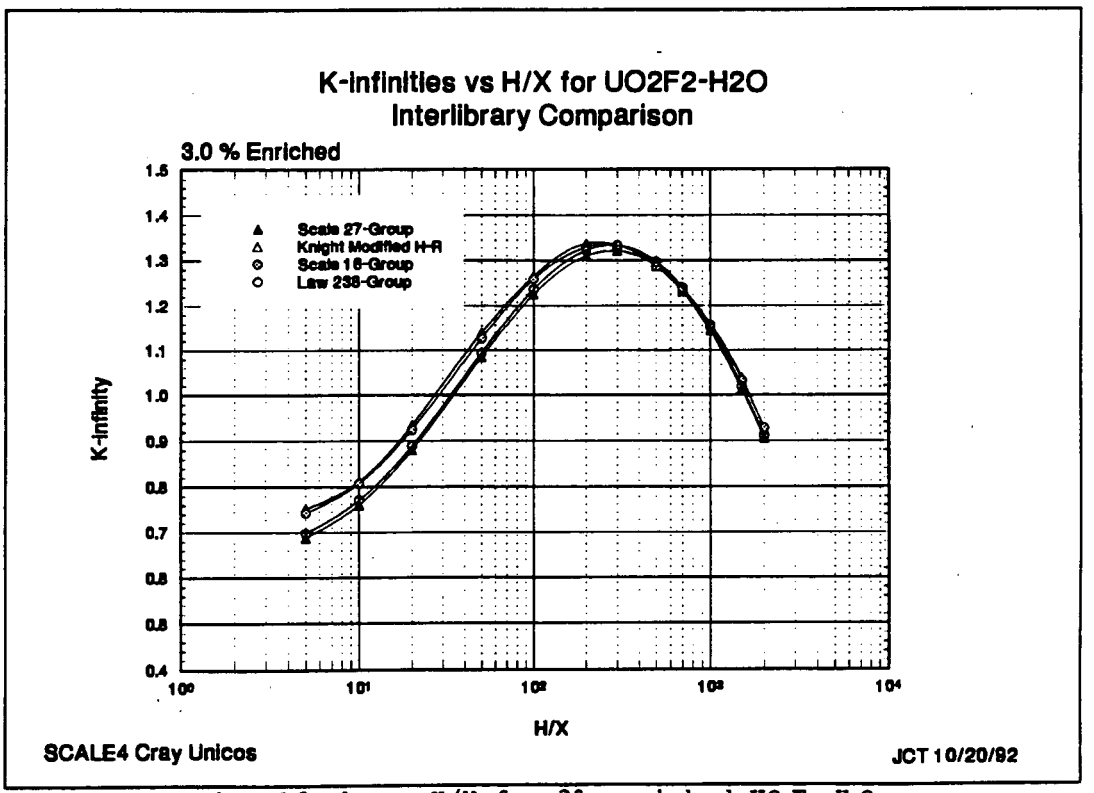

Fig. 16. k_∞ vs H/X for 3% enriched UO_2F_2–H_2O.

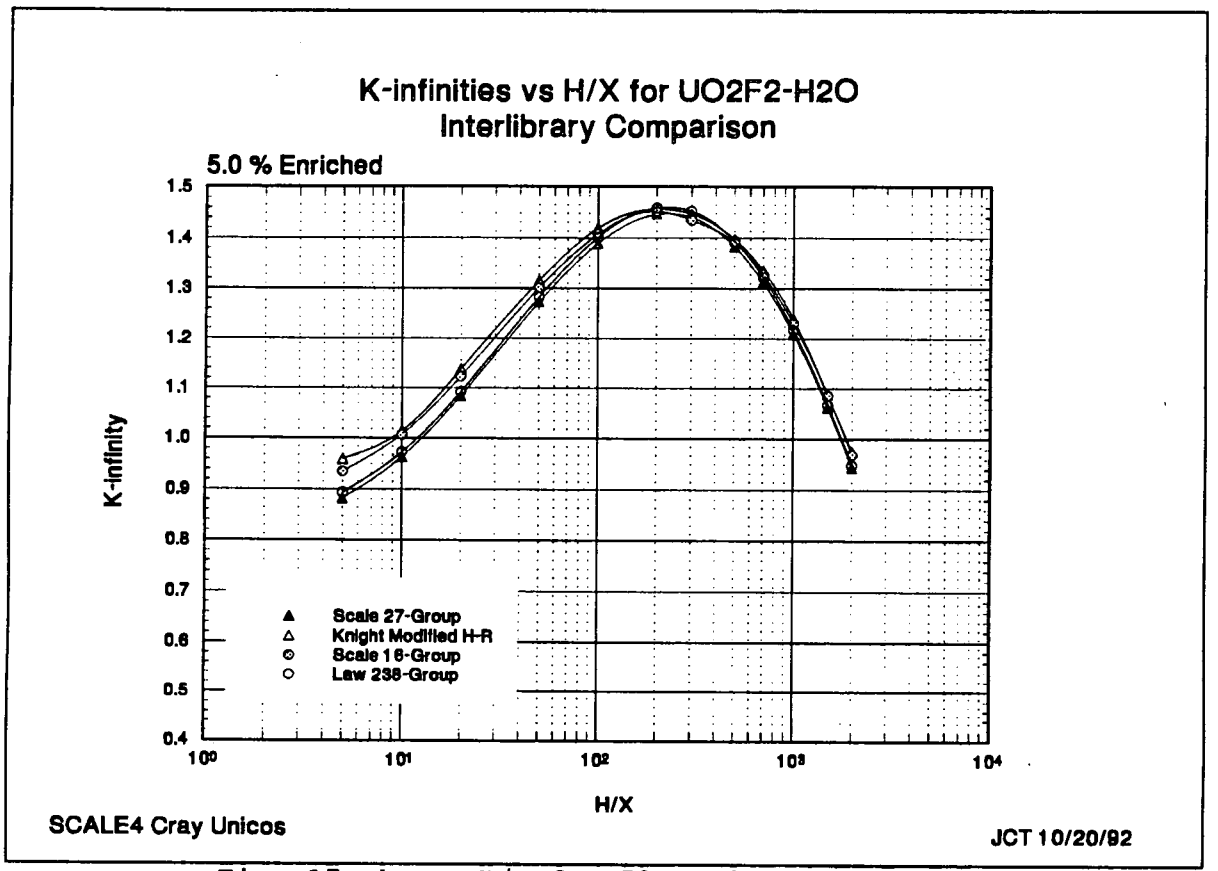

Fig. 17. k_∞ vs H/X for 5% enriched UO_2F_2–H_2O.

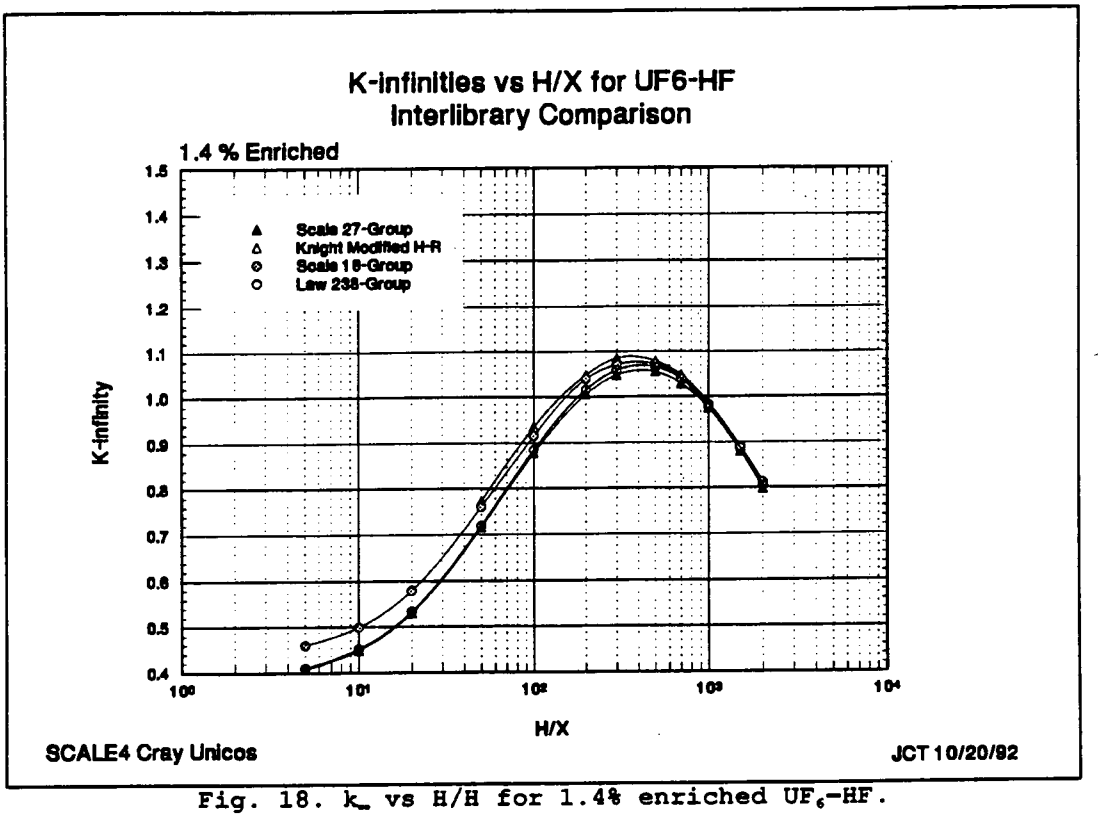

Fig. 18. k_∞ vs H/H for 1.4% enriched UF_6-HF.

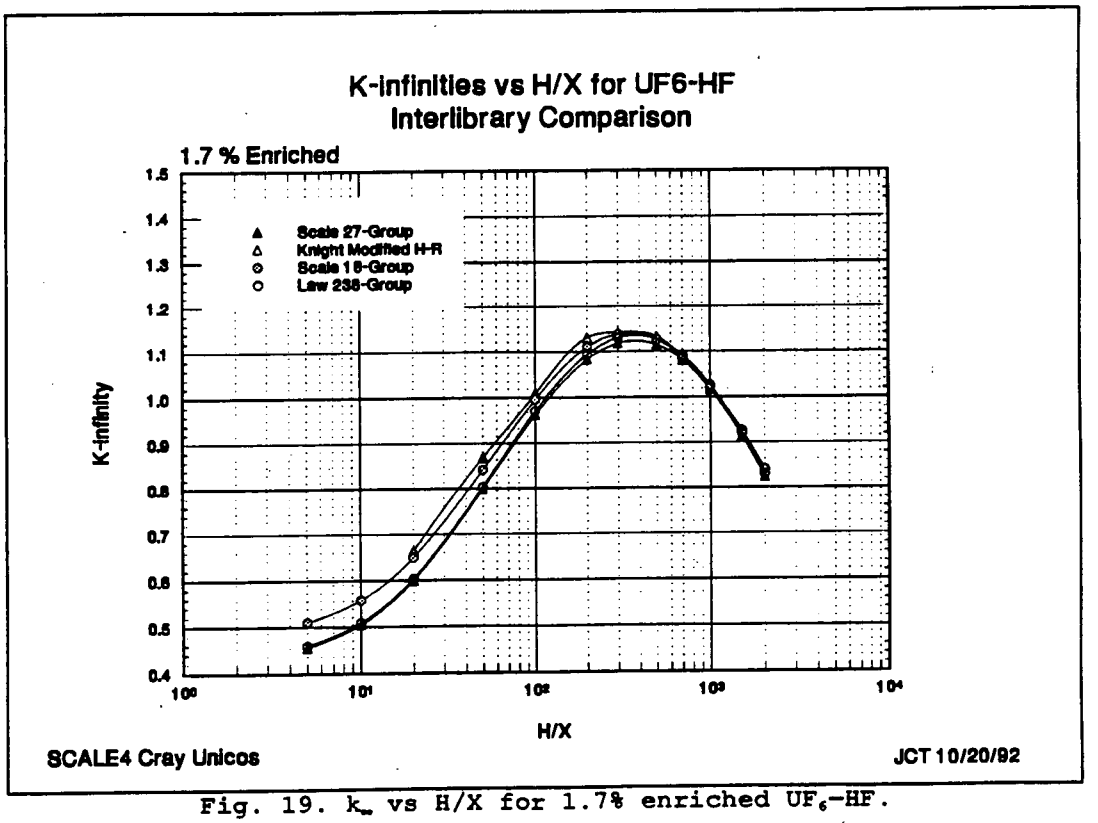

Fig. 19. k_∞ vs H/X for 1.7% enriched UF_6-HF.

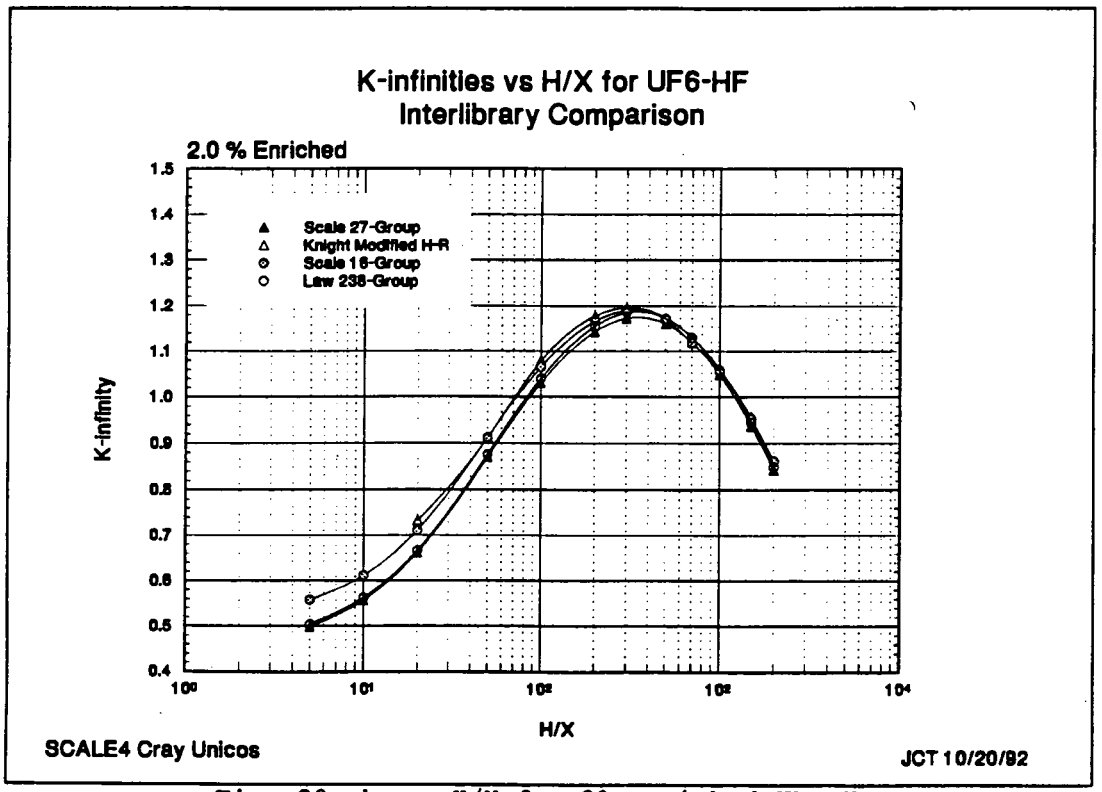

Fig. 20. k_∞ vs H/X for 2% enriched UF_6-HF.

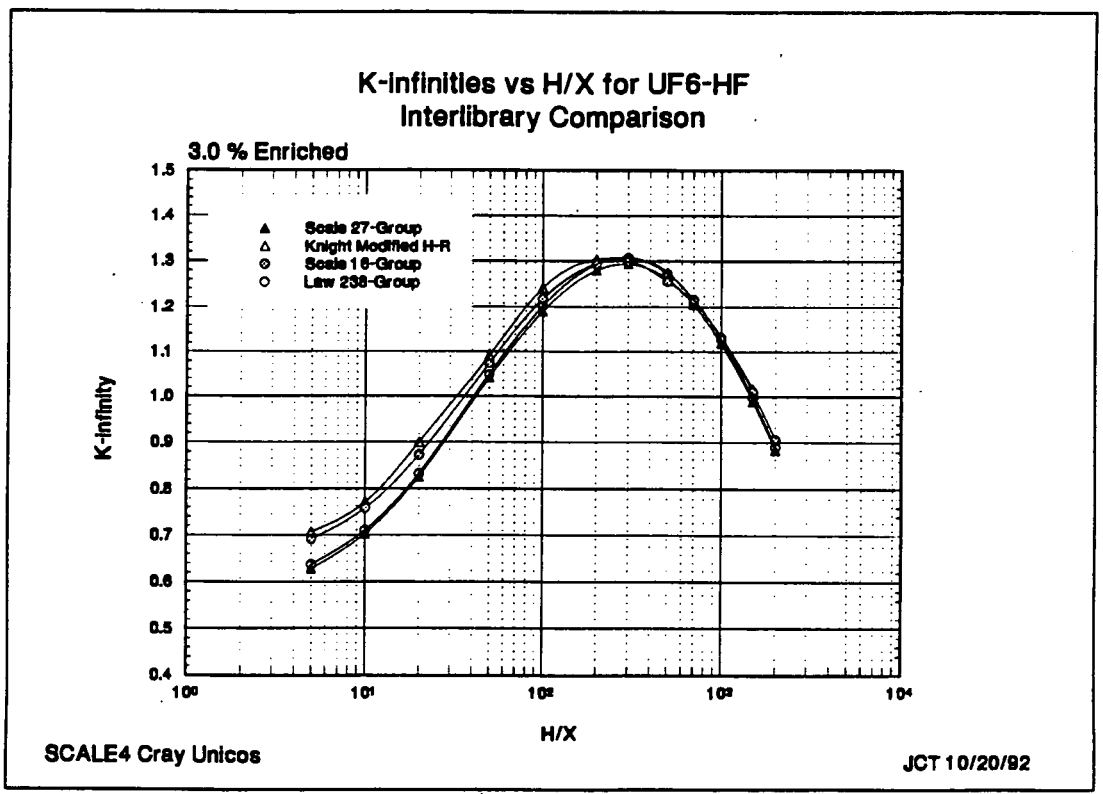

Fig. 21. k_∞ vs H/X for 3% enriched UF_6-HF.

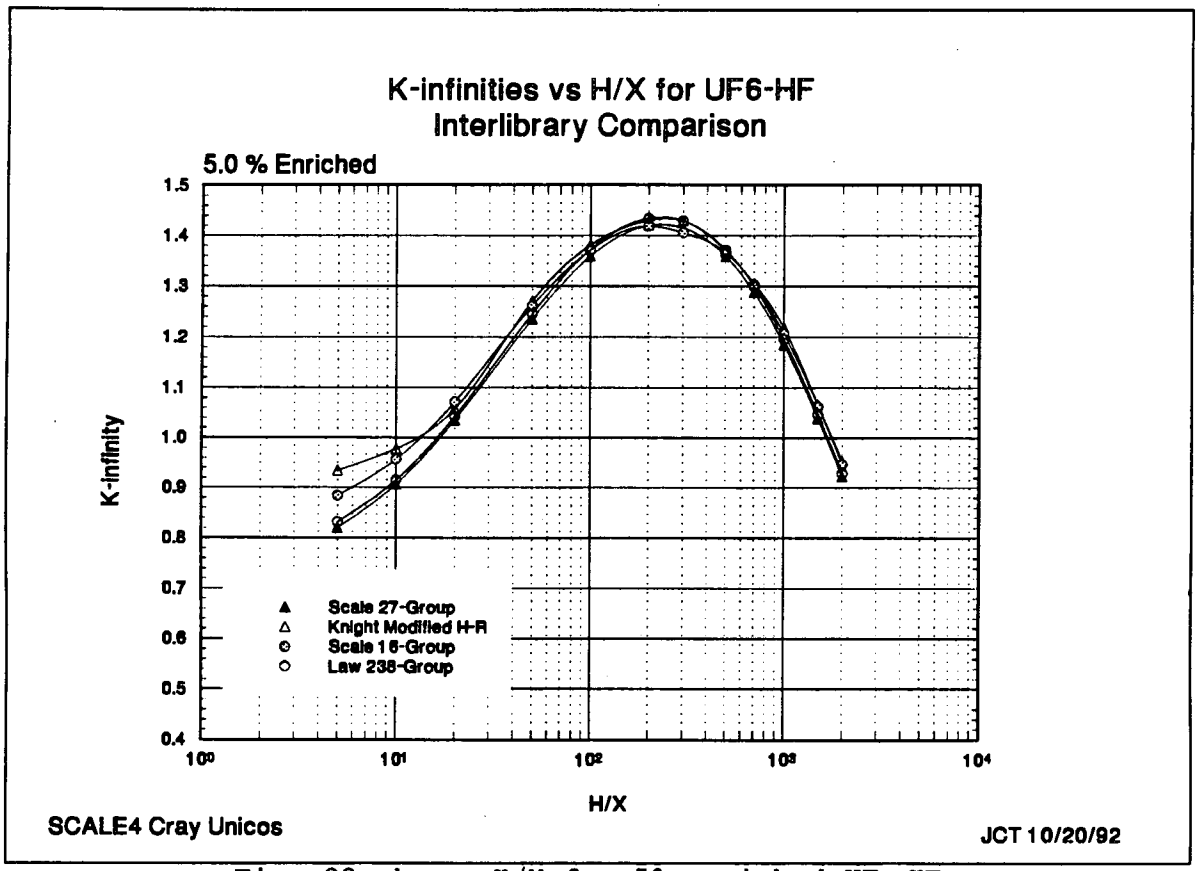

Fig. 22. k_∞ vs H/X for 5% enriched UF_6-HF.

that were made to ^{238}U from ENDF/B-IV to ENDF/B-V. They are also consistent with the fact that the unresolved resonance region for ^{235}U and ^{238}U were processsed at σ_p = 50,000 in the SCALE 27-group library.)

Of interest is the departure between the Knight-modified Hansen-Roach calculations and the 27-group calculations as a function of H/X and enrichment. There is a significant difference in calculated k_∞ over a range of H/X from 5 to 500 at 1.4% enrichment. The differences at 5% enrichment do not become significant until the H/X ratio is below about 100. In both cases, the differences in the infinite media multiplication are much greater at the lower values of k_∞. The relatively good agreement between the libraries at H/X = 500 for all the systems may help explain why there has not been more evidence in validations of an inadequacy in either library.

In general, minimum-mass systems occur at an H/X of around 500 for hydrogen-moderated uranium systems. Most critical experiments designed for low-enriched uranium have been designed to study the moderation region around minimum mass. This is especially true for enrichments much below 5%. The minimum volume system for 5% enriched uranium occurs at an H/X of about 200. As the enrichment gets smaller, the H/X at which minimum volume occurs moves toward an H/X of 500. There are fewer critical experiments with systems of low-enriched uranium at moderation levels below optimum because of the tremendous quantities of uranium required to attain criticality. Of the critical experiments that have been performed at low enrichment, low H/X, many have utilized "drivers" to attain criticality.

The trends between calculations performed with the Knight-modified Hansen-Roach cross sections, the SCALE 16-group library, and the LAW 238-group library as compared with the SCALE 27-group library are presented graphically in Figs. 23 through 30. These figures were generated by dividing the calculated k_∞ predicted by a library by the k_∞ predicted by the SCALE 27-group library. The results are presented on both log scales and linear scales. Figures 23 though 26 show that the 1983 Knight-modified Hansen-Roach (KMHR) calculations have a significant trend that is a function of both the enrichment and H/X ratio. The 5% results range from 0.5% higher at H/X = 300 to about 9% higher at H/X = 5 with a minima at H/X = 300. The 1.4% results range from 1.2% higher at H/X = 2000 to 8% higher at H/X = 50.

The infinite media ratios for the SCALE 16-group library are shown in Figs. 27 and 28 for the UO_2F_2–H_2O system. The SCALE 16-group calculations show the same general trends seen in the 1983 calculations. If the trends observed with both the Knight-modified Hansen-Roach and SCALE 16-group cross sections compared with the SCALE 27-group continue at higher enrichments, then there is a region of enrichments above 5% where the Hansen-Roach libraries will underpredict k_∞ with respect to the 27-group library.

Figures 29 and 30 show the ratio of the LAW-238 library against the 27-group library. The calculations using the LAW-238 library range from 0.5 to 1.5% higher than the 27-group library over the H/X range at all enrichments.

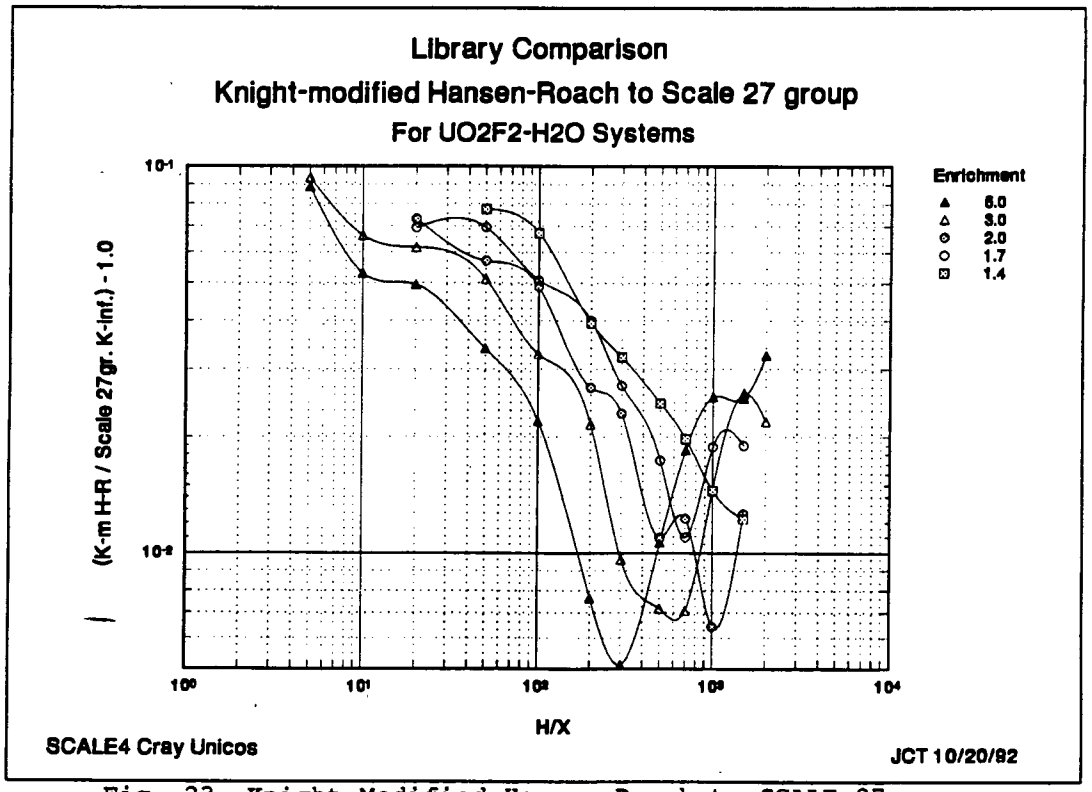

Fig. 23. Knight-Modified Hansen-Roach to SCALE 27-group library comparison - UO_2F_2-H_2O.

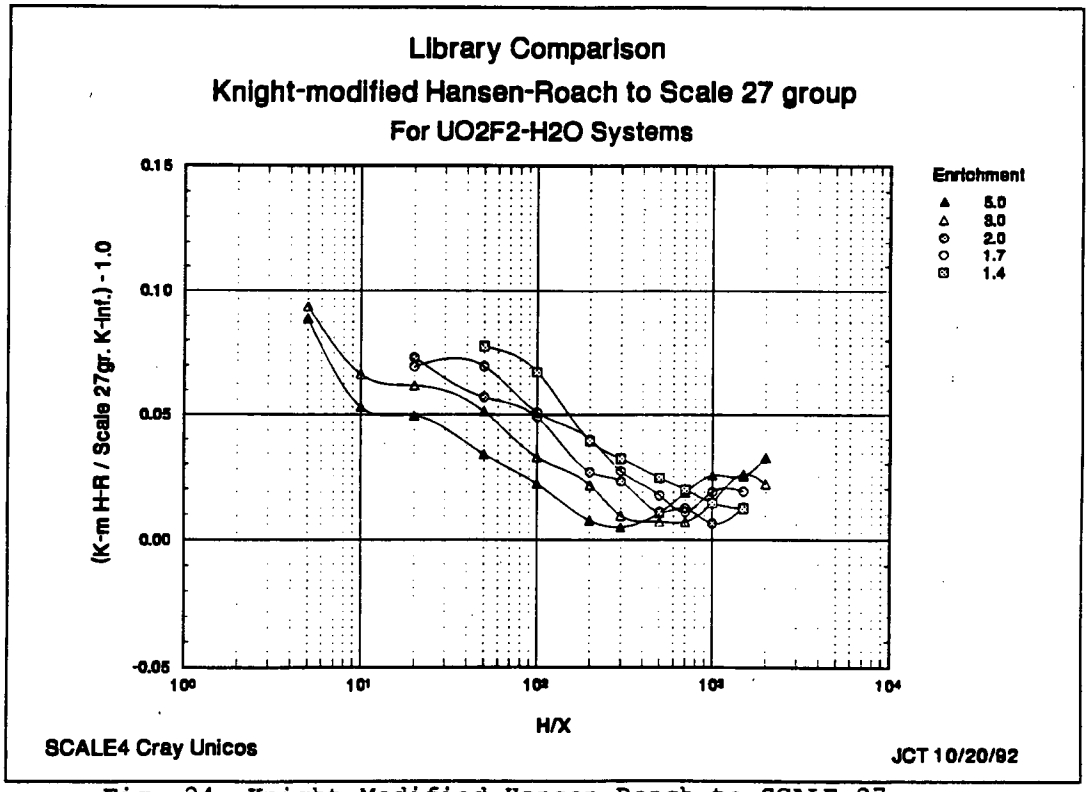

Fig. 24. Knight-Modified Hansen-Roach to SCALE 27-group library comparison - UO_2F_2-H_2O.

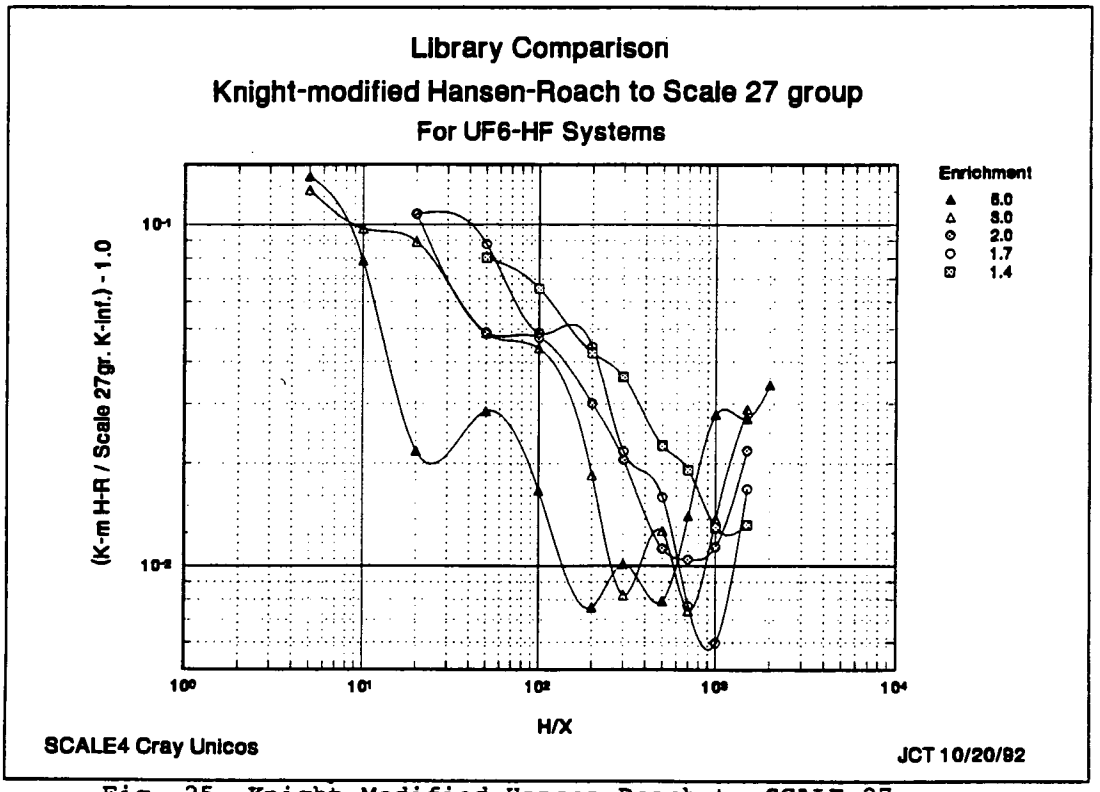

Fig. 25. Knight-Modified Hansen-Roach to SCALE 27-group library comparison - UF_6-HF.

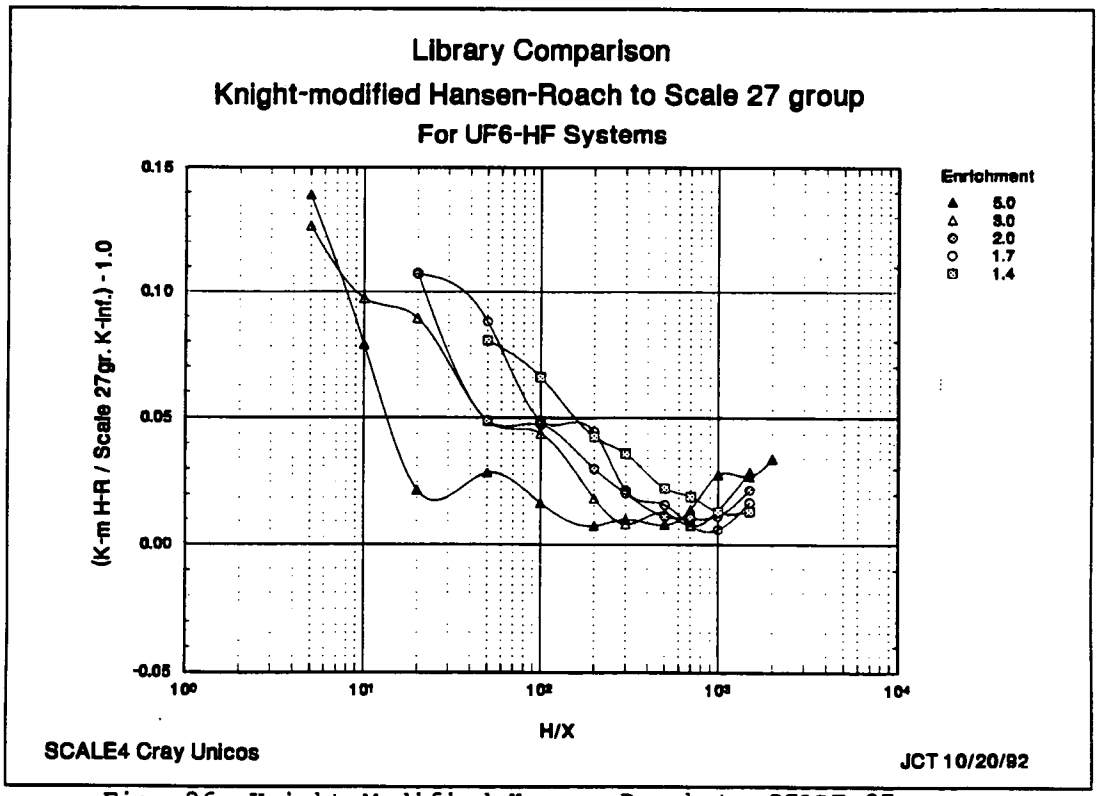

Fig. 26. Knight-Modified Hansen-Roach to SCALE 27-group library comparison - UF_6-HF.

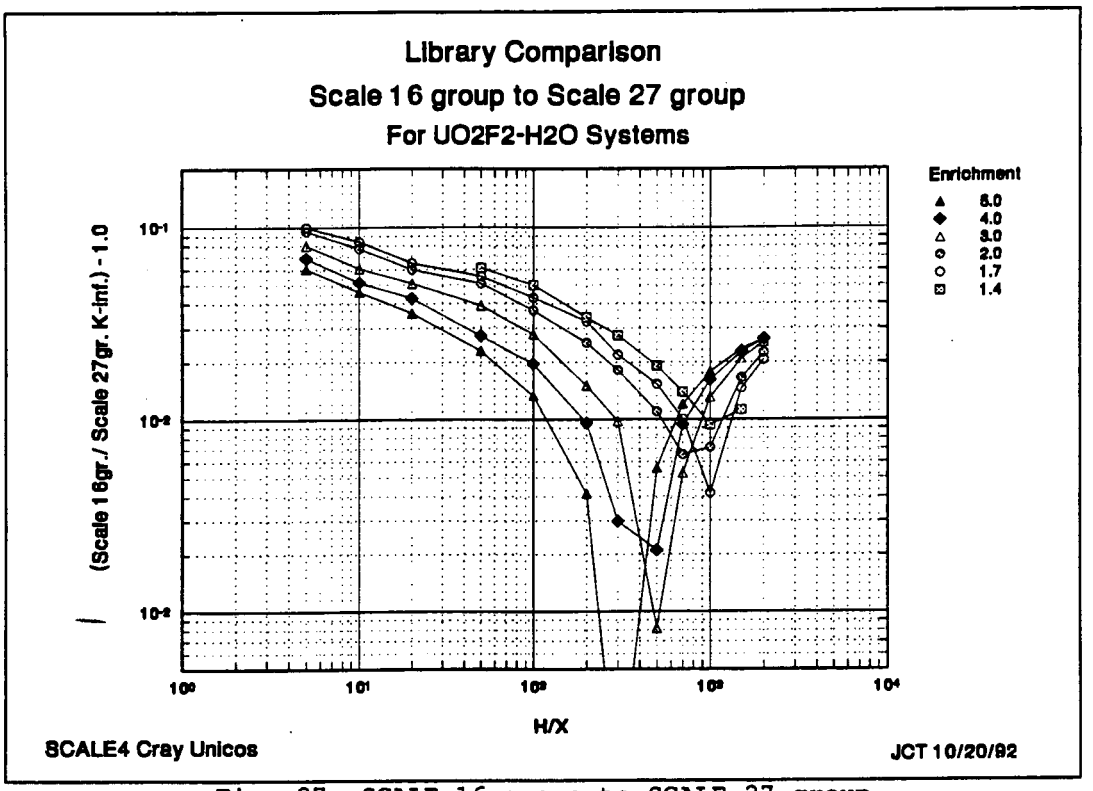

Fig. 27. SCALE 16-group to SCALE 27-group library comparison - UO_2F_2-H_2O.

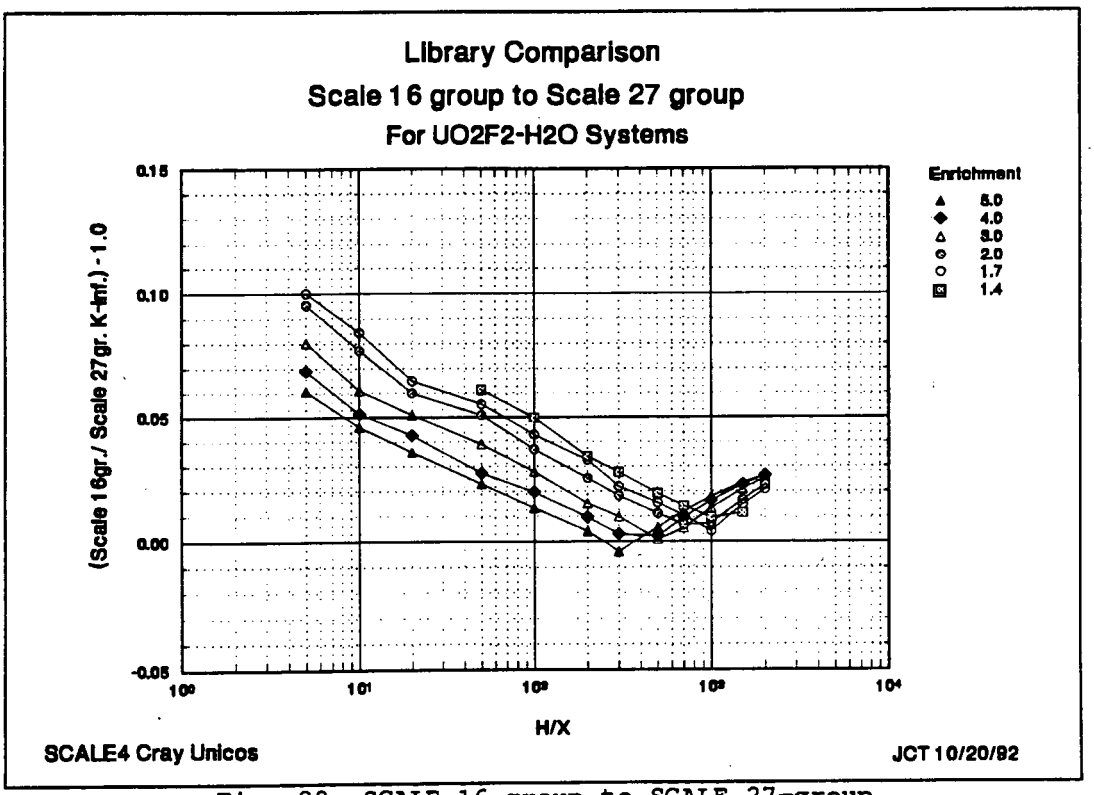

Fig. 28. SCALE 16-group to SCALE 27-group library comparison - UO_2F_2-H_2O.

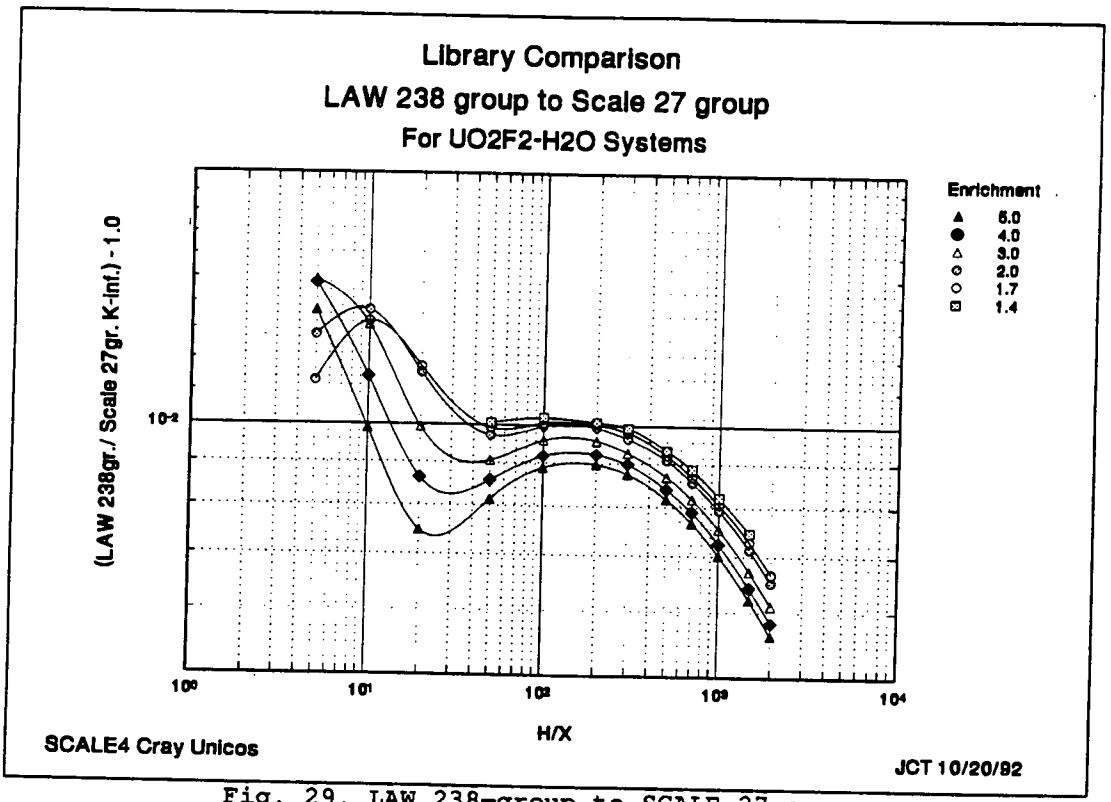

Fig. 29. LAW 238-group to SCALE 27-group library comparison - UO_2F_2-H_2O.

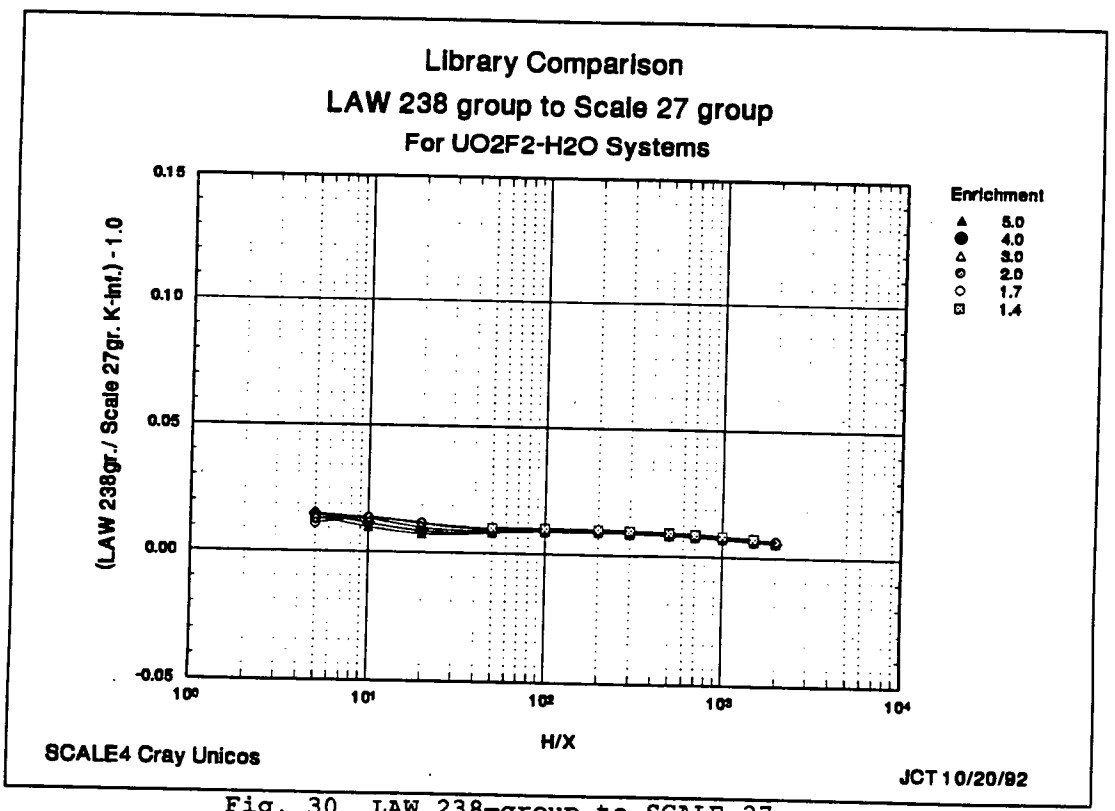

Fig. 30. LAW 238-group to SCALE 27-group library comparison - UO_2F_2-H_2O.

While the interlibrary comparison indicates that there is a difference in the infinite media multiplication factors predicted, it does not demonstrate which library is correct. Additional testing of the adequacy of the ENDF/B libraries was done using the ROLAIDS code.

3.2 ROLAIDS CALCULATIONS

The interlibrary comparison did not indicate which cross-section library should be considered more correct for the minimum-mass study. The possibility of poor resonance region cross-section processing could cause poor results for the ENDF/B libraries and exhibit the type of trends observed. The resonance region cross-section processing of the ENDF/B libraries was tested using the ROLAIDS code.

The ROLAIDS code performs a multiregion, energy-pointwise, resolved resonance treatment and was designed for use in cases where the Nordheim treatment implemented in NITAWL may not be adequate. ROLAIDS uses an energy-pointwise library and can more accurately reproduce the flux shape across the resonance region. ROLAIDS also treats resonance overlap. Several of the 1.4% and 5% enriched UO_2F_2–H_2O calculations were rerun using ROLAIDS-processed cross sections. The results of these calculations are presented in Table 3.

Table 3. ROLAIDS comparison

Enrichment	H/X	SCALE 27-group ROLAIDS	ENDF/B-IV NITAWL	LAW 238-group ROLAIDS	ENDF/B-V NITAWL
5.0	5	0.866579	0.881333	0.889335	0.893399
	10	0.946088	0.963163	0.969576	0.972681
	200	1.43972	1.44607	1.45673	1.45904
	2000	0.942285	0.943632	0.948294	0.948921
1.4	5	0.45088	0.462036	0.463756	0.466234
	100	0.907377	0.920974	0.929367	0.930380

The results in Table 3 indicate that ROLAIDS consistently underpredicts NITAWL for the ENDF/B-IV calculations. This result is in the opposite direction of that required to explain the difference between the 27-group and Hansen-Roach calculations. The difference between ROLAIDS and NITAWL results for the ENDF/B-IV cross sections has been observed in the past.[23]

There appears to be good agreement between the ENDF/B-V ROLAIDS and NITAWL calculations. The ENDF/B-V results are 0.5 to 1% greater than the ENDF/B-IV NITAWL results, which is the general trend expected from ENDF/B-IV to ENDF/B-V. The inconsistency of the ENDF/B-IV ROLAIDS calculations raises questions about the reliability of those results. The ENDF/B-V results indicate that there is probably not a problem in the NITAWL resonance-region cross sections for these systems.

The ROLAIDS results did not demonstrate a significant inadequacy of the 27-group calculations. Critical experimental data were reviewed to determine if there were experiments that would test the regions of the cross sections where the largest differences occurred. The Physical Constants Test Reactor (PCTR) series of experiments was identified as a possible candidate.

3.3 THE PCTR ANALYSIS

The PCTR experiments are a series of experiments which were performed at Hanford Experimental Development Laboratory (HEDL) in the 1950s and early 1960s. A series of experiments performed in 1957 for UO_2–H_2O mixtures at enrichments near 1% was of particular interest because it included k_∞ measurements for systems with an infinite media multiplication factor of less than 1.0. The trends in the Hansen-Roach and the 27-group calculations indicate that the lower the enrichment, the larger the disagreement in calculated k_∞. Table 4 gives the experimentally measured values for k_∞ along with those calculated using the 27-group and Hansen-Roach libraries. Selected cases were analyzed with ROLAIDS and the LAW 238-group library. Both the Hansen-Roach dE/E and X(E) hydrogen were used to determine if the high-energy scattering was impacting these results.

The results presented in Table 4 lead to the following observations:

1. The SCALE 27-group ENDF/B-IV library gives consistently better results when compared with the results using the Knight-modified Hansen-Roach cross sections. The ratio of the results of the Knight-modified Hansen-Roach calculations to the SCALE 27-group library calculations follow the same general trends as those observed in Fig. 23.
2. The 27-group calculations appear to be consistently 0.5 to 1% low relative to the experimental values.
3. The ENDF/B-IV results using ROLAIDS tend to underpredict both the measured k_∞ and that calculated with the SCALE 27-group library using NITAWL.
4. The LAW-238 ENDF/B-V library appears to give good overall agreement for the few cases in which this library was used.

Table 4. PCTR results

% Enrich.	H/U	Experimental k_∞	XSDRNPM results: 27-group	XSDRNPM results: Hansen-Roach dE/E	XSDRNPM results: Hansen-Roach X/E	XSDRNPM results: ROLAIDS ENDF/B-IV	XSDRNPM results: ROLAIDS ENDF/B-V	KENO results: 27-group k ± σ	KENO results: 27-group AEG	KENO results: Hansen-Roach k ± σ	KENO results: Hansen-Roach AEG
1.006	3.83	0.986 + 0.005	0.97973	1.01432	1.01259	0.974135	0.988313	0.98384 ± 0.00273	22.492	1.01247 ± 0.00217	14.390
	6.23	0.986 + 0.007	0.97543	0.99786	0.99667	---	---	0.97362 ± 0.00216	23.342	0.99547 ± 0.00223	14.855
	6.95	0.974 + 0.005	0.96799	0.98935	0.98827	---	---	0.97131 ± 0.00212	23.484	0.98970 ± 0.00233	14.953
	7.52	0.960 + 0.005	0.96109	0.98120	---		0.956988	0.96074 ± 0.00191	23.581	0.98221 ± 0.00202	15.013
1.071	3.78	1.005 + 0.006	0.99961	1.03483	1.03309	---	---	0.99959 ± 0.00234	22.450	1.03680 ± 0.00240	14.381
	5.84	1.005 + 0.006	1.00167	1.02515	1.02390	0.996922	1.00953	1.00080 ± 0.00196	23.232	1.02968 ± 0.00231	14.822
	7.14	0.992 + 0.007	0.98992	1.01100	1.00994	---	---	0.99244 ± 0.00234	23.527	1.01080 ± 0.00181	14.977
1.157	3.73	1.031 + 0.006	1.02347	1.05935	1.05758	1.01756	1.03260	1.02300 ± 0.00239	22.390	1.06058 ± 0.00257	14.371
	5.99	1.031 + 0.005	1.02876	1.05199	1.05076	---	---	1.02786 ± 0.00237	23.275	1.05228 ± 0.00206	14.845
	6.90	1.030 + 0.007	1.02167	1.04340	1.04231	---	---	1.02520 ± 0.00208	23.477	1.04610 ± 0.00238	14.966
	7.52	1.019 + 0.005	1.01530	1.03564	---	---	---	1.01564 ± 0.00226	23.592	1.03485 ± 0.00226	15.016

The case for 1.006% enrichment at H/U = 3.83 was selected for further study to determine the cause of the poor performance of the Knight-modified Hansen-Roach cross sections. The SCALE 16-group library is based on the Knight-modified cross sections which have been put into a form that can be processed by BONAMI. BONAMI performs an iteration and calculates the σ_p on a groupwise basis as opposed to selecting a specific σ_p cross-section set. To test if there is a sensitivity to the manner in which σ_p's are calculated, the σ_p's for ^{235}U and ^{238}U were calculated by the KENO-IV methodology. The results using the Knight-modified Hansen-Roach cross sections gave k_∞ values within a few tenths of a percent of the SCALE 16-group library.

All the Hansen-Roach calculations considered up to this point have been ORNL Knight-modified versions of the cross sections. It was of interest to determine if the poor performance of the Hansen-Roach calculations could be attributed to the Knight modifications. Several calculations were performed using the original Hansen-Roach cross-section library. The σ_p methodology proposed by Hopper-Renier of ξ weighting was used,[24] with one modification. The modification involves adding into the σ_p calculation the background self-shielding for the nuclide being considered. The original Hansen-Roach library using this σ_p formalism gave a value of k_∞ = 0.99317 and is in relatively good agreement with experiment. This represents a 2% improvement. The significant improvement of the calculated k_∞ value suggests that there is an inadequacy in the manner in which the Knight modifications were applied to the original Hansen-Roach cross sections. The systems considered in the minimum-mass study may have extended into the range of extrapolation of the Knight modifications, and the results of the analysis with the Knight-modified Hansen-Roach cross sections may be significantly biased.

Additional comparisons using the modified Hopper-Renier σ_p weighting were performed for the 5% enriched UO_2F_2-H_2O system at H/X = 5. The use of this formulation with the original Hansen-Roach library improved the agreement to the SCALE 27-group library but did not account for all of the difference. A series of calculations were performed in which the cross sections in the original Hansen-Roach library were replaced by ENDF/B-V cross sections processed into the same group structure. The results of these replacement calculations are presented in Table 5.

As shown in Table 5, the use of the Hopper-Renier formulation and the original Hansen-Roach library (Case 01A) yields a 0.7% reduction in the infinite media multiplication factor compared to the SCALE-4 16-group library. The replacement of the Hansen-Roach fluorine in Case 01A yields a 1% reduction in infinite media multiplication, and the replacement of oxygen yields an 0.8% reduction. Replacement of the Hansen-Roach hydrogen with ENDF/B-V hydrogen yields a slight increase in k_∞. Replacement of H, O, and F in Case 01A with ENDF/B-V cross sections yields a 1.5% reduction in the calculated k_∞.

It appears that the Knight-modified Hansen-Roach cross sections are not well suited for the range of systems encountered in the minimum-mass study. Both the Knight-modified and original Hansen-Roach libraries tend to overpredict the infinite media multiplication factor and thus underpredict the critical radii. This is a reverse in trend compared with the observations of

Table 5. H-R replacement calculations for $U(5)O_2F_2$ and water at H/X = 5

Case	Description	k_∞
Ref.	SCALE-4 16-group	0.934757
01A	Original H-R library	0.928203
01B	Case 01A except ENDF/B-V F	0.918825
01C	Case 01A except ENDF/B-V O	0.921045
01D	Case 01A except ENDF/B-V H	0.931194
01E	Case 01A except ENDF/B-V F & O	0.911973
01F	Case 01A except ENDF/B-V F,O & H	0.914886

Stratton.[25] The reversal of calculational trends for the original library may be due to the use of different σ_p formulations.

It also appears that one might expect a 0.5 to 1% negative bias in the value of k_∞ predicted by the SCALE 27-group ENDF/B-IV NITAWL-processed cross-section library for the range of systems analyzed. This bias may be accounted for using the procedures outlined in Sect. 2. The ROLAIDS-processed ENDF/B-IV cross sections tend to underpredict the NITAWL-processed library and significantly underpredict the measured k_∞'s in the PCTR experiments analyzed.

The LAW 238-group ENDF/B-V library gave good results for the PCTR calculations and appears to be the most reliable of the libraries tested.

An important conclusion of the investigation into the discrepancies between calculations with the Knight-modified Hansen-Roach cross sections and the SCALE 27-group library is that there are areas of application that have not been validated. Infinite media measurements and critical experiments at the lower range of moderation level may need to be included in future validations. If these experiments are not available, then new critical experiments are needed.

It is apparent that the σ_p formalism used with the Hansen-Roach library must be consistent between the validation and the subsequent application. The trends and bias observed will be related to this formalism. This statement can be generalized. In validation of a criticality code, the code, cross sections, and cross-section processing methodology are being validated. In application, care must be taken to ensure that the code, cross sections, and processing methodology are consistent with the validation. If the application is inconsistent with the validation, trends and bias may be introduced which have not been properly taken into account in establishing the calculational acceptance criteria.

4. EFFECTS OF MODERATION LEVEL ON THE NEUTRON SPECTRUM

The significant disagreement between the calculations using the SCALE 27-group and Knight-modified Hansen-Roach libraries was not expected. Both of these libraries have been in use for years and have been validated against substantially the same set of critical experiments. Large differences between the two libraries have not been previously encountered. The large differences between the libraries seen in the minimum-mass study suggest that the libraries are being used outside of their respective validation. The purpose of this section is to briefly review the adequacy of the parameters used to demonstrate the area of applicability and range of applicability of a particular set of validation problems in relation to another (unknown) system.

In the strictest sense, one should have critical experiments (benchmarks) that are directly related to the unknown systems being calculated. The adequacy of the codes and cross sections for use in predicting criticality for the unknown system should be demonstrated by calculating the benchmarks (this is commonly called the "validation" of the code and cross sections). Virtually all the critical experiments used for benchmarking codes were performed decades ago. In practice, the criticality engineer must review the data base of old experiments and find those directly applicable to the systems under consideration. In the absence of directly applicable experiments, those that appear to encompass the unknown system parameters must be used for validation, since there is little chance of obtaining new experiments in a timely manner.

Common parameters in establishing the range of applicability of a validation include the fissile material compound, the uranium enrichment, the moderator compound, the level of moderation, and the system geometry and reflective conditions. Another parameter which has been used is the average energy group of the neutron-causing fission (AEG).[26,27,28]

The systems considered in the minimum-mass study have low-enriched uranium in the form of UO_2F_2 or UF_6 as the uranium compound. The moderators considered are H_2O and HF over a range of moderation levels. Fully H_2O-reflected spherical geometry was considered. The fissile materials, moderators, moderation levels, and geometries are those one might expect to encounter (routinely) in a gaseous diffusion plant or in the analysis of UF_6 transportation and storage.

There are a number of critical experiments for low-enriched uranium. These cover an enrichment range from near 1 to 5%. A number of these experiments involve UO_2F_2 as the fissile compound. There are no critical experiments that involve low-enriched UF_6. Experiments with UF_4 are generally used to validate cross sections for UF_6 systems.

The moderation levels for the critical experiments for H_2O-moderated UO_2F_2 cover a range from H/U = 15 to H/U = 100. At moderator ratios much below H/U = 15, the system is no longer a "free-flowing" solution, but more like syrup; at moderation ratios below H/U = 9, the systems become more comparable to toothpaste; below H/U = 4, one has mixtures of solid hydrated uranyl fluoride compounds. Critical experiments with other materials, such as UF_4 or uranium oxides, are used to evaluate the cross sections at the lower moderation levels. There

are a number of experiments involving these compounds with paraffin, sterotex, or water as the moderator. There are no low-enriched critical experiments that have HF as a moderator.

The lack of experiments with liquid HF may be of significant importance. There are no thermal-scattering data in ENDF for HF. The cross sections used for hydrogen in calculations involving HF are those for water-bound hydrogen. There is no reason to expect that the neutron thermal scattering in water and HF are the same. The only way to evaluate the acceptability of this approximation is through evaluation of the thermal-scattering kernel in HF and through experimentation with HF as a moderator.

In establishing an acceptable set of validation experiments for the calculations performed in Sect. 2, observe that there are few critical experiments performed in spherical geometry for low-enriched uranium. This is because of the difficulties involved in manufacturing the spherical vessels in combination with the appropriate size for criticality. It is rare that a partially filled spherical experiment is described because the calculational codes available twenty years ago could not handle these systems. Slab, cylindrical, and spherical geometries must be considered collectively in order to establish an adequate benchmark data base.

The AEG has been used as a parameter to establish the range of applicability of validations. The AEG has embedded information related to the moderation level and leakage of a system. It also has embedded information on the spectral effects of the reflector. Using the AEG as a parameter tends to smear all of the critical experiments involving different geometries, fissile compounds, moderators, and moderation levels into the same group. The unknown system can be related through its AEG to the group of validation experiments.

The AEG for several of the infinite media systems in the minimum moderator mass study were calculated using KENO V.a. The systems considered were UO_2F_2–H_2O at 5% enrichment, UO_2F_2–H_2O at 1.4% enrichment, and UF_6–HF at 5% enrichment. The results are presented in Table 6, along with XSDRNPM results. There is excellent agreement between KENO V.a and XSDRNPM for both of the cross-section libraries considered.

Additional details of the neutron spectrum for the SCALE 27-group calculations in Table 6 were obtained from the system summary tables of the XSDRNPM calculations and are presented in Tables 7 through 9. Included in these tables is the percentage of the flux, absorptions, and fissions for five energy regions. This enables one to determine what the important cross-section regions are for the problem. The energy region boundaries were chosen to correspond roughly to the following energy regions: (1) fission spectrum (groups 1–7 of the 27-group library); (2) unresolved resonance region (groups 8 and 9); (3) top of the ^{238}U resolved resonance region (groups 10–12); (4) the ^{235}U resolved resonance region and the bottom of the ^{238}U resolved resonance region (groups 13–15); and (5) the thermal region (groups 16–27). The percentage of the generating flux which occurs in each of the five energy regions is also given in Table 7.

Table 6. Intercomparison of XSDRNPM and KENO V.a results

	27-Group				Hansen-Roach			
H/X	XSDRN k_∞	KENO V.a k	Dev.	AEG	XSDRN k_∞	KENO V.a k	Dev.	AEG
5% enriched UO_2F_2–H_2O								
5	0.881333	0.88112	0.00209	10.0848	0.934757	0.93707	0.00249	7.6242
10	0.963163	0.96512	0.00253	12.2513	1.00741	1.00759	0.00239	9.0192
20	1.08401	1.08783	0.00279	15.3618	1.12277	1.11931	0.00332	10.8151
50	1.27189	1.26804	0.00319	19.3531	1.30100	1.30207	0.00290	13.0341
100	1.38902	1.39477	0.00356	21.7170	1.40743	1.40793	0.00321	14.2131
200	1.44607	1.44711	0.00296	23.2340	1.45203	1.45073	0.00287	14.9778
500	1.38267	1.38230	0.00291	24.3418	1.39039	1.39216	0.00281	15.5130
1500	1.06147	1.06229	0.00186	24.8981	1.08629	1.08505	0.00187	15.7762
1.4% enriched UO_2F_2–H_2O								
100	0.920974	0.91856	0.00262	19.6329	0.966783	0.96463	0.00262	12.9369
200	1.04172	1.04320	0.00288	21.8093	1.07727	1.07574	0.00302	14.0912
500	1.08382	1.08377	0.00208	23.5369	1.10453	1.10765	0.00222	15.0118
1500	0.903401	0.90499	0.00171	24.4997	0.913548	0.91644	0.00153	15.5316
5% enriched UF_6–HF								
10	0.905968	0.90803	0.00267	12.8951	0.955991	0.95210	0.00245	9.4568
50	1.23487	1.23205	0.00323	19.7314	1.26124	1.25983	0.00305	13.2370
200	1.41973	1.42274	0.00293	23.3646	1.41898	1.41686	0.00285	15.0473

Table 7. Selected spectral information for $U(5)O_2F_2$–H_2O systems

H/X	H/U	Group	Flux %	Absorptions %	Fissions %	AEG	Generating flux
5	0.25	<7	45.82	15.28	22.39	10.08	44.5
		8-9	33.62	25.07	13.35		11.9
		10-12	17.72	43.31	40.47		13.2
		13-15	2.10	11.39	9.69		8.1
		(> 16)	0.74	4.95	14.10		22.3
10	0.51	< 7	47.45	13.14	20.85	12.25	
		8-9	28.16	16.94	8.18		
		10-12	18.75	40.47	33.66		
		13-15	3.71	16.78	12.46		
		(> 16)	1.93	12.67	24.85		
20	1.01	< 7	48.61	10.49	15.17	15.36	
		8-9	23.17	10.38	4.40		
		10-12	18.62	33.33	23.29		
		13-15	5.43	19.93	12.11		
		(> 16)	4.17	25.87	45.03		
50	2.53	< 7	48.73	6.84	8.63	19.35	
		8-9	18.15	4.89	1.74		
		10-12	17.16	21.94	11.53		
		13-15	6.95	18.69	8.20		
		(> 16)	9.01	47.64	69.90		
100	5.06	< 7	47.20	4.50	5.17	21.72	
		8-9	15.40	2.63	0.85		
		10-12	15.63	14.81	6.23		
		13-15	7.35	15.30	5.17		
		(> 16)	14.42	62.76	82.58		
200	10.1	< 7	43.86	2.78	2.96	23.23	
		8-9	13.11	1.38	0.42		
		10-12	13.90	9.67	3.31		
		13-15	7.18	11.68	3.05		
		(> 16)	22.95	74.49	90.26		
500	15.2	<7	36.68	1.43	1.41	24.34	
		8-9	10.29	0.58	0.18		
		10-12	11.26	5.37	1.49		
		13-15	6.25	7.81	1.49		
		(> 16)	35.52	84.81	95.43		
500	50.6	<7	26.84	0.71	0.65	24.89	
		8-9	7.29	0.20	0.08		
		10-12	8.13	2.62	0.67		
		13-15	4.73	4.69	0.71		
		(> 16)	53.01	91.78	97.89		

Table 8. Selected spectral information for $U(1.4)O_2F_2$-H_2O systems

H/X	H/U	Group	Flux %	Absorptions %	Fissions %	AEG
100	0.08	< 7	43.78	8.12	13.11	19.63
		8-9	19.18	6.90	1.14	
		10-12	17.76	22.92	7.49	
		13-15	7.01	18.56	5.52	
		(> 16)	12.27	43.50	72.74	
500	7.09	< 7	37.45	3.27	4.53	23.54
		8-9	11.68	1.65	0.22	
		10-12	12.35	9.69	1.76	
		13-15	6.39	11.56	1.66	
		(> 16)	32.13	73.83	91.83	
1500	21.3	< 7	28.40	1.51	2.22	24.49
		8-9	8.03	0.58	0.09	
		10-12	8.80	5.11	0.76	
		13-15	4.92	7.52	0.78	
		(> 16)	49.85	85.28	96.15	

Table 9. Selected spectral information for $U(5)F_6$-HF

H/X	H/U	Group	Flux %	Absorptions %	Fissions %	AEG
10	0.51	< 7	38.01	9.85	15.73	12.89
		8-9	33.59	17.47	8.72	
		10-12	21.79	41.88	35.38	
		13-15	4.33	17.78	13.31	
		(> 16)	2.28	13.02	26.86	
50	2.53	< 7	42.46	5.86	6.73	19.73
		8-9	20.66	5.04	1.79	
		10-12	19.09	22.37	11.70	
		13-15	7.72	19.14	8.37	
		(> 16)	9.97	47.59	71.41	
200	10.1	< 7	39.17	2.80	2.36	23.36
		8-9	14.36	1.44	0.43	
		10-12	14.99	9.79	3.32	
		13-15	7.74	11.89	3.06	
		(>16)	23.74	74.08	90.83	

A desirable characteristic of group cross sections is that the spectral flux used to generate the cross sections be similar to the spectral flux of the system being analyzed. As these two fluxes get farther apart, more energy groups are required to adequately represent the cross sections. As the generating flux and true flux become significantly different, it is likely that the library will yield unacceptable calculational results.

The information presented in Tables 7 through 9 is depicted graphically in Figs. 31–44. In each of these figures the fine-group (218-group) and broad-group (27-group) generating spectrums are shown as a function of energy.

For UO_2F_2 at H/X = 5, the AEG = 10.08 when using the SCALE 27-group library. This corresponds to an energy of about 3 keV. The majority of the flux is in the fission spectrum region with smaller, about equal amounts in the resolved and unresolved regions. There is a very small flux in the thermal region. The increased importance of the thermal flux over the fluxes in the other regions may be seen by the large fission contribution in the thermal region. This type of system tests the resonance region of the fissile material and the scattering matrices of the moderating material. One of the validation documents for KENO V.a and the SCALE 27-group library was reviewed to determine if this AEG range had been validated.[28] The review indicated that AEGs greater than about 13 were validated for low-enriched uranium. Any systems with an AEG less than 13 must be considered outside the range of validation.

As the H/X ratio is increased, the AEG becomes larger (the system becomes more thermal). The flux in the unresolved resonance region becomes smaller, and then the flux in the resolved resonance regions becomes smaller. The relative amount of fissions in the thermal region grows rapidly. The figures demonstrate that the AEG is closely related to the moderation level of the system. At an H/X of about 20, the AEG comes into the range of the validation. However, virtually all of the validation criticals in the AEG range from 13 to 20 involve heterogeneous systems or had highly enriched uranium drivers in order to reach criticality. It may not be appropriate to use AEG to relate homogeneous calculations to heterogeneous or driven benchmark experiments (i.e., the AEG of the unknown system is within the range of AEG validated, but the unknown system is outside the area of applicability of the validation).

There is good agreement between the generating flux and the calculated flux at H/X = 200. It might be expected that the cross sections would be more reliable at this moderation level. The AEG for this range is on the order of 23. There appear to be numerous critical experiments with a calculated AEG between 22 and 25. Above H/X = 200, there is a gradual decrease in the flux in the resonance region; the flux in the fission spectrum region is nearly constant.

The flux plots for 1.4% UO_2F_2–H_2O are similar to those for 5% enrichment, except there is a slight spectral hardening that can be seen in the AEG at a given H/X. The 5% UF_6-HF systems show a slight spectral softening when compared with the 5% UO_2F_2-H_2O system at the H/X. The effects of enrichment on the AEG are given in Table 10 for several of the predicted critical systems from Sect. 2.

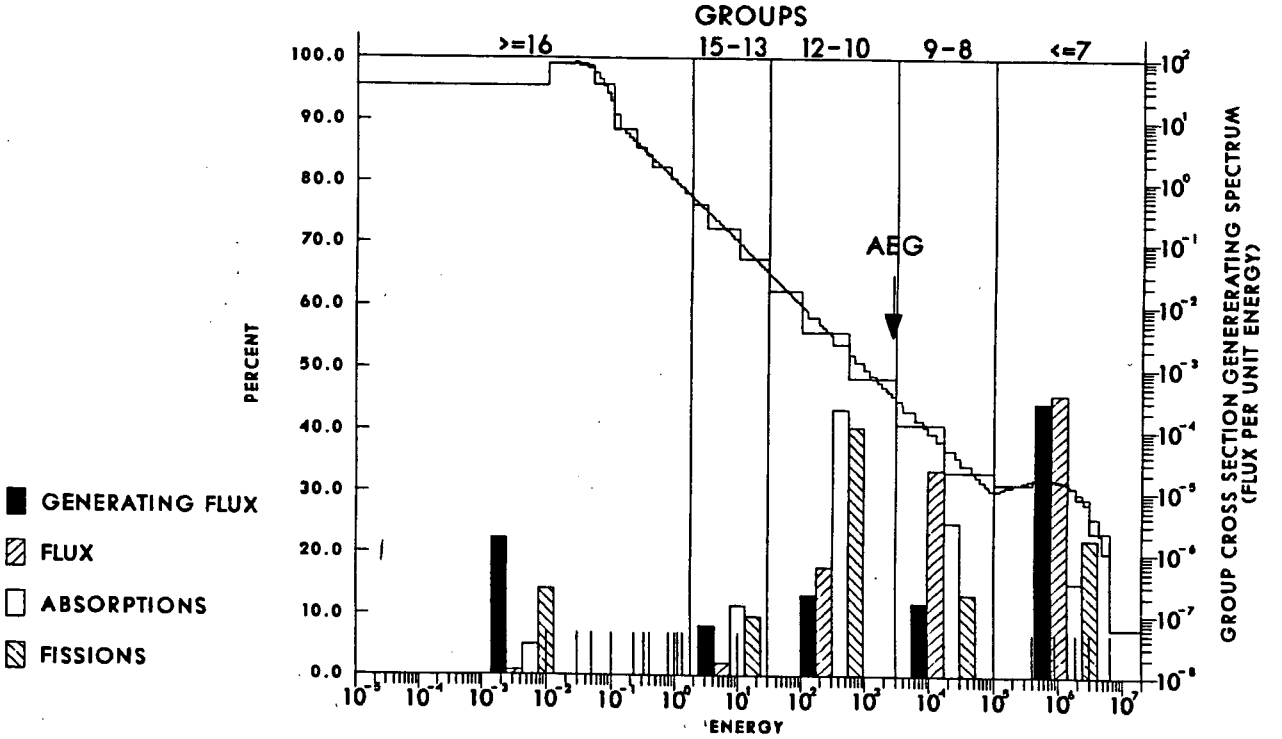

Fig. 31. UO_2F_2-H_2O 5.0% enriched H/X = 5.

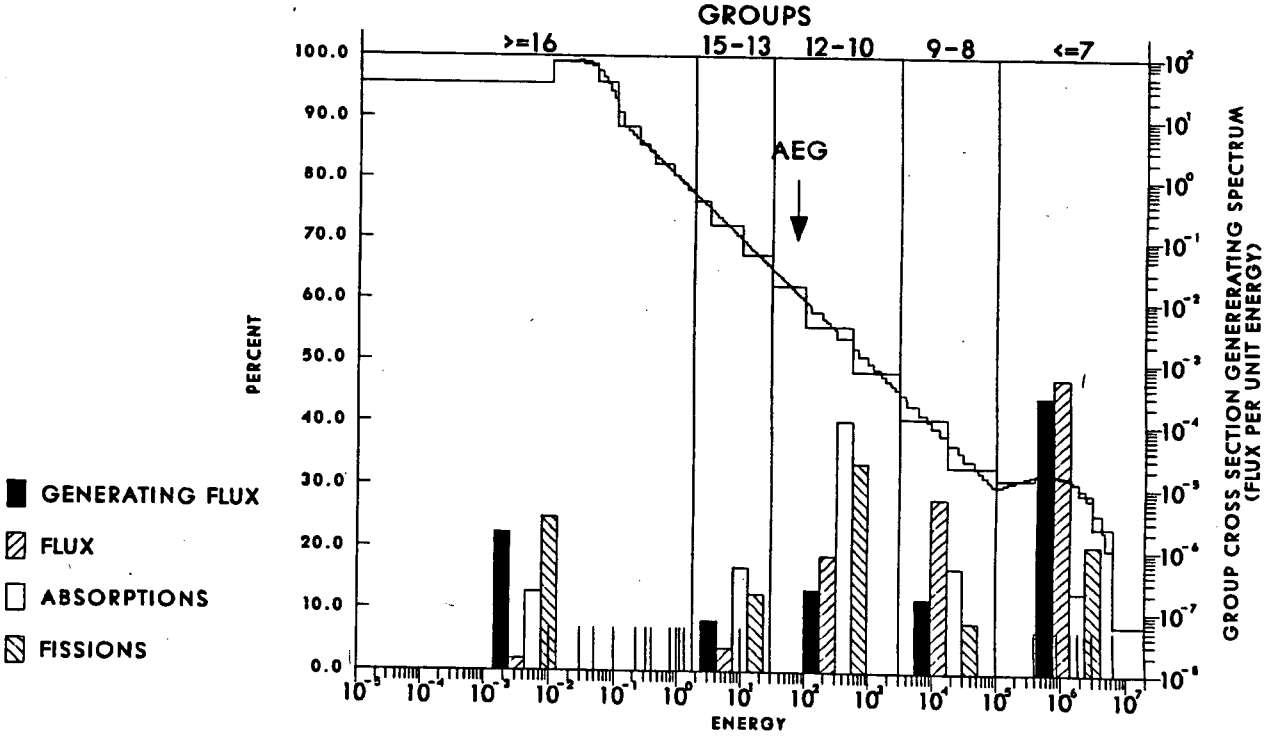

Fig. 32. UO_2F_2-H_2O 5.0% enriched H/X = 10.

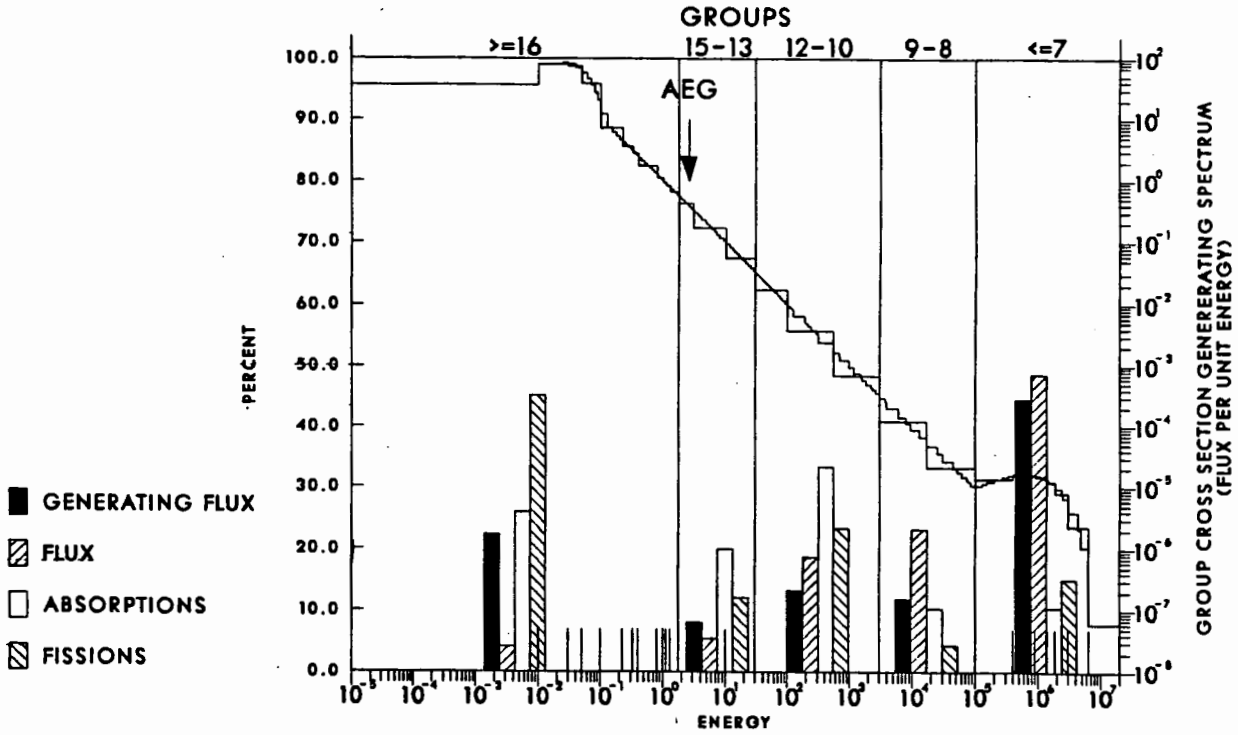

Fig. 33. UO_2F_2-H_2O 5.0% enriched H/X = 20

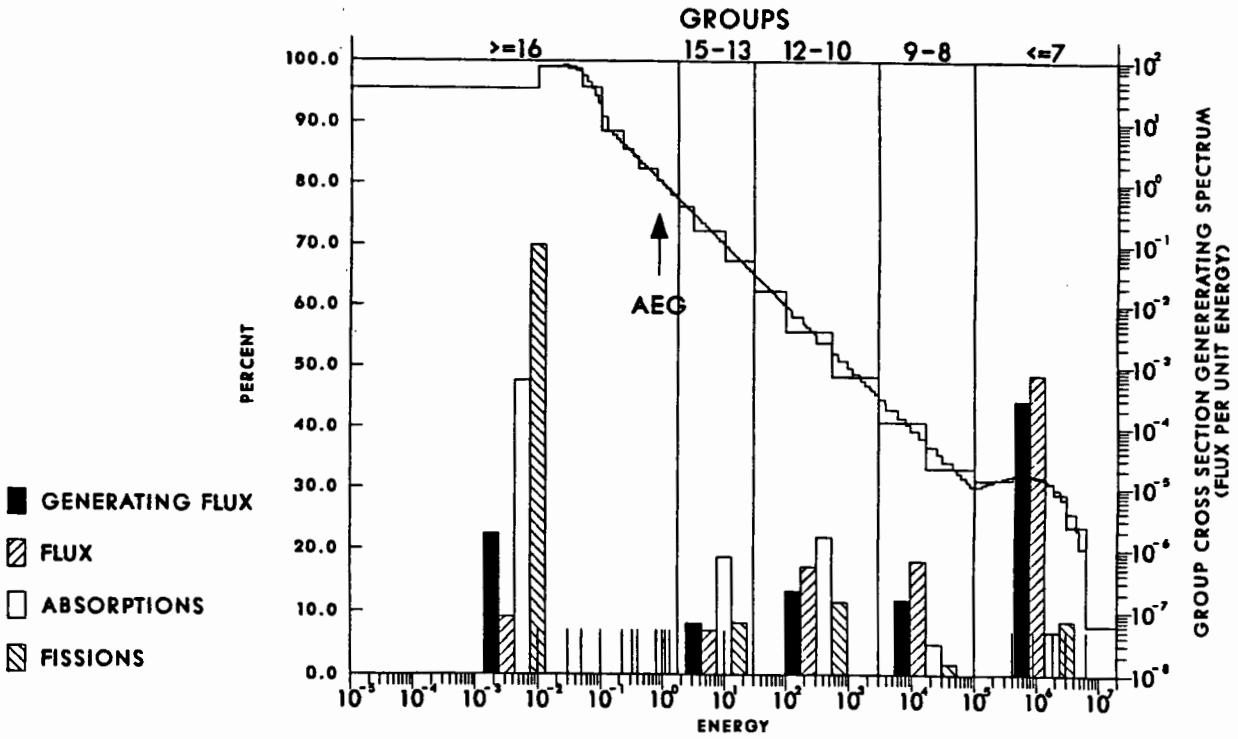

Fig. 34. UO_2F_2-H_2O 5.0% enriched H/X = 50.

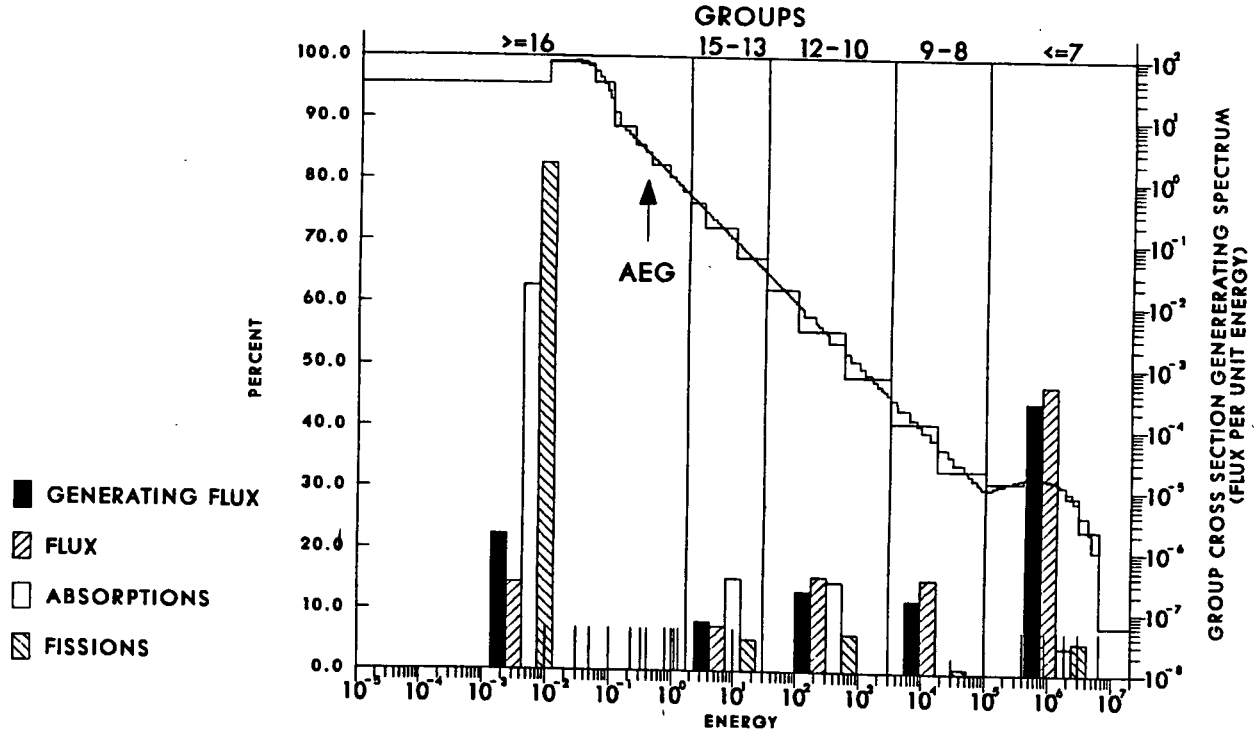

Fig. 35. UO_2F_2-H_2O 5.0% enriched H/X = 100.

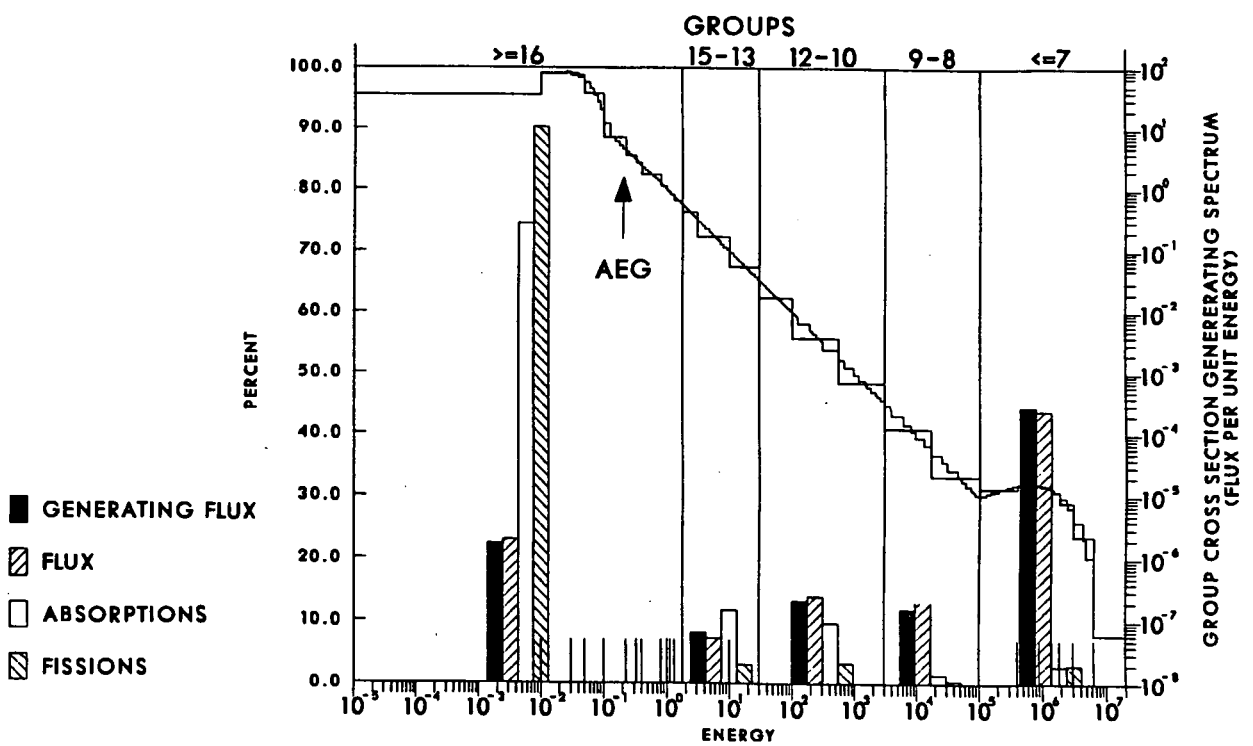

Fig. 36. UO_2F_2-H_2O 5.0% enriched H/X = 200.

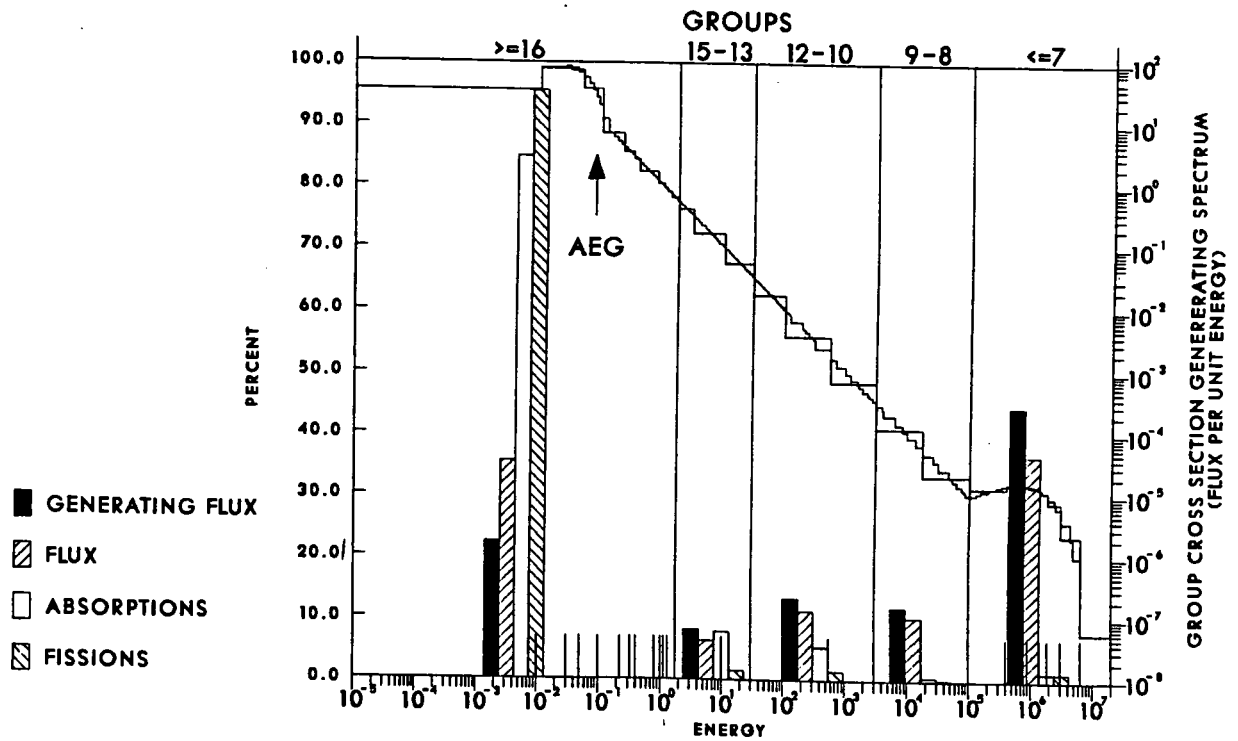

Fig. 37. UO_2F_2-H_2O 5.0% enriched H/X = 500.

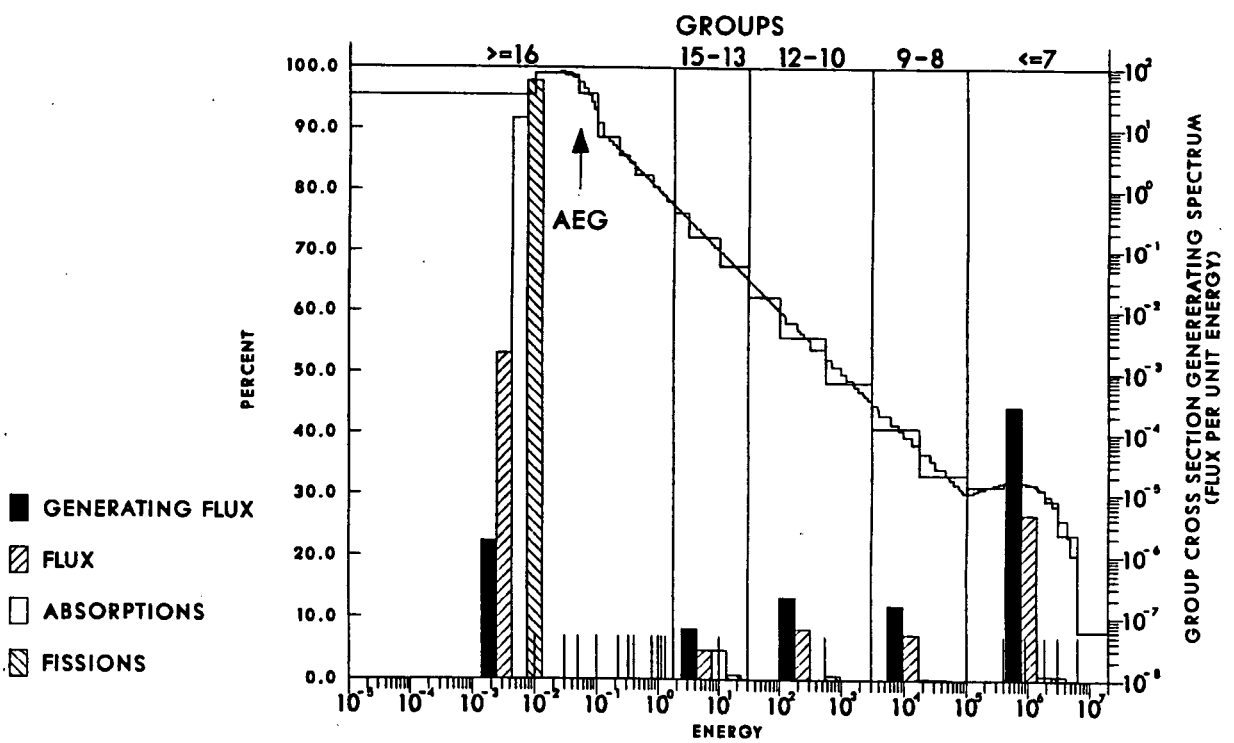

Fig. 38. UO_2F_2-H_2O 5.0% enriched H/X = 1500.

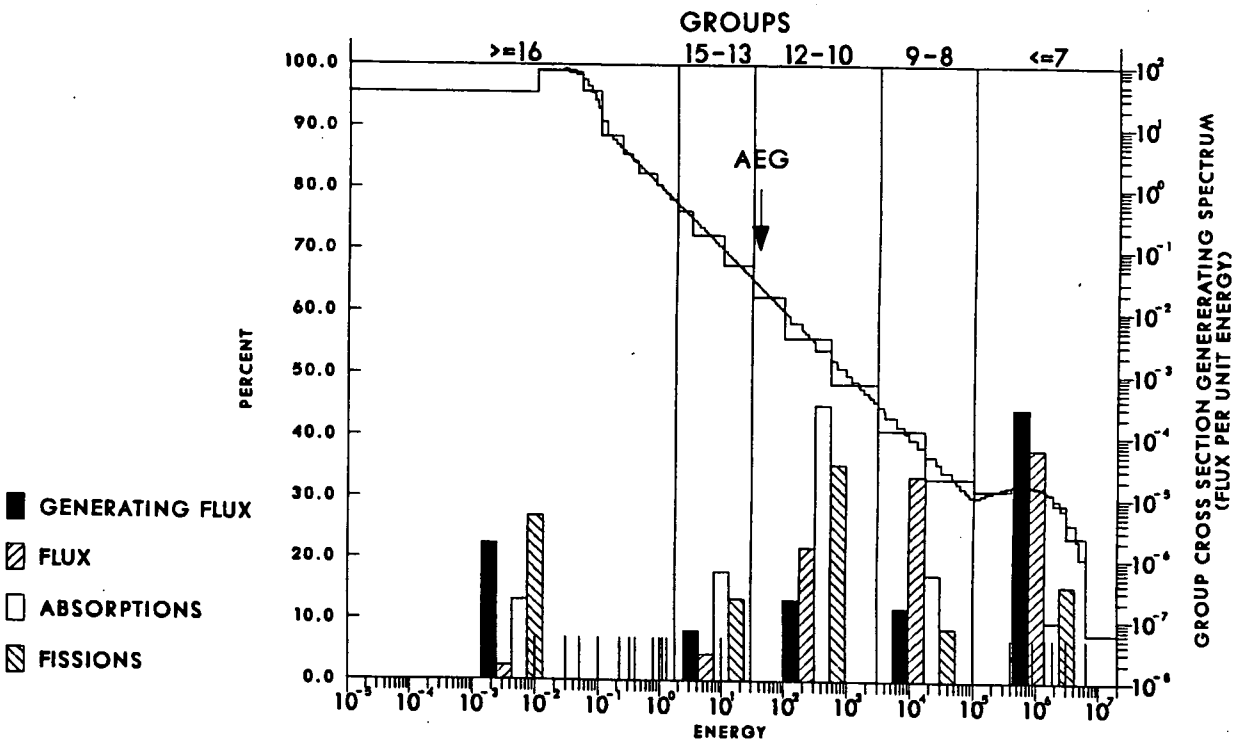

Fig. 39. UF_6-HF 5.0% enriched H/X = 10.

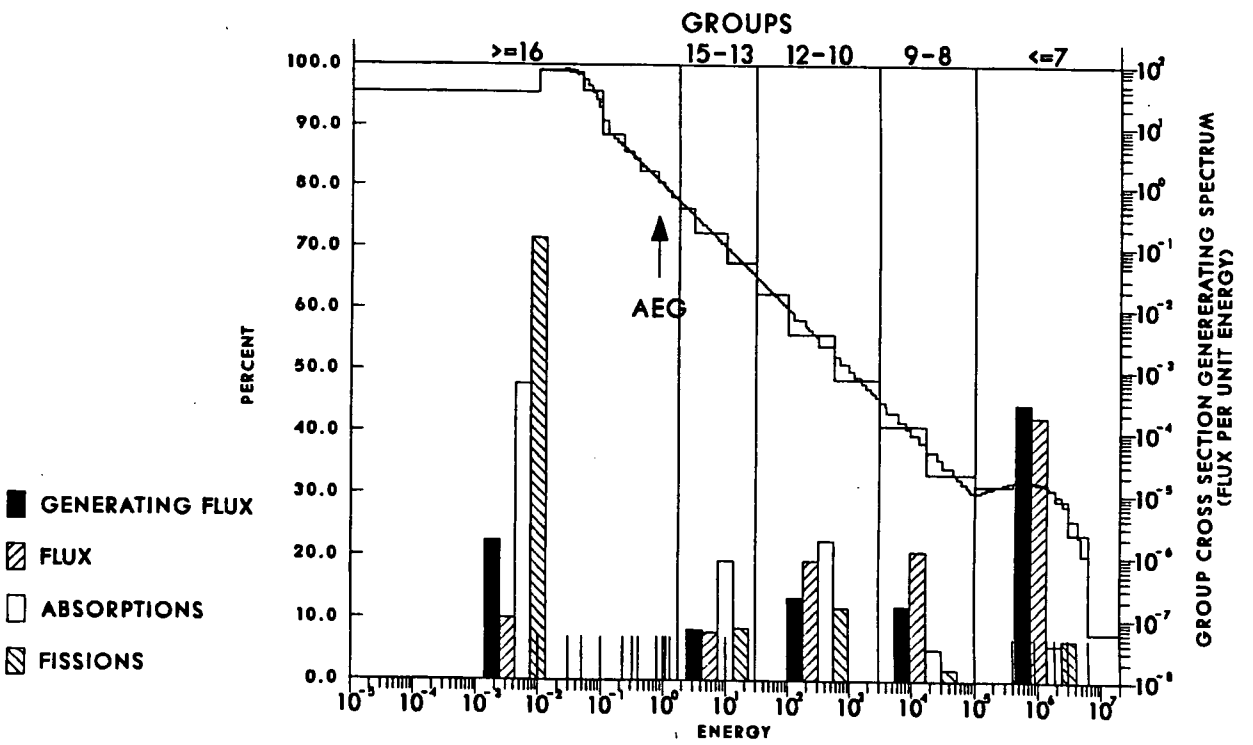

Fig. 40. UF_6-HF 5.0% enriched H/X = 50.

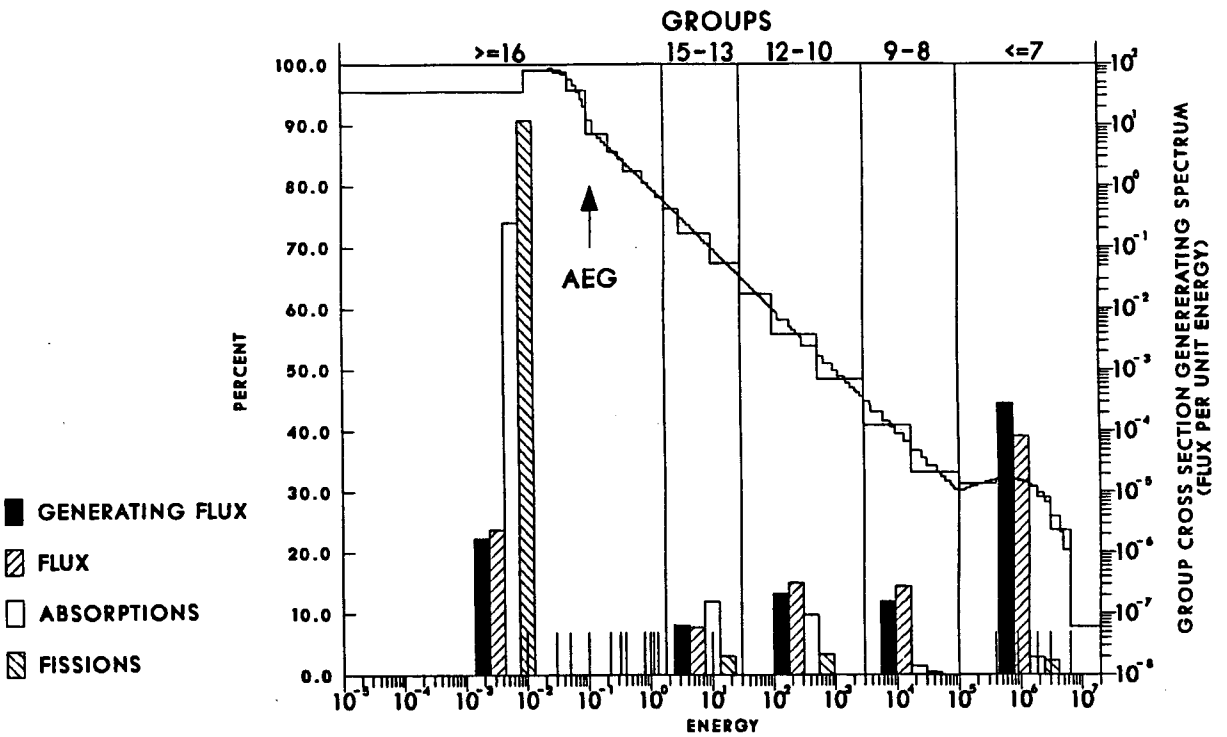

Fig. 41. UF_6-HF 5.0% enriched H/X = 200.

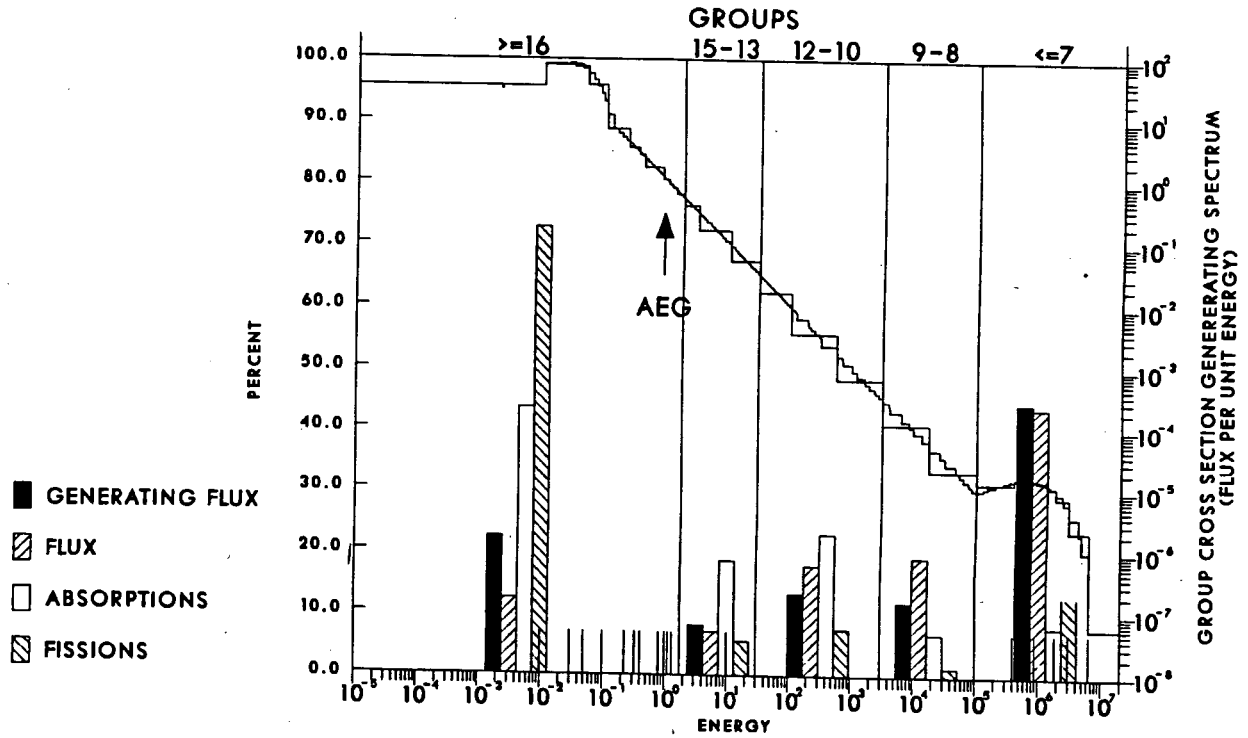

Fig. 42. UO_2F_2-H_2O 1.4% Enriched H/X = 100.

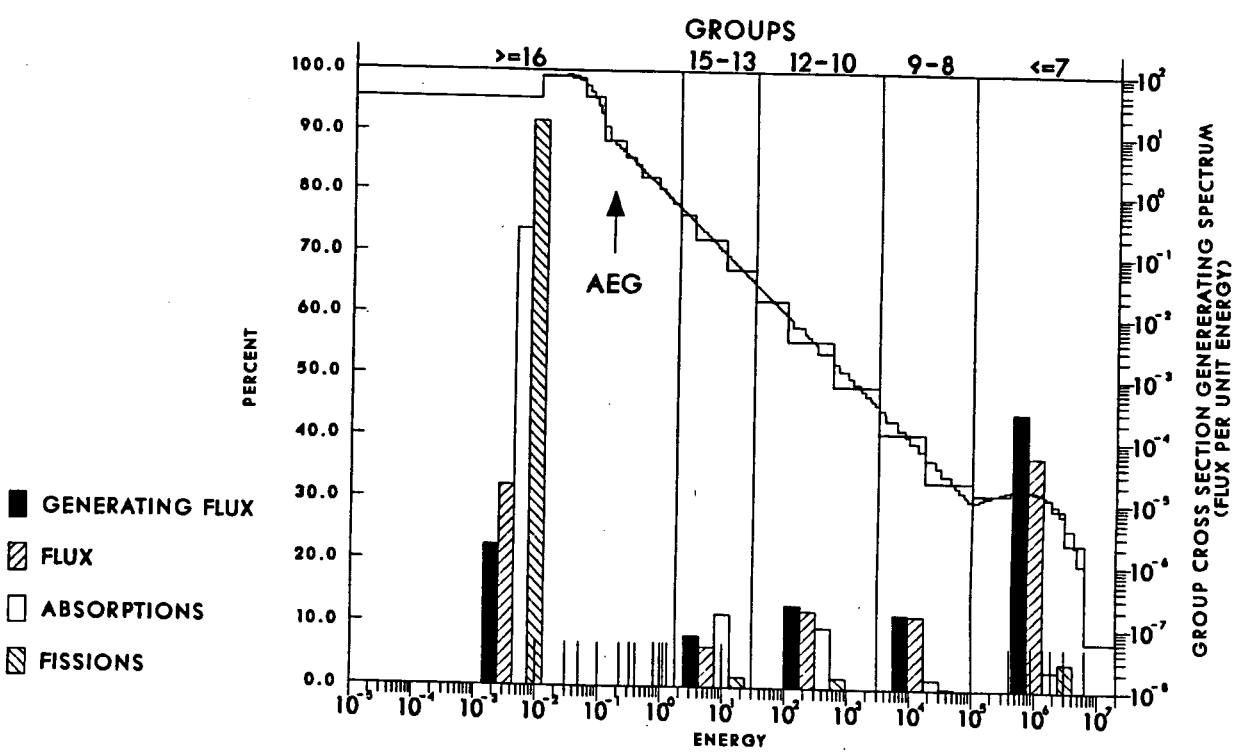

Fig. 43. UO_2F_2-H_2O 1.4% Enriched H/X = 500.

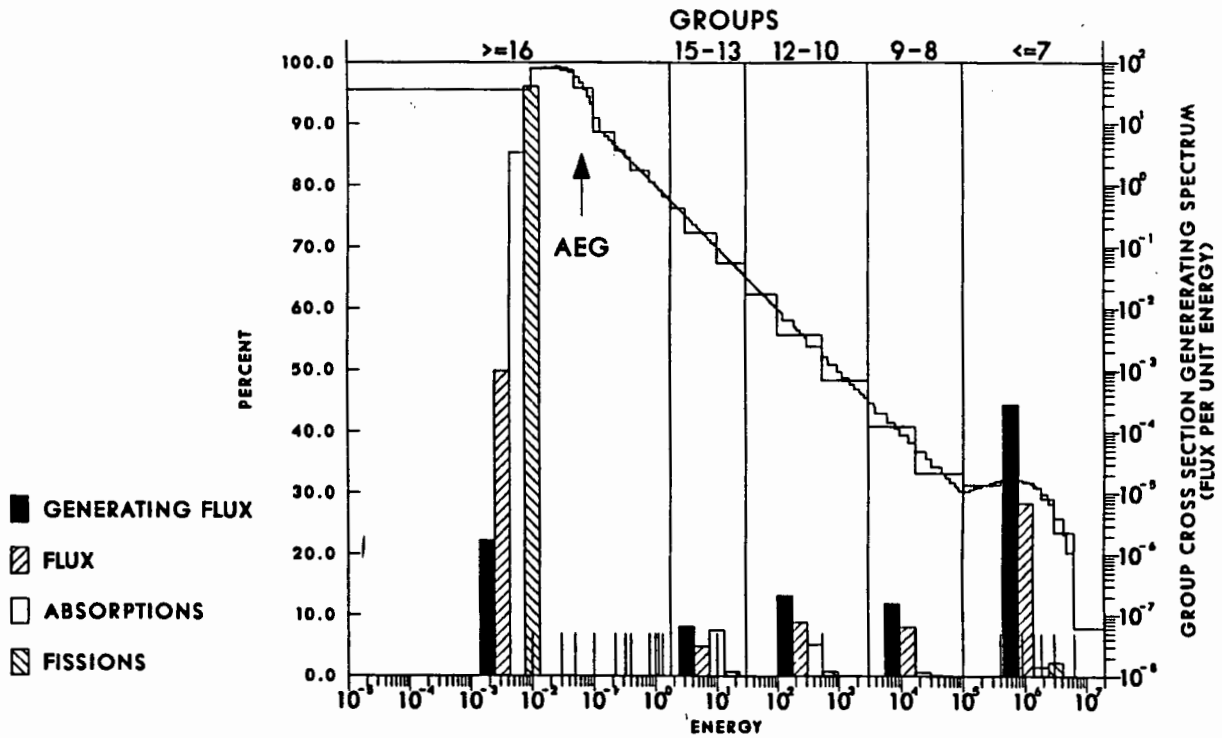

Fig. 44. UO_2F_2-H_2O 1.4% Enriched H/X = 1500.

Table 10. AEG for several calculated critical spheres

UO_2F_2-H_2O	Enrichment	H/X	KENO V.a Results $k_{eff} \pm \sigma$	AEG
	5	100	0.9927 ± 0.0041	21.99
	4	100	1.0054 ± 0.0047	21.77
	3	100	0.9867 ± 0.0038	21.34
	2	100	1.0018 ± 0.0031	20.59
		200	0.9904 ± 0.0035	22.34
	1.7	200	0.9960 ± 0.0030	22.18
	1.4	200	0.9949 ± 0.0030	22.83
UF_6-HF				
	5	100	1.0007 ± 0.0044	22.24
	4	100	0.9978 ± 0.0041	22.03
	3	100	0.9937 ± 0.0038	21.66
	2	200	0.9985 ± 0.0033	22.73
	1.7	200	0.9980 ± 0.0033	22.54
	1.4	200	0.9964 ± 0.0024	22.21

Information derived from analyses similar to these could be useful for selecting critical experiments that test specific cross-section regions. If a cross-section inadequacy is suspected in some energy range, experiments could be chosen that have characteristics that enhance the flux in that energy range and increase the sensitivity to the inadequacy.

Further study should be performed related to the use of the AEG in grouping different types of critical experiments. There is evidence that the AEG should not be used for comparison of latticed or driven systems to homogeneous systems. Grouping of reflected systems and unreflected systems and systems of differing geometries by use of the AEG should be evaluated. It may be that more detailed information on the flux distribution, fissions, absorptions, and leakage should be used rather than the AEG.

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APPENDIX A

DENSITY RELATIONSHIPS

The purpose of this appendix is to present relationships for uranium density as a function of H/U ratio for uranium compounds. Water and HF have been considered as the principal moderators. The density of homogeneous mixtures may be estimated based on the principle of additive molar volume. One form of this is given in Eq. (A.1), where the uranium density in a mixture is expressed as a function of the H/U:

$$\rho_u = \frac{M_u}{\frac{V_{uc}}{N} + \left(\frac{H}{U} - M * Y\right) * \frac{V_m}{M}}, \qquad \text{(A.1)}$$

where

ρ_u = uranium density,

M_u = molecular weight of uranium at a given enrichment,

V_{uc} = molar volume of the uranium compound (M_{uc}/ρ_{uc}),

N = number of uranium atoms in the uranium compound,

$\frac{V_{uc}}{N}$ = specific molar volume of uranium compound,

V_m = molar volume of the moderating compound (M_m/ρ_m),

M = number of hydrogen atoms in the moderating compound,

$\frac{V_m}{M}$ = specific molar volume of hydrogenous compound,

$\frac{H}{U}$ = the H/U moderating ratio,

Y = number of hydrated-moderating molecules in uranium compound (hydrated water for water-moderated systems, hydrated HF for HF moderated systems).

In Eq. (A.1) M is used for molecular weight, ρ is used for density, and V is used for molar volume ($V = M/\rho$). The subscripts u, uc, and m refer to uranium, uranium compound, and moderating compound, respectively. The form of Eq. (A.1) is general and requires a minimum of tabulated data to represent a large number of systems. The "specific molar volume" (V_{uc}/N and V_m/M) used in Eq. (A.1) is a contrived quantity which is defined as the molar volume (the molecular weight of a compound divided by its density) divided by the number of atoms of the nuclide of interest in the compound, the number of uranium atoms for the compound and the number of hydrogen atoms for the hydrogenous moderator. Eq. (A.1) could be simplified but, in doing so, the physical significance of the quantities which are involved is lost. As it stands, Eq. (A.1) is quite general and may be easily adapted for use on more complex mixtures and solutions.

The quantity defined as the specific molar volume has the interesting property that the ratio of the molecular weight of a compound divided by the theoretical density of that compound is nearly constant, independent of the isotopic distribution of the elements in the molecule. For example, the specific molar volume for the uranium compound is independent of the uranium enrichment in the compound. This is because the theoretical density of the uranium compound has the same variation with enrichment as the molecular weight of uranium. Table A.1 lists several uranium compounds and moderating materials. The molecular weight and theoretical densities are given along with the specific molar volumes. Variations of the theoretical density of the mixtures due to temperature may be taken into account by using the appropriate theoretical density of the compound in computing the specific molar volume. The values listed in Table A.1 are based on a temperature of 23°C. The density variation as a function of temperature is given in Table A.2 for several of the compounds.

The use of Eq. (A.1) with the specific molar volumes given in Table A.1 should yield maximum uranium densities for a given H/U and are therefore conservative. (Note that the molecular weights given in Table A.1 are not consistent with those in SCALE-4.0. The molecular weights in Table A.1 are those values that were used in the original testing of the density relationships. Revising the molecular weights to those in SCALE-4.0 would not significantly affect the specific molar volumes tabulated, but revisions were not done here to maintain traceability to my notes.)

Uranyl fluoride and uranyl nitrate form solutions when moderated by water. They also form water hydrates at low H/U ratios. This complicates the theoretical predictions of the uranium density. Because of these characteristics, the uranyl fluoride and uranyl nitrate systems have been treated in more detail.

E. J. Barber suggested that the relationship for uranyl fluoride be discontinuous at H/U = 4 in order to account for the various hydrates which exist. Only mixtures of hydrated salts exist at H/U < 4. Given this consideration, the density of uranyl fluoride may be estimated by Eqs. (A.2) and (A.3), where Eq. (A.3) is the specific form of Eq. (A.1).

Table A.1. Properties of uranium and moderating compounds

Compound	Molecular weight (M°)	Wt % U in compound	Density (g/cc) @23°C	Specific molar volume (V_{uc}/N) or (V_m/M)
U	238.029	100.00	19.05	12.4950
UO_2	270.028	88.15	10.96	24.6376
U_3O_8	842.082	84.80	8.30	33.8187
UF_6(solid)	352.019	67.62	5.075[a]	69.3633
UO_2F_2-$2H_2O$	344.057	69.18	4.76	72.2809
$UO_2(NO_3)_2 \cdot 6H_2O$	502.134	47.40	2.745[a]	182.927
H_2O	18.016	---	0.9977[a]	9.0287
HF(liquid)	20.0063	---	0.9516[a]	21.0239
HNO_3	63.0128	---	1.9447	32.4023

[a]The density is a function of temperature as given in Table 2.
The tabulated volume is at 23°C.

Table A.2. Temperature variation of several compounds

Compound	Density @ t °C (g/cc)	Notes
UF_6(solid)	5.194 - 0.005168*t	(1)
UF_6(liquid)	1.670 + 0.15203*(230.2-t)$^{1/2}$	(2)
$UO_2(NO_3)_2 \cdot 6H_2O$	2.745*[1 - (t - 23.)*0.0015]	(3)
H_2O	0.99987/(1. - 6.427-5*t + 8.5053-6*t^2 - 6.79-8*t^3)	(4)
HF(liquid)	1.0020 - 0.0022625*t + 3.125-6*t^2	(5)
HF(solid)	1.562 - 0.000979*t	(5)
HNO_3	1.95 - (t - 20.)*0.00176	(3)

[a]Sources of data:

(1) E. J. Barber, *Estimation of Pressures Developed by Retrained Solid UF_6*, K/ET-307 (1979).

(2) E. J. Barber, *Relationship of Pressure to Temperature Rise in Overfilled Cylinders*," K/ET-194 (1979).

(3) Fit to measured data by W. C. Jordan, ORNL, 1988.

(4) Fit to specific volume data for water 15 < t < 30°C.

(5) I. G. Ryss, *Chemistry of Fluorine and Its Inorganic Compounds*, AEC-tr-3927 Part 1, Chapter 3 - Hydrogen Flouride. Data for solid - p. 65 (LeBoucher, Fischer, Biltz). Data for liquid - p. 66 (Simons and Bouknight).

URANYL FLUORIDE

H/U < 4

$$\rho_u = 4.96 - 0.32 * \left(\frac{H}{U}\right) . \tag{A.2}$$

H/U ≥ 4

$$\rho_u = \frac{M_u}{V_{UO_2F_2 \cdot 2H_2O} + \left(\frac{H}{U} - 4\right) * \frac{V_{H_2O}}{2}} . \tag{A.3}$$

URANYL NITRATE

$$\rho_u = \frac{M_u * \left[1 + \frac{M^+}{1000} * \left(V_{H_2O} - V_{HNO_3}\right)\right]}{V_{UNH} + \left(\frac{H}{U} - 12\right) * \frac{V_{H_2O}}{2}} . \tag{A.4}$$

It was found that, for uranyl nitrate, the use of theoretical densities in Eq. (A.1) did not yield accurate uranium densities over the full range of H/U. In addition, the inclusion of the excess acid into Eq. (A.1) and the use of theoretical densities for the excess acid gave unreasonable density effects. The molar volume of uranyl nitrate hexahydrate and nitric acid given in Table A.1 were adjusted for a best fit to data on uranyl nitrate solutions with excess acid using Eq. (A.4). Equation (A.4) is the specific form of Eq. (A.1) for uranyl nitrate, including the excess acid. Equation (A.4) is similar to that in ARH-600, but is believed to be a better estimate for the nitric acid system.

Mixtures of various hydrate forms must be assumed for H/U ratios less than 12 in uranyl nitrate systems. Only limited information was found for these systems. It is believed that the formulations in Eq. (A.4) may significantly overpredict uranium densities at H/U < 12.

Table A.3 gives the theoretical density for UO_2F_2-H_2O mixtures as predicted by Eqs. (A.2) and (A.3). Table A.4 gives the theoretical density for UF_6-HF mixtures as predicted by Eq. (A.1). Tables A.3 and A.4 were used in the calculations presented in Sect. 2. Tables A.3 and A.4 list the physical properties of UO_2F_2-H_2O and UF_6-HF mixtures predicted at 20°C. The uranium density, uranium compound density, and moderator densities are tabulated for the specified H/X (and corresponding H/U) moderation ratios. Uranium enrichments of 5, 4, 3, 2, 1.7, and 1.4% ^{235}U were considered.

Table A.3. Physical properties of UO_2F_2–H_2O mixtures

		UO_2F_2–H_20		
H/X	H/U	U den.	UO_2F_2 den.	H_2O den.
5.0E+00 % Enriched				
5.000E+00	2.532E-01	4.8790E+00	6.3143E+00	4.6776E-02
1.000E+01	5.064E-01	4.7980E+00	6.2095E+00	9.1999E-02
2.000E+01	1.013E+00	4.6359E+00	5.9997E+00	1.7778E-01
5.000E+01	2.532E+00	4.1498E+00	5.3706E+00	3.9785E-01
1.000E+02	5.064E+00	2.9054E+00	3.7601E+00	5.5710E-01
2.000E+02	1.013E+01	1.8648E+00	2.4134E+00	7.1513E-01
3.000E+02	1.519E+01	1.3730E+00	1.7769E+00	7.8980E-01
5.000E+02	2.532E+01	8.9889E-01	1.1633E+00	8.6180E-01
7.000E+02	3.545E+01	6.6817E-01	8.6474E-01	8.9683E-01
1.000E+03	5.064E+01	4.8243E-01	6.2436E-01	9.2504E-01
1.500E+03	7.596E+01	3.2968E-01	4.2667E-01	9.4824E-01
2.000E+03	1.013E+02	2.5040E-01	3.2407E-01	9.6027E-01
4.0E+00 % Enriched				
5.000E+00	2.026E-01	4.8952E+00	6.3351E+00	3.7540E-02
1.000E+01	4.051E-01	4.8304E+00	6.2512E+00	7.4087E-02
2.000E+01	8.102E-01	4.7007E+00	6.0834E+00	1.4420E-01
5.000E+01	2.026E+00	4.3118E+00	5.5801E+00	3.3067E-01
1.000E+02	4.051E+00	3.2708E+00	4.2330E+00	5.0167E-01
2.000E+02	8.102E+00	2.1769E+00	2.8172E+00	6.6777E-01
3.000E+02	1.215E+01	1.6313E+00	2.1111E+00	7.5061E-01
5.000E+02	2.026E+01	1.0866E+00	1.4062E+00	8.3331E-01
7.000E+02	2.836E+01	8.1462E-01	1.0542E+00	8.7461E-01
1.000E+03	4.051E+01	5.9225E-01	7.6646E-01	9.0838E-01
1.500E+03	6.077E+01	4.0705E-01	5.2679E-01	9.3649E-01
2.000E+03	8.102E+01	3.1009E-01	4.0130E-01	9.5122E-01
3.0E+00 % Enriched				
5.000E+00	1.519E-01	4.9114E+00	6.3559E+00	2.8245E-02
1.000E+01	3.038E-01	4.8628E+00	6.2930E+00	5.5931E-02
2.000E+01	6.077E-01	4.7655E+00	6.1672E+00	1.0962E-01
5.000E+01	1.519E+00	4.4739E+00	5.7897E+00	2.5729E-01
1.000E+02	3.038E+00	3.9877E+00	5.1606E+00	4.5866E-01
2.000E+02	6.077E+00	2.6144E+00	3.3833E+00	6.0140E-01
3.000E+02	9.115E+00	2.0092E+00	2.6001E+00	6.9328E-01
5.000E+02	1.519E+01	1.3734E+00	1.7773E+00	7.8980E-01
7.000E+02	2.127E+01	1.0432E+00	1.3500E+00	8.3992E-01
1.000E+03	3.038E+01	7.6674E-01	9.9225E-01	8.8190E-01
1.500E+03	4.558E+01	5.3183E-01	6.8825E-01	9.1756E-01
2.000E+03	6.077E+01	4.0711E-01	5.2684E-01	9.3649E-01

Table A.3 (continued)

UO_2F_2-H_2O				
H/X	H/U	U den.	UO_2F_2 den.	H_2O den.
2.0E+00 % Enriched				
5.000E+00	1.013E-01	4.9276E+00	6.3767E+00	1.8890E-02
1.000E+01	2.026E-01	4.8952E+00	6.3347E+00	3.7531E-02
2.000E+01	4.051E-01	4.8304E+00	6.2509E+00	7.4068E-02
5.000E+01	1.013E+00	4.6359E+00	5.9992E+00	1.7772E-01
1.000E+02	2.026E+00	4.3118E+00	5.5798E+00	3.3058E-01
2.000E+02	4.051E+00	3.2717E+00	4.2338E+00	5.0167E-01
3.000E+02	6.077E+00	2.6147E+00	3.3836E+00	6.0140E-01
5.000E+02	1.013E+01	1.8655E+00	2.4141E+00	7.1513E-01
7.000E+02	1.418E+01	1.4500E+00	1.8764E+00	7.7819E-01
1.000E+03	2.026E+01	1.0869E+00	1.4065E+00	8.3331E-01
1.500E+03	3.038E+01	7.6684E-01	9.9235E-01	8.8190E-01
2.000E+03	4.051E+01	5.9240E-01	7.6661E-01	9.0838E-01
1.7E+00 % Enriched				
5.000E+00	8.609E-02	4.9325E+00	6.3829E+00	1.6071E-02
1.000E+01	1.722E-01	4.9049E+00	6.3473E+00	3.1963E-02
2.000E+01	3.443E-01	4.8498E+00	6.2760E+00	6.3209E-02
5.000E+01	8.609E-01	4.6845E+00	6.0621E+00	1.5264E-01
1.000E+02	1.722E+00	4.4090E+00	5.7056E+00	2.8732E-01
2.000E+02	3.443E+00	3.8581E+00	4.9926E+00	5.0283E-01
3.000E+02	5.165E+00	2.8746E+00	3.7199E+00	5.6197E-01
5.000E+02	8.609E+00	2.0901E+00	2.7048E+00	6.8103E-01
7.000E+02	1.205E+01	1.6421E+00	2.1249E+00	7.4905E-01
1.000E+03	1.722E+01	1.2425E+00	1.6079E+00	8.0970E-01
1.500E+03	2.583E+01	8.8401E-01	1.1440E+00	8.6411E-01
2.000E+03	3.443E+01	6.8606E-01	8.8781E-01	8.9416E-01
1.4E+00 % Enriched				
5.000E+00	7.090E-02	4.9373E+00	6.3891E+00	1.3248E-02
1.000E+01	1.418E-01	4.9146E+00	6.3598E+00	2.6374E-02
2.000E+01	2.836E-01	4.8693E+00	6.3011E+00	5.2261E-02
5.000E+01	7.090E-01	4.7331E+00	6.1249E+00	1.2700E-01
1.000E+02	1.418E+00	4.5063E+00	5.8314E+00	2.4183E-01
2.000E+02	2.836E+00	4.0525E+00	5.2442E+00	4.3495E-01
3.000E+02	4.254E+00	3.1917E+00	4.1303E+00	5.1384E-01
5.000E+02	7.090E+00	2.3763E+00	3.0751E+00	6.3761E-01
7.000E+02	9.925E+00	1.8927E+00	2.4493E+00	7.1101E-01
1.000E+03	1.418E+01	1.4501E+00	1.8765E+00	7.7819E-01
1.500E+03	2.127E+01	1.0434E+00	1.3503E+00	8.3992E-01
2.000E+03	2.836E+01	8.1489E-01	1.0545E+00	8.7461E-01

Table A.4. Physical properties of UF_6-HF systems

		UF_6-HF		
H/X	H/U	U den.	UF_6 den.	HF den.
5.0E+00 % Enriched				
5.000E+00	2.532E-01	3.1959E+00	4.7273E+00	6.8051E-02
1.000E+01	5.064E-01	2.9840E+00	4.4138E+00	1.2707E-01
2.000E+01	1.013E+00	2.6345E+00	3.8969E+00	2.2439E-01
5.000E+01	2.532E+00	1.9496E+00	2.8837E+00	4.1512E-01
1.000E+02	5.064E+00	1.3602E+00	2.0119E+00	5.7924E-01
2.000E+02	1.013E+01	8.4765E-01	1.2538E+00	7.2196E-01
3.000E+02	1.519E+01	6.1567E-01	9.1067E-01	7.8656E-01
5.000E+02	2.532E+01	3.9788E-01	5.8853E-01	8.4720E-01
7.000E+02	3.545E+01	2.9391E-01	4.3474E-01	8.7616E-01
1.000E+03	5.064E+01	2.1115E-01	3.1232E-01	8.9920E-01
1.500E+03	7.596E+01	1.4371E-01	2.1257E-01	9.1798E-01
2.000E+03	1.013E+02	1.0892E-01	1.6111E-01	9.2767E-01
4.0E+00 % Enriched				
5.000E+00	2.026E-01	3.2424E+00	4.7958E+00	5.5225E-02
1.000E+01	4.051E-01	3.0657E+00	4.5344E+00	1.0443E-01
2.000E+01	8.102E-01	2.7643E+00	4.0887E+00	1.8833E-01
5.000E+01	2.026E+00	2.1348E+00	3.1576E+00	3.6361E-01
1.000E+02	4.051E+00	1.5475E+00	2.2889E+00	5.2714E-01
2.000E+02	8.102E+00	9.9822E-01	1.4765E+00	6.8007E-01
3.000E+02	1.215E+01	7.3672E-01	1.0897E+00	7.5288E-01
5.000E+02	2.026E+01	4.8344E-01	7.1505E-01	8.2340E-01
7.000E+02	2.836E+01	3.5975E-01	5.3211E-01	8.5783E-01
1.000E+03	4.051E+01	2.5998E-01	3.8454E-01	8.8561E-01
1.500E+03	6.077E+01	1.7780E-01	2.6298E-01	9.0850E-01
2.000E+03	8.102E+01	1.3510E-01	1.9982E-01	9.2039E-01
3.0E+00 % Enriched				
5.000E+00	1.519E-01	3.2902E+00	4.8664E+00	4.2025E-02
1.000E+01	3.038E-01	3.1520E+00	4.6619E+00	8.0517E-02
2.000E+01	6.077E-01	2.9076E+00	4.3004E+00	1.4855E-01
5.000E+01	1.519E+00	2.3589E+00	3.4889E+00	3.0129E-01
1.000E+02	3.038E+00	1.7945E+00	2.6542E+00	4.5841E-01
2.000E+02	6.077E+00	1.2137E+00	1.7952E+00	6.2010E-01
3.000E+02	9.115E+00	9.1697E-01	1.3562E+00	7.0272E-01
5.000E+02	1.519E+01	6.1582E-01	9.1082E-01	7.8656E-01
7.000E+02	2.127E+01	4.6358E-01	6.8565E-01	8.2894E-01
1.000E+03	3.038E+01	3.3817E-01	5.0017E-01	8.6386E-01
1.500E+03	4.558E+01	2.3308E-01	3.4474E-01	8.9311E-01
2.000E+03	6.077E+01	1.7782E-01	2.6301E-01	9.0850E-01

Table A.4 (continued)

		UF_6-HF		
H/X	H/U	U den.	UF_6 den.	HF den.
2.0E+00 % Enriched				
5.000E+00	1.013E-01	3.3395E+00	4.9390E+00	2.8432E-02
1.000E+01	2.026E-01	3.2432E+00	4.7967E+00	5.5225E-02
2.000E+01	4.051E-01	3.0665E+00	4.5352E+00	1.0443E-01
5.000E+01	1.013E+00	2.6355E+00	3.8979E+00	2.2439E-01
1.000E+02	2.026E+00	2.1354E+00	3.1582E+00	3.6361E-01
2.000E+02	4.051E+00	1.5479E+00	2.2893E+00	5.2714E-01
3.000E+02	6.077E+00	1.2139E+00	1.7953E+00	6.2010E-01
5.000E+02	1.013E+01	8.4798E-01	1.2541E+00	7.2196E-01
7.000E+02	1.418E+01	6.5157E-01	9.6365E-01	7.7663E-01
1.000E+03	2.026E+01	4.8356E-01	7.1517E-01	8.2340E-01
1.500E+03	3.038E+01	3.3821E-01	5.0021E-01	8.6386E-01
2.000E+03	4.051E+01	2.6005E-01	3.8461E-01	8.8561E-01
1.7E+00 % Enriched				
5.000E+00	8.609E-02	3.3546E+00	4.9612E+00	2.4275E-02
1.000E+01	1.722E-01	3.2717E+00	4.8386E+00	4.7351E-02
2.000E+01	3.443E-01	3.1176E+00	4.6107E+00	9.0241E-02
5.000E+01	8.609E-01	2.7316E+00	4.0399E+00	1.9767E-01
1.000E+02	1.722E+00	2.2644E+00	3.3489E+00	3.2772E-01
2.000E+02	3.443E+00	1.6872E+00	2.4953E+00	4.8838E-01
3.000E+02	5.165E+00	1.3445E+00	1.9884E+00	5.8377E-01
5.000E+02	8.609E+00	9.5609E-01	1.4140E+00	6.9188E-01
7.000E+02	1.205E+01	7.4180E-01	1.0971E+00	7.5152E-01
1.000E+03	1.722E+01	5.5515E-01	8.2104E-01	8.0348E-01
1.500E+03	2.583E+01	3.9113E-01	5.7846E-01	8.4913E-01
2.000E+03	3.443E+01	3.0193E-01	4.4653E-01	8.7396E-01
1.4E+00 % Enriched				
5.000E+00	7.090E-02	3.3698E+00	4.9836E+00	2.0081E-02
1.000E+01	1.418E-01	3.3006E+00	4.8813E+00	3.9338E-02
2.000E+01	2.836E-01	3.1704E+00	4.6888E+00	7.5573E-02
5.000E+01	7.090E-01	2.8349E+00	4.1927E+00	1.6894E-01
1.000E+02	1.418E+00	2.4099E+00	3.5641E+00	2.8723E-01
2.000E+02	2.836E+00	1.8541E+00	2.7420E+00	4.4195E-01
3.000E+02	4.254E+00	1.5065E+00	2.2281E+00	5.3868E-01
5.000E+02	7.090E+00	1.0958E+00	1.6206E+00	6.5301E-01
7.000E+02	9.925E+00	8.6102E-01	1.2734E+00	7.1835E-01
1.000E+03	1.418E+01	6.5162E-01	9.6370E-01	7.7663E-01
1.500E+03	2.127E+01	4.6367E-01	6.8574E-01	8.2894E-01
2.000E+03	2.836E+01	3.5987E-01	5.3223E-01	8.5783E-01

APPENDIX B

TABLES OF CALCULATED VALUES FOR SECTION 2

Tables B.1 and B.2 give the calculated infinite media multiplication values predicted using SCALE-4 and the SCALE 27-group ENDF/B-IV cross-section library for each system listed in Tables A.3 and A.4. The CSAS1X control sequence prepares input data and executes BONAMI, NITAWL, and XSDRNPM.

Tables B.3 and B.4 list critical parameters at each enrichment and several H/X moderation ratios predicted using XSDRNPM and the 27-group ENDF/B-IV cross-section library in SCALE-4.

Table B.1. k_∞ for UO_2F_2–H_2O systems using the SCALE 27-group library

	% Enrichment					
H/X	5.0	4.0	3.0	2.0	1.7	1.4
5.000E+00	8.81333-1	7.93512-1	6.87041-1	5.55748-1	5.10421-1	4.62036-1
1.000E+01	9.63163-1	8.73875-1	7.60571-1	6.13581-1	5.60951-1	5.03967-1
2.000E+01	1.08401	9.96199-1	8.79551-1	7.16552-1	6.54776-1	5.85342-1
5.000E+01	1.27189	1.19358	1.08394	9.16725-1	8.47631-1	7.65433-1
1.000E+02	1.38902	1.32164	1.22466	1.07018	1.00338	9.20974-1
2.000E+02	1.44607	1.39075	1.30964	1.17623	1.11675	1.04172
3.000E+02	1.44016	1.39206	1.32102	1.20227	1.14849	1.07998
5.000E+02	1.38267	1.34382	1.28586	1.18737	1.14215	1.08382
7.000E+02	1.31182	1.27903	1.22992	1.14571	1.10666	1.05588
1.000E+03	1.20866	1.18222	1.14238	1.07355	1.04134	9.99196-1
1.500E+03	1.06147	1.04178	1.01201	9.60152-1	9.35683-1	9.03401-1
2.000E+03	9.43632-1	9.28235-1	9.04946-1	8.64176-1	8.44828-1	8.19175-1

Table B.2. k_∞ for UF_6–HF systems using the SCALE 27-group library

	% Enrichment					
H/X	5.0	4.0	3.0	2.0	1.7	1.4
5.000E+00	8.19499-1	7.32459-1	6.27232-1	4.98597-1	4.54192-1	4.06768-1
1.000E+01	9.05968-1	8.15744-1	7.02198-1	5.56021-1	5.04333-1	4.48155-1
2.000E+01	1.03490	9.44869-1	8.25771-1	6.60869-1	5.99098-1	5.29825-1
5.000E+01	1.23487	1.15383	1.04069	8.68930-1	7.98222-1	7.14412-1
1.000E+02	1.35879	1.28932	1.18946	1.03050	9.61796-1	8.77323-1
2.000E+02	1.41973	1.36315	1.28013	1.14342	1.08243	1.00551
3.000E+02	1.41511	1.36606	1.29357	1.17236	1.11749	1.04753
5.000E+02	1.35838	1.31893	1.26010	1.16015	1.11419	1.05488
7.000E+02	1.28783	1.25467	1.20497	1.11975	1.08021	1.02881
1.000E+03	1.18510	1.15841	1.11825	1.04883	1.01633	9.73798-1
1.500E+03	1.03887	1.01903	9.89123-1	9.37008-1	9.12395-1	8.79951-1
2.000E+03	9.22151-1	9.06687-1	8.83307-1	8.42411-1	8.22988-1	7.97281-1

Table B.3. Critical parameters for UO_2F_2–H_2O using the SCALE 27-group library

Enrichment	H/X	Critical radius (cm)	Critical volume (l)	Critical mass (kg U)	H_2O kg
5.0	100	22.078	45.078	130.970	25.113
	200	19.621	31.641	59.004	22.627
	300	19.705	32.049	44.003	25.312
	500	21.423	41.184	37.020	35.492
	700	24.384	60.730	40.578	54.464
4.0	100	25.478	69.276	226.588	34.754
	200	21.696	42.779	93.126	28.567
	300	21.384	40.960	66.818	30.745
	500	23.020	51.098	55.523	42.580
	700	26.233	75.619	61.601	66.137
3.0	100	30.860	123.105	490.906	56.463
	200	25.709	71.178	186.088	42.806
	300	24.660	62.816	126.210	43.549
	500	26.125	74.689	102.578	58.989
	700	29.608	108.722	113.419	91.318
2.0	100	68.944	1372.708	5918.842	453.790
	200	37.622	223.056	729.772	111.901
	300	33.551	158.199	413.643	95.141
	500	34.222	167.882	313.184	120.057
	700	39.136	251.083	364.070	195.390
1.7	200	44.494	368.972	1423.531	185.530
	300	40.725	282.925	813.296	158.995
	500	40.492	278.097	581.251	189.392
	700	47.253	441.954	725.733	331.046
1.4	200	83.483	2437.153	9876.563	1060.040
	300	59.670	889.932	2840.396	457.283
	500	55.461	714.581	1698.059	455.624
	700	68.124	1324.308	2506.518	941.569

Table B.4. Critical parameters for UF_6–HF using the SCALE 27-group library

Enrichment	H/X	Critical radius (cm)	Critical volume (l)	Critical mass (kg U)	HF kg
5.0	-100	39.110	250.583	340.843	145.148
	200	35.663	189.995	161.049	137.169
	300	36.331	200.873	123.476	157.749
	500	40.611	280.556	111.628	237.687
	700	47.171	439.657	129.220	385.210
4.0	100	45.456	393.425	608.825	207.390
	200	39.366	255.536	255.081	173.782
	300	39.538	258.900	190.737	194.921
	500	43.763	351.083	169.728	289.082
	700	50.552	541.133	194.673	464.200
3.0	100	59.984	904.055	1622.327	414.428
	200	46.900	432.123	524.468	267.959
	300	45.667	398.929	365.806	280.335
	500	49.565	510.051	314.100	401.186
	700	57.337	789.575	366.031	654.510
2.0	200	71.473	1529.377	2367.323	806.196
	300	63.723	1083.870	1315.710	672.108
	500	66.185	1214.416	1029.800	876.760
	700	78.155	1999.673	1302.927	1553.006
1.7	200	98.741	4032.563	6803.740	1969.423
	300	79.674	2118.549	2848.348	1236.745
	500	80.837	2212.683	2115.524	1530.911
	700	98.213	3968.218	2943.624	2982.195
1.4	200	575.878	799981.737	1483246.139	353551.929
	300	133.151	9888.306	14896.733	5326.633
	500	123.624	7914.017	8672.180	5167.932
	700	183.862	26035.418	22417.016	18702.543

APPENDIX C

RESULTS OF THE 1983 MINIMUM MODERATOR MASS STUDY

This appendix contains tables of results from the 1983 minimum-mass study. These values were calculated using the ANISN computer code and the Knight-modified Hansen-Roach cross sections as distributed with KENO-IV.

Tables C.1 and C.2 give calculated infinite media multiplication factors. Tables C.3 and C.4 give calculated critical parameters.

Table C.1. k_∞ for UO_2F_2–H_2O systems using the Knight-modified Hansen-Roach cross sections

H/X	5.0%	3.0%	2.0%	1.7%	1.4%
5	0.9596	0.75144	---	---	---
10	1.01418	0.81097	---	---	---
20	1.13762	0.93385	0.76892	0.70014	---
50	1.31498	1.13937	0.96895	0.90647	0.82472
100	1.41953	1.26473	1.12249	1.05437	0.98281
200	1.45713	1.33779	1.20778	1.16135	1.08281
300	1.44752	1.33372	1.22991	1.17967	1.11475
500	1.39738	1.29507	1.20037	1.16200	1.11031
700	1.33602	1.23862	1.15981	1.11883	1.07671
1000	1.23932	1.15913	1.08045	1.06095	1.01371
1500	1.08818	1.03825	0.97231	0.95344	0.91448
2000	0.974296	0.92476	---	---	---

Table C.2. k_∞ UF_6–HF systems using the Knight-modified Hansen-Roach cross sections

H/X	5.0%	3.0%	2.0%	1.7%	1.4%
5	0.93340	0.70650	---	---	---
10	0.97734	0.77054	---	---	---
20	1.05741	0.89957	0.73193	0.66329	---
50	1.27002	1.09127	0.91130	0.86840	0.77178
100	1.38137	1.24161	1.07914	1.00864	0.93487
200	1.43047	1.30376	1.17781	1.13043	1.04833
300	1.42941	1.30419	1.19639	1.14176	1.08529
500	1.36910	1.27605	1.17318	1.13194	1.07863
700	1.30585	1.21392	1.13145	1.08849	1.04848
1000	1.21809	1.13357	1.06076	1.02241	0.98644
1500	1.06701	1.01770	0.95743	0.92775	0.89154
2000	0.95356	---	---	---	---

Table C.3. Critical parameters for UO_2F_2-H_2O using the Knight-modified Hansen-Roach cross sections

% Enrichment	H/X	Critical radius (cm)	Critical volume (l)	Critical mass (kgU)	Moderator mass (kg H_2O)
5.0	100	21.1	39.35	118.8	22.8
	200	19.3	30.11	58.1	22.3
	300	20.4	35.56	48.0	27.6
	500	21.8	43.40	38.6	37.0
	700	24.2	59.37	39.3	52.9
3.0	100	31.8351	135.147	494.463	56.849
	200	24.1569	59.049	162.231	37.303
	300	23.8979	57.170	119.891	41.351
	500	26.8948	81.488	109.8865	63.169
2.0	100	56.8322	768.904	3100.06	237.598
	200	35.2383	183.287	608.845	93.330
	300	30.9211	123.8379	340.2074	78.226
	500	33.0577	151.324	291.691	111.786
1.7	200	42.6778	325.608	1146.009	149.321
	300	36.7800	208.413	623.195	121.802
	500	37.4104	219.314	480.231	156.433
	700	45.7854	402.040	667.508	304.410
1.4	200	66.3662	1224.417	4567.199	490.07
	300	49.9523	522.1017	1701.268	273.827
	500	47.3765	445.428	1115.530	299.250
	700	58.1412	823.2668	1613.3559	553.092

Table C.4. Critical parameters for UF_6–HF systems using the Knight-modified Hansen-Roach cross sections

% Enrichment	H/X	Critical radius (cm)	Critical volume (l)	Critical mass (kgU)	Moderator mass (kg HF)
5.0	100	34.1565	166.920	270.644	115.182
	200	30.8937	123.509	127.585	108.590
	300	30.9320	123.9689	93.956	119.956
	500	34.2626	168.481	83.314	177.292
	700	38.7159	243.084	89.2119	265.769
3.0	100	48.3653	473.904	995.198	254.114
	200	40.0466	269.021	391.586	199.977
	300	39.3874	255.953	285.081	218.388
	500	41.6399	302.425	229.208	292.646
2.0	200	57.8921	812.730	1487.297	506.365
	300	53.0730	626.195	911.489	465.504
	500	55.9314	732.919	757.105	644.412
	700	65.1432	157.966	926.952	1104.636
1.7	200	70.7364	1482.578	2939.952	850.77
	300	65.3421	168.605	1873.508	813.255
	500	66.3236	222.061	1416.613	1024.882
	700	82.2357	329.538	2114.755	2141.931
1.4	200	128.326	8851.820	19154.453	4565.05
	300	89.8978	043.237	5429.439	1940.946
	500	90.7661	132.273	4136.480	2464.470
	700	117.168	737.762	7062.522	5891.216

APPENDIX D

TABLES OF CALCULATED VALUES FOR SECTION 3.1

This appendix contains tables of results used in Sect. 3.1 for cross-section comparisons. The CSAS1X control sequence of SCALE-4 was used to obtain calculated infinite media multiplication factors for selected systems.

Tables D.1 and D.2 give values of k_∞ predicted using the SCALE 16-group library that is included in SCALE-4.

Tables D.3 and D.4 give values k_∞ predicted using the LAW-238 ENDF/B-V fine-group library generated at ORNL. This library is not part of SCALE and was used as an independent reference.

Table D.1. k_∞ for UO_2F_2-H_2O systems using the SCALE 16-group library

H/X	5.0%	4.0%	3.0%	2.0%	1.7%	1.4%
5	0.934757	0.848083	0.742242	0.608830	0.561554	0.510214
10	1.00741	0.918760	0.806853	0.660984	0.608319	0.5540329
20	1.12277	1.03860	0.924300	0.759448	0.697177	0.627266
50	1.30100	1.22618	1.12624	0.963198	0.894538	0.812195
100	1.40743	1.34749	1.25882	1.10972	1.04646	0.966783
200	1.45203	1.40403	1.32935	1.20591	1.15315	1.07727
300	1.43457	1.39620	1.33385	1.22408	1.17363	1.10979
500	1.39039	1.34665	1.28691	1.20039	1.15961	1.10453
700	1.32754	1.29103	1.23640	1.15321	1.11777	1.07062
1000	1.23018	1.20132	1.15732	1.08121	1.04568	1.00856
1500	1.08629	1.06537	1.03308	0.976061	0.949311	0.913548
2000	0.968434	0.952739	0.927977	0.883590	0.862263	0.833990

Table D.2. k_∞ for UF_6-HF systems using the SCALE 16-group library

H/X	5.0%	4.0%	3.0%	2.0%	1.7%	1.4%
5	0.883584	0.796980	0.690648	0.557223	0.510242	0.459340
10	0.955991	0.868747	0.757425	0.610425	0.557175	0.498894
20	1.07160	0.985383	0.872498	0.710573	0.648872	0.578675
50	1.26124	1.18240	1.07332	0.911512	0.841283	0.759657
100	1.37101	1.30734	1.21788	1.06582	0.995713	0.915161
200	1.41898	1.36945	1.29441	1.16658	1.10986	1.03932
300	1.40541	1.36426	1.30034	1.18955	1.13726	1.07102
500	1.36569	1.32168	1.25578	1.16873	1.12608	1.07165
700	1.30333	1.26649	1.21177	1.11961	1.08642	1.04002
1000	1.20640	1.17737	1.13324	1.05670	1.02062	0.976927
1500	1.06327	1.04244	1.01019	0.953121	0.926089	0.890630
2000	0.946341	0.930792	0.906228	0.861898	0.840716	0.812401

Table D.3. k_∞ for UO_2F_2-H_2O systems using the LAW-238 ENDF/B-V library

H/X	5.0%	4.0%	3.0%	2.0%	1.7%	1.4%
5	0.893399	0.805225	0.697273	0.562855	0.516176	0.466234
10	0.972681	0.883838	0.770575	0.621987	0.568406	0.510019
20	1.09211	1.00479	0.888273	0.724829	0.662461	0.592253
50	1.28224	1.20381	1.09375	0.925627	0.856034	0.773132
100	1.40136	1.33376	1.23639	1.08084	1.01347	0.930380
200	1.45904	1.40357	1.32218	1.18791	1.12794	1.05223
300	1.45275	1.40456	1.33326	1.21385	1.15975	1.09070
500	1.39397	1.35510	1.29703	1.19816	1.15267	1.09394
700	1.32187	1.28913	1.23998	1.15552	1.11627	1.06524
1000	1.21714	1.19078	1.15099	1.08207	1.04974	1.00741
1500	1.06806	1.04847	1.01881	0.966998	0.942495	0.910142
2000	0.948921	0.933630	0.910468	0.869800	0.850457	0.824790

Table D.4. k_∞ for UF_6-HF systems using the LAW-238 ENDF/B-V library

H/X	5.0%	4.0%	3.0%	2.0%	1.7%	1.4%
5	0.831253	0.743318	0.636440	0.504124	0.458321	0.409286
10	0.914564	0.824171	0.709937	0.561783	0.508820	0.451284
20	1.04227	0.951865	0.832172	0.666011	0.603294	0.533053
50	1.24555	1.16386	1.04940	0.875412	0.803793	0.718858
100	1.37243	1.30237	1.20142	1.04023	0.970495	0.884678
200	1.43456	1.37757	1.29385	1.15561	1.09380	1.01576
300	1.42961	1.38034	1.30735	1.18501	1.12951	1.05866
500	1.37158	1.33204	1.27295	1.17230	1.12596	1.06606
700	1.29970	1.26653	1.21670	1.13104	1.09121	1.03937
1000	1.19527	1.16862	1.12843	1.05879	1.02611	0.983292
1500	1.04695	1.02719	0.997328	0.945162	0.920473	0.887886
2000	0.928778	0.913395	0.890095	0.849232	0.829783	0.804005

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