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NUCLEAR CRITICALITY DATA FOR URANIUM MASS
AND SPHERE VOLUME OF HOMOGENEOUS
WATER-REFLECTED AND -MODERATED ADU

November 1987

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Nuclear Criticality Data for Uranium Mass
and Sphere Volume of Homogeneous
Water-Reflected and -Moderated ADU

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The criticality calcuation to search for critical uranium mass and sphere volume, and subcritical uranium mass limit and sphere volume limit of homogeneous water-reflected and -moderated ammonium diuranate(ADU) was carried out with the JACS code system developed in Japan Atomic Energy Research Institute(JAERI) for criticality safety. Criticality calculations to search for these values were performed with the multigroup constant library MGCL and the multigroup Monte Carlo program KENO-IV of the JACS system. Uranium enrichment, uranium concentration, types of ADU, condition of the reflection and geometry were assumed as follows:

^{235}U enrichment :	3, 4 and 5 wt%
Uranium concentration :	\leq (theoretical density of ADU)
Types of ADU :	ADU(II), ADU(III) and ADU(IV)
Reflector :	30 cm thick water reflector was assumed around ADU
Geometry :	sphere

* Nagoya University

Calculated critical and subcritical sphere radii under these conditions were converted into sphere volumes and uranium masses. These values show that (1) subcritical mass limit of three kinds of ADU described above decrease in order of ADU(IV), (III), (II), while (2) subcritical volume limit of ADU(III) and (IV) are less than that of ADU(II).

There is a mixture of ADU(II),(III) and (IV) in the ADU process at nuclear fuel fabrication facility. From our results, the ADU mixture with less than 5wt% enrichment can be safely handled up to 34.5 kg by uranium mass or 24.5l by volume at the same time in the ADU process.

Keywords : Ammonium Diuranate, Critical Size, Subcritical Size Limit, Mass, Volume, JACS, MGCL, KENO-IV

水反射体付き均質 ADU-H₂O の臨界質量・体積
及び未臨界極限質量・体積

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(1987 年 10 月 15 日受理)

原研で開発した臨界安全性評価コードシステム JACS に収められている多群定数ライブラリー MGCL、多群モンテカルロ計算プログラム KENO-IV を用いて均質 ADU-H₂O の臨界条件（ちょうど臨界となるウラン質量及び球体積、臨界上安全と考えられる最大のウラン質量及び球体積）を計算した。ADU の組成、形状、外部反射条件は次のように設定した。

²³⁵ U 濃縮度	3, 4, 5 wt %
ウラン濃度	≤(ADU の理論密度)
組 成	ADU(II), ADU(III), ADU(IV)
外部反射条件	厚さ 30cm の水
形 状	球

計算で得られた半径から、対応するウラン質量及び球体積を求めた。この 2 種類の値のウラン濃度に対する最小値（最小ウラン質量、最小球体積）を ADU の種類で比較すると、(1) 最小ウラン質量は ADU(IV), (III), (II) の順で小さくなり、一方、(2) ADU(III) 及び(IV) の最小球体積は ADU(II) よりも小さくなつた。

軽水炉燃料加工工場の ADU プロセスでは、ADU(II), ADU(III) 及び ADU(IV) が混在していると一般に考えられている。本計算結果によれば、²³⁵U 濃縮度が 5 wt % 以下の ADU-H₂O の場合、臨界上安全と考えられる最大のウラン質量及び球体積は（制限ウラン質量、制限球体積）それぞれ 34.5 kg — ADU(II), 24.5 l — ADU(III) となつた。よって、ADU プロセスでは、一度に最大で 34.5 kg のウランを含む ADU-H₂O あるいは 24.5 l の ADU-H₂O を臨界上安全に取扱うことができる。

Contents

1. Introduction	1
2. Calculation Method	2
3. Preparation for Criticality Calculation	3
3.1 A Model for KENO-IV	3
3.2 Temperature	3
3.3 MGCL	4
3.4 KENO-IV input parameters	4
3.5 Atomic Number Densities	4
4. Results of Dimension Search	5
5. Discussions	5
References	7

Appendices

A.1 Composition of ADU	25
A.2 Atomic Number Densities of ADU-H ₂ O	25
A.3 Atomic Number Density of Water	27
A.4 Results of KENO-IV Calculation	27
A.5 Maximum Uranium Concentration of ADU-H ₂ O	27

目 次

1. 序	1
2. 計算方法	2
3. 臨界計算のための各パラメータ	3
3.1 KENO-IV 計算モデル	3
3.2 温度	3
3.3 MGCL	4
3.4 KENO-IV 入力データ	4
3.5 原子個数密度	4
4. 計算結果	5
5. 検討	5
参考文献	7

付録

A.1 ADUの組成	25
A.2 ADU-H ₂ Oの原子個数密度	25
A.3 水の原子個数密度	27
A.4 KENO-IV の計算結果	27
A.5 ADU-H ₂ Oの最大ウラン濃度	27

1. Introduction

Fuel fabrication facility for light water reactor has a chemical process, known as the ADU process, in which UF_6 gas is converted into UO_2 powder. ADU(Ammonium Diuranate) is produced in the middle of the process. The following compositions of ADU are reported¹⁾ as a result of chemical analysis.

ADU(I)	$\text{UO}_3 \cdot 2\text{H}_2\text{O}$
ADU(II)	$3\text{UO}_3 \cdot \text{NH}_3 \cdot 5\text{H}_2\text{O}$
ADU(III)	$2\text{UO}_3 \cdot \text{NH}_3 \cdot 3\text{H}_2\text{O}$
ADU(IV)	$3\text{UO}_3 \cdot 2\text{NH}_3 \cdot 4\text{H}_2\text{O}$

It is considered that ADU mixture in the process consists of ADU(II),ADU(III) and ADU(IV), and that there is seldom or no ADU(I) in the mixture.

In reference to ADU, the criticality handbook²⁾ published in West Germany is the only one data source for the criticality parameters such as uranium mass, sphere volume, infinite cylinder diameter and infinite slab thickness. While it is considered that the composition of ADU is $(\text{NH}_4)_2\text{U}_2\text{O}_7$ in the handbook. It is reported that the composition can not be observed in the ADU process¹⁾. According to the report, the criticality data of West Germany are not adequate for evaluating criticality safety in the ADU process.

So we calculated critical uranium mass and sphere volume, and subcritical uranium mass limit and sphere volume limit of homogeneous water-moderated ADU(II)^{*1)}, ADU(III)^{*1)} and ADU(IV)^{*1)} with water reflector using the criticality safety code system JACS³⁾. Calculation for ADU(I) was not performed, since it can be hardly observed in the ADU process. The criticality calculations for ADU were performed on the following conditions.

^{235}U enrichment :	3,4 and 5 wt%
Uranium concentration :	\leq (Theoretical density of ADU)
Types of ADU :	ADU(II), ADU(III) and ADU(IV)
Reflector :	30 cm thick water

*1) Water-moderated ADU is often expressed as ADU- H_2O . This report uses this expression

Geometry	Sphere
Desired k_{eff} :	0.986 (for critical)
	0.965 (for subcritical limit)

Calculated results shown in this report can be applied to the criticality safety analysis for the ADU process.

2. Calculation Method

Calculations were performed using the following library and programs, which are all contained in criticality safety code system JACS.

MGCL library (137 energy-groups, 300 k)

AND program

MAIL program

KENO-IV program

MGCL³⁾ is a multigroup constant library constructed with a code system MGCL-PROCESSOR³⁾ from evaluated nuclear data file ENDF/B-IV⁴⁾. AND⁵⁾ is a program calculating atomic number density of various nuclear materials. MAIL³⁾ is a program which generates effective macroscopic cross sections from MGCL and atomic number densities. KENO-IV⁴⁾ is a multigroup Monte Carlo program which can calculate neutron multiplication factor k_{eff} and can perform dimension search and array search corresponding to a desired k_{eff} .

Figure 1 shows a flow chart of the calculation to search a critical size or a subcritical limit size of homogeneous ADU-H₂O.

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Figure 1 shows a flow chart of the calculation to search a critical size or a subcritical limit size of homogeneous ADU-H₂O.

The calculation in Fig.1 have three steps, these are:

- (1) calculation of atomic number densities of the nuclides in ADU-H₂O,
- (2) generation of a macroscopic cross section set of ADU-H₂O and water as a reflector for KENO-IV,
- (3) dimension search calculation on sphere of water-reflected ADU-H₂O corresponding to the desired k_{eff} .

Desired k_{eff} values used in the calculation are listed in Table 1. They were derived from a statistical analysis⁷⁾. This table has two kinds of k_{eff} values proper to the JACS system, one corresponds to critical k_{eff} , another to subcritical limit k_{eff} , respectively. These values are based on about 400 of calculated k_{eff} values with the JACS system for many critical experiments. The critical k_{eff} is the value of the most probable calculated k_{eff} for a critical state. Subcritical limit k_{eff} is the value to assure a nuclear fuel system of subcriticality. As the calculated k_{eff} with the JACS code system for a nuclear fuel system is lower than this value, the system is safe on criticality. In accordance with this table, a critical k_{eff} value and a k_{eff} value of subcritical limit for the low enriched ADU-H₂O are 0.986 and 0.965 respectively

3. Preparation for Criticality Calculation

3.1 A Model for KENO-IV

Figure 2 shows a model of water-reflected homogeneous ADU-H₂O for KENO-IV. The model consists of spherical ADU-H₂O region and 30 cm thick reflector region outside the ADU-H₂O. A neutron across over the outermost boundary of the model is assumed not to return at all.

3.2 Temperature

Temperature of the ADU-H₂O and reflector were assumed to be 20

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⁹⁰C. Atomic number densities of the composite isotopes in the ADU-H₂O region and the reflector region were calculated on this assumption.

3.3 MGCL

Ten kinds of MGCL libraries are available in the JACS system. They have different temperature or energy-group structure each other. The MGCL library with 137 energy-group and 300 k of temperature was selected for the MAIL calculation. 300 k was the nearest temperature to 20° c described in section 3.2.

3.4 KENO-IV Input Parameters

Parameters entered to KENO-IV are as follows. The desired k_{eff} values were selected from Table 1. In some cases, 600 neutrons per generation and 203 generations were entered to execute more accurate dimension search.

Number of energy groups :	137,
Number of neutrons per generation :	300,
Number of generations :	103,
Number of generations to be skipped :	3,
Neutron distribution at start :	flat,
Search constant for sphere radius :	1.0,
Condition of search completion :	$\pm 1\sigma$,
Boundary condition :	see Fig.2,
Desired k_{eff} corresponding to critical :	0.986,
Desired k_{eff} corresponding to subcritical limit :	0.965.

3.5 Atomic number densities

Atomic number densities of the composite nuclides in the homogeneous ADU-H₂O and water were calculated with the AND program. The calculated results are tabulated in Appendix.

4. Results of Dimension Search

Dimension search with KENO-IV gives a size of nuclear fuel material corresponding to desired k_{eff} . In the case of a spherical geometry, sphere radius of the fuel material is calculated and printed out. Results of the dimension search for the water-moderated homogeneous ADU-H₂O are shown in Appendix.

Sphere volume and uranium mass of the fuel material is given from the sphere radius as shown in Equations (1) and (2) below.

$$V = (1/1000) \cdot (4/3)\pi r^3 \quad (1)$$

$$M = V \cdot C \quad (2)$$

where,

$r[\text{cm}]$: radius of homogeneous ADU-H₂O sphere
corresponding to desired k_{eff} ,

$V[\ell]$: volume of the sphere,

$C[\text{g/cm}^3]$: uranium concentration in homogeneous ADU-H₂O,

$M[\text{kg}]$: uranium mass in the sphere.

Figures 3.1.1 through Fig.3.6.2 show uranium mass curves and sphere volume curves with two parameters of ²³⁵U enrichment and uranium concentration. Each data on the curves was calculated in accordance with Eqs. (1) and (2).

5. Discussions

(1) Minimum Values of Critical Mass and Volume, and Subcritical mass limit and volume limit

Table 2 shows minimum values on critical and subcritical limit curves drawn in Figs.3.1.1 through 3.6.2. The minimum critical mass and the minimum subcritical mass limit increase in order of ADU(II), ADU(III), ADU(IV). The minimum critical volume and the minimum

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subcritical volume limit increase in order of ADU(III), ADU(IV), ADU(II). These facts imply that the composition of ADU(II) is suitable to obtain criticality safety mass limit in the ADU process, on the other hand, ADU(III) is suitable to obtain volume limit.

Table 2 reveals that the mixture of ADU(II), ADU(III) and ADU(IV) with less than 5 wt% ^{235}U enrichment can be safely handled up to 34.5 kg by uranium mass or 24.5 l by volume at the same time in the ADU process.

(2) Effect of Nitrogen in ADU on reactivity

Figure 3.7 shows a comparison of the critical sphere volumes among 3wt% enriched ADU(II), ADU(III) and ADU(IV). In the left half of the figure, it can be observed that the critical sphere volume increases in order of ADU(II), ADU(III), ADU(IV). This order seems to depend on nitrogen concentration in ADU, since nitrogen has ~20 barn of capture cross section for the thermal neutron and it effects to reduce the reactivity. So, the critical sphere volume of ADU(II), which has the lowest nitrogen/uranium atom ratio in the three kinds of ADUs, is the smallest in ADUs in the region of low uranium concentration.

In the region of high uranium concentration, in the right half of the figure, the effect of nitrogen is not so strong because of harder neutron spectrum than in the lower uranium concentration region. Therefore, the amount of the critical sphere volume only depends on hydrogen/uranium atom ratio, and the critical sphere volume increase in order of ADU(IV), ADU(III), ADU(II).

Figure 3.8 shows a comparison of critical uranium mass among 3wt% enriched ADU(II), ADU(III) and ADU(IV). The same situation as in Fig.3.7 can be observed in Fig.3.8.

References

- 1) E.H.P.Cordfunke, "On The Uranates of Ammonium-I, The Ternary System NH₃-UO₃-H₂O," J.Inorg.Nucl.Chem., Vol.24, pp.303 to 307 (1962)
- 2) W.Heinicke, H.Krug, W.Thomas, W.Weber and B.Gmal, "Handbuch zur Kritikalität--- Teil I,II,III," Gesellschaft fur Reaktorsicherheit mbH (1985)
- 3) Y.Naito, S.Tsuruta,T.Matsumura and T.Ohuchi, "MGCL-Processor: A Computer Code System for Processing Multigroup Constant Library MGCL," JAERI-M9396 (1981)
- 4) ENDF/B Summary Documentation, BNL-NCS-17541(ENDF-201), 2nd Edition (ENDF/B-IV) (1975)
- 5) Y.Komuro, T.Sakai and S.Nakamaru, "Caluculation Methods of Atomic Number Density for Various Nuclear Materials," JAERI-M 86-037 (in Japanese)
- 6) L.M.Petrie and N.F.Cross, "KENO-IV, An Improved Monte Carlo Criticality Program," ORNL-4938 (1975)
- 7) H.Okuno and Y.Naito, "Evaluation of Calculational Errors with the Nuclear Criticality Safety Analysis Code System JACS," JAERI-M 87-057 (1987) (in Japanese)

Table 1 Critical k_{eff} and subcritical limit k_{eff} in JACS

Category		Critical k_{eff}	Subcritical limit k_{eff}
Homo	• Low enriched uranium	0.986	0.965
Homo	• High enriched uranium	0.985	0.954
Homo	• Plutonium	1.008	0.980
Homo	• Mixed oxide	1.013	0.980
Homo	• Mix a)	1.010	0.980
Hetero	• Low enriched uranium	0.995	0.978
Hetero	• Plutonium	1.004	0.964
Hetero	• Mixed oxide	0.997	0.980

a) $\text{UO}_2(\text{NO}_3)_2 - \text{Pu}(\text{NO}_3)_4$ solution

Table 2 Minimum values of critical curves and subcritical limit curves of homogeneous water-reflected and -moderated ADU

Type of A D U	^{235}U enrichment [wt%]	Uranium mass [kg] (a)	Sphere volume [l] (c)	Sphere volume [l] (d)
(II)	3	109	94	61
	4	60.5	52.5	37.8
	5	41.5	34.5	30.9
(III)	3	114	95	55
	4	62	53	36.0
	5	41	36.15	28
(IV)	3	122	102	57
	4	64	52.9	35.8
	5	41	36.5	27

(a) Minimum critical mass

(b) Minimum subcritical mass limit

(c) Minimum critical sphere volume

(d) Minimum subcritical sphere volume limit

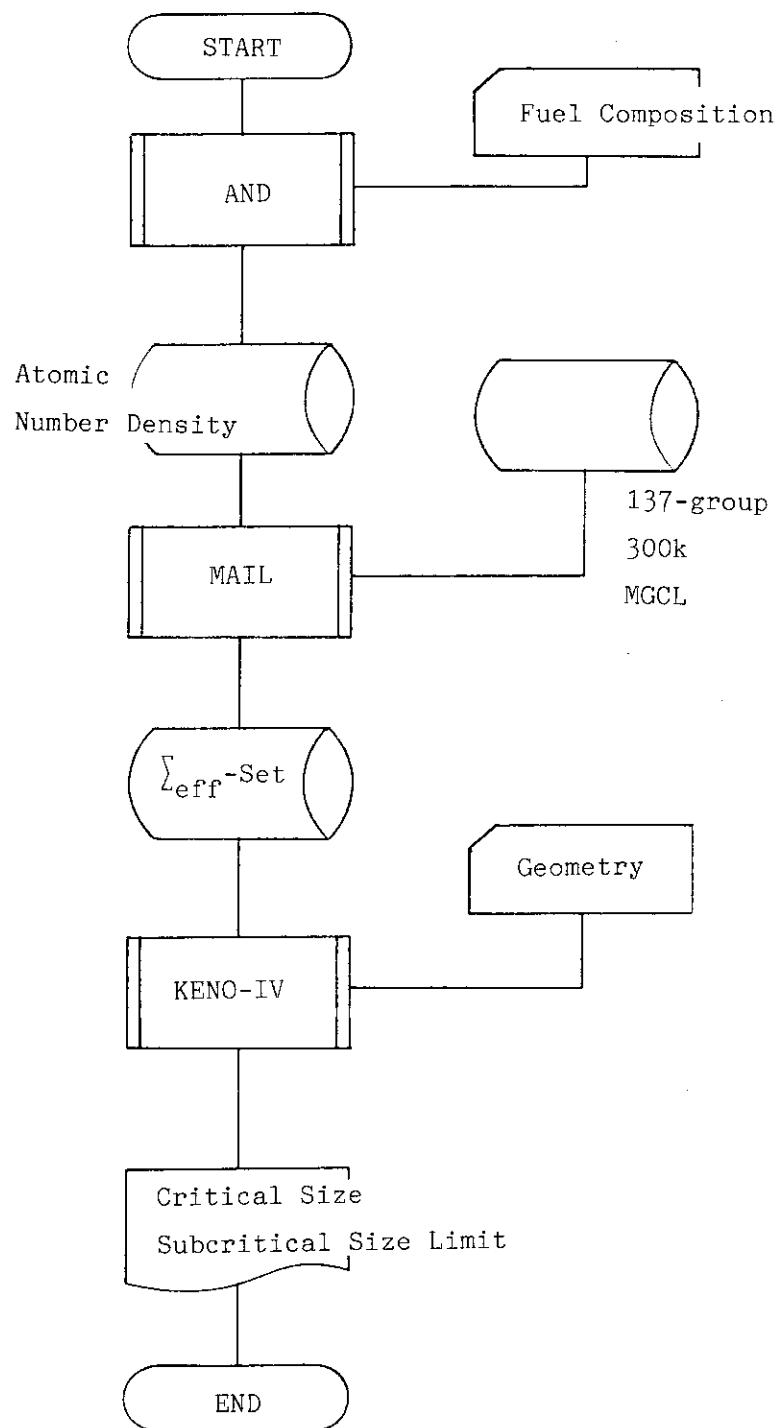


Fig.1 Flow of the dimension search with JACS

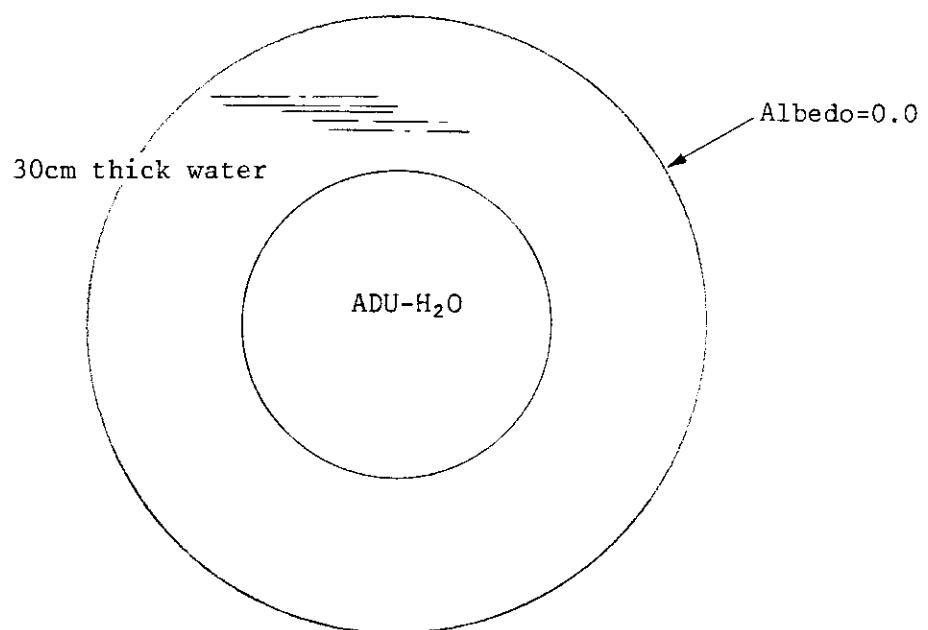


Fig.2 The model of water reflected ADU- H_2O sphere for KENO-IV

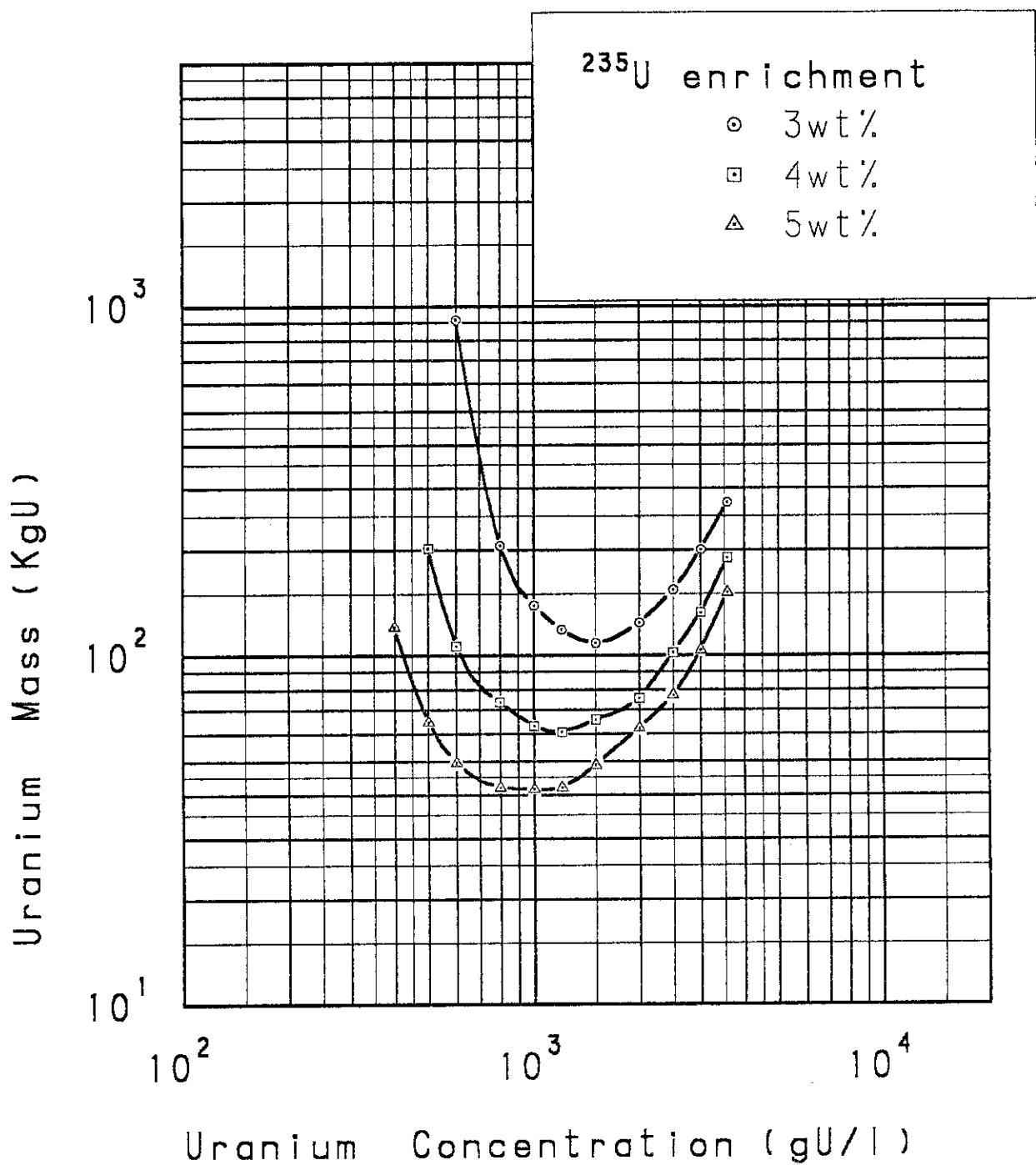


Fig. 3.1.1 Critical uranium mass of homogeneous water-reflected ADU(II)-H₂O

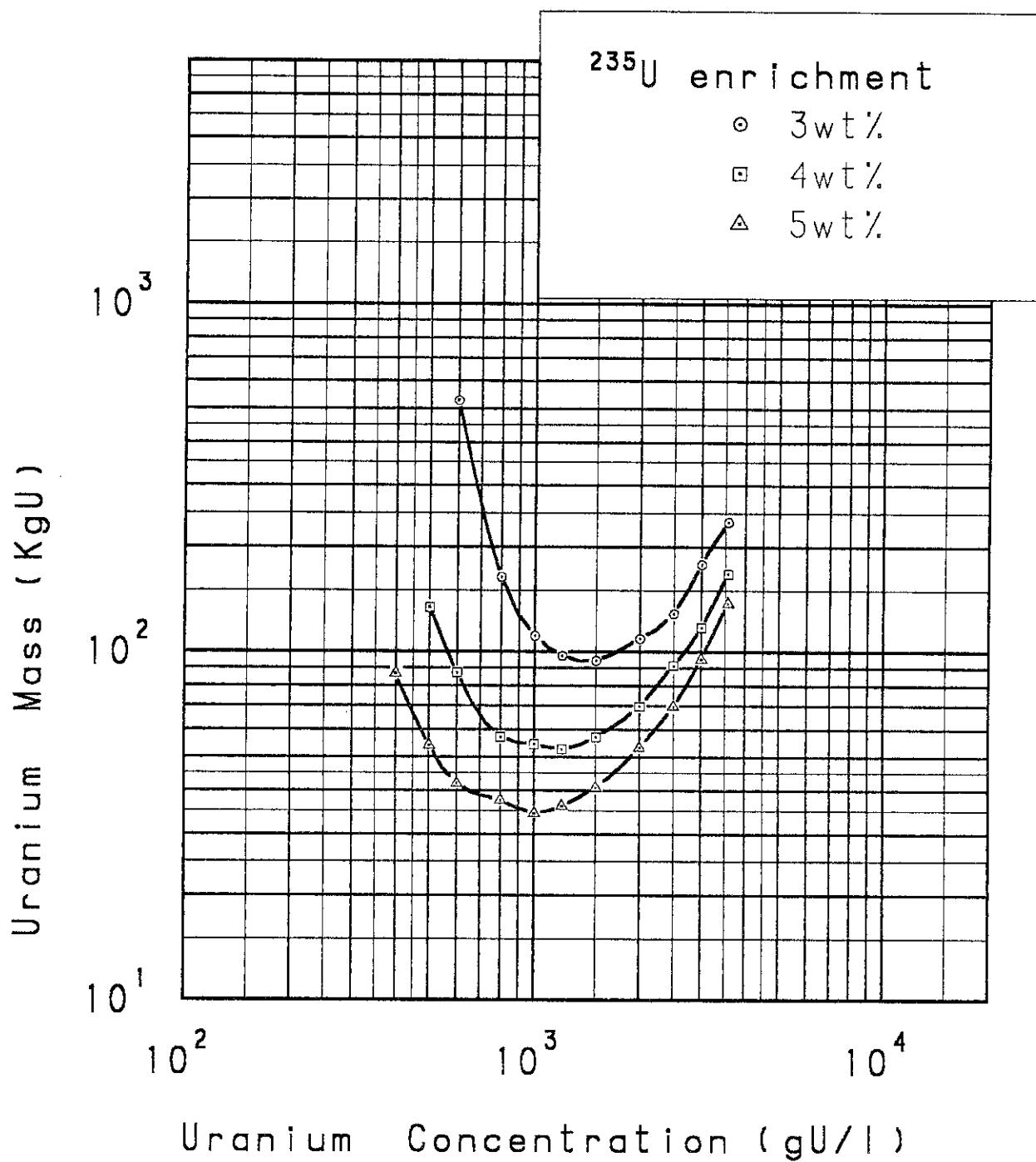


Fig. 3.1.2 Subcritical uranium mass limit of homogeneous water-reflected ADU(II)-H₂O

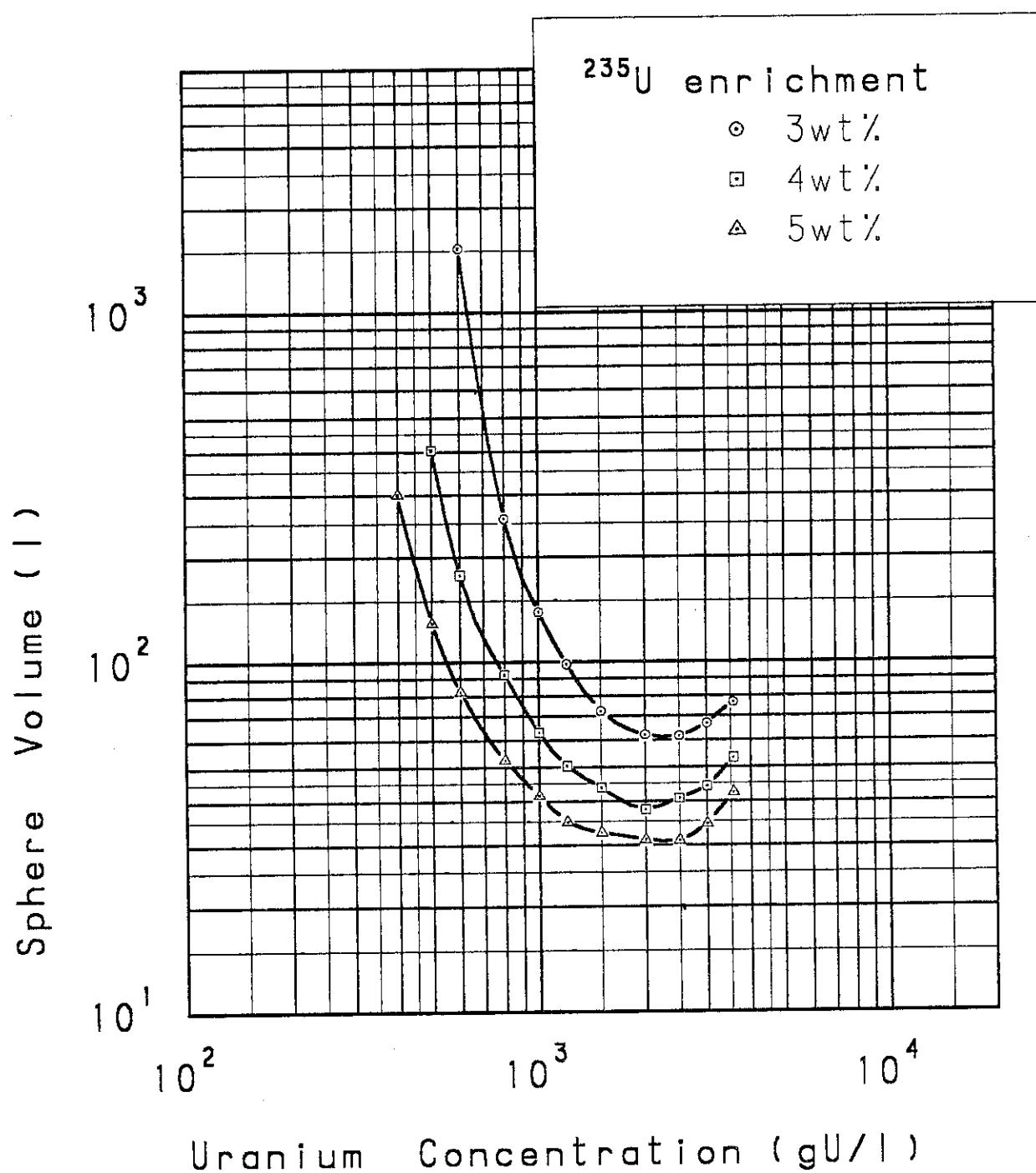


Fig. 3.2.1 Critical sphere volume of homogeneous water-reflected
ADU(II)-H₂O

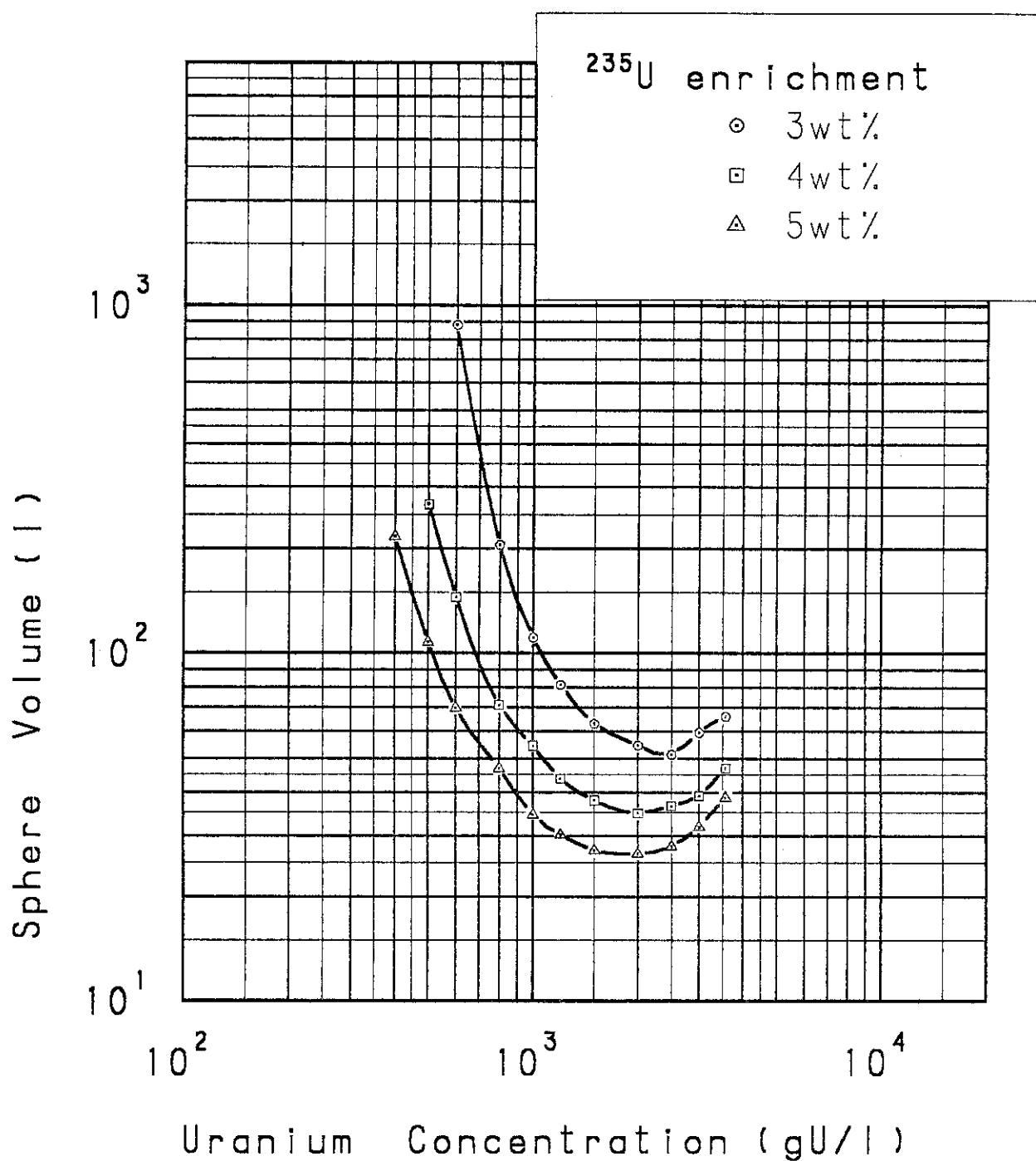


Fig. 3.2.2 Subcritical sphere volume limit of homogeneous water-reflected ADU(II)-H₂O

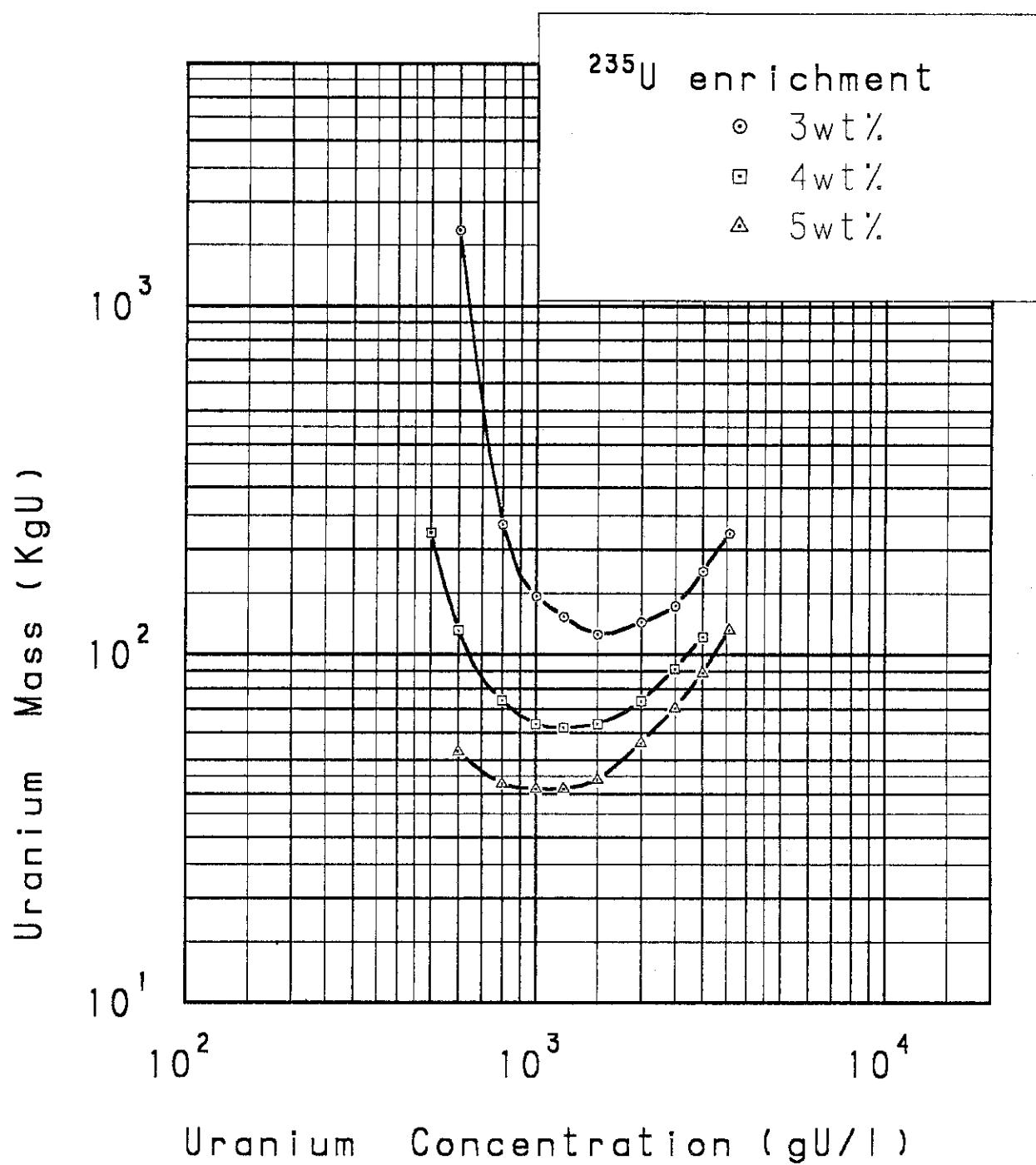


Fig. 3.3.1 Critical uranium mass of homogeneous water-reflected
ADU(III)- H_2O

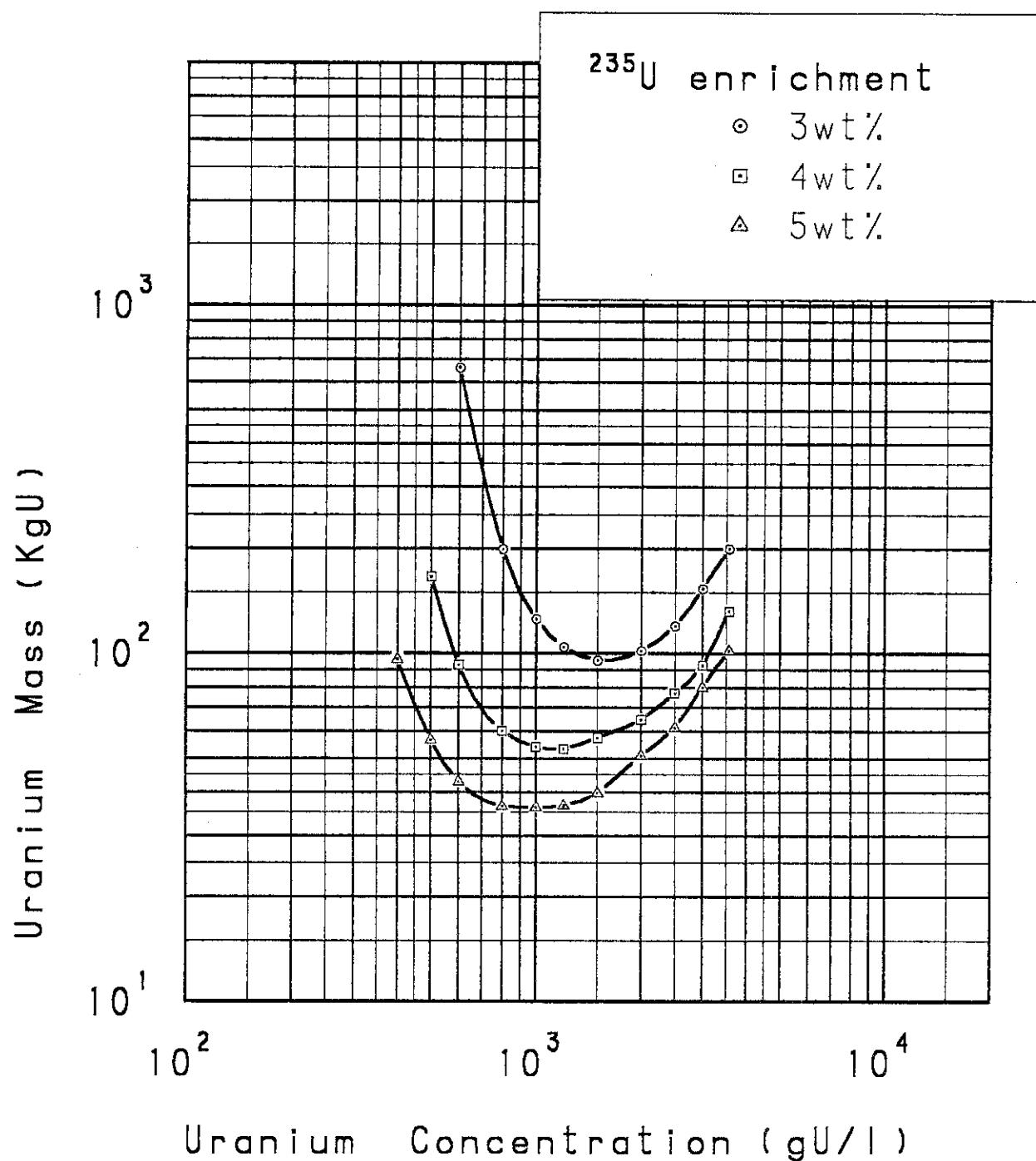


Fig. 3.3.2 Subcritical uranium mass limit of homogeneous water-reflected ADU(III)-H₂O

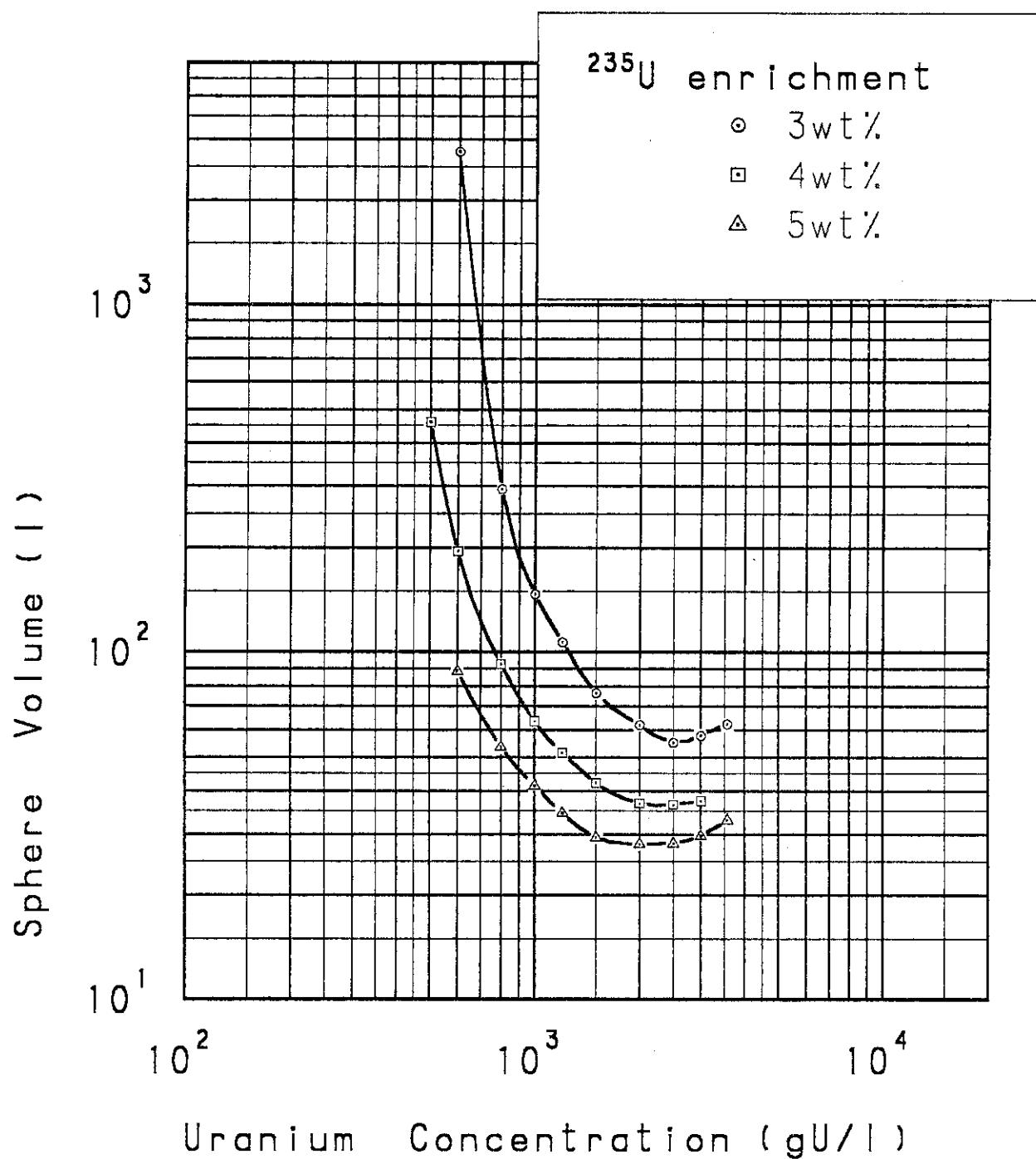


Fig. 3.4.1 Critical sphere volume of homogeneous water-reflected ADU(III)-H₂O

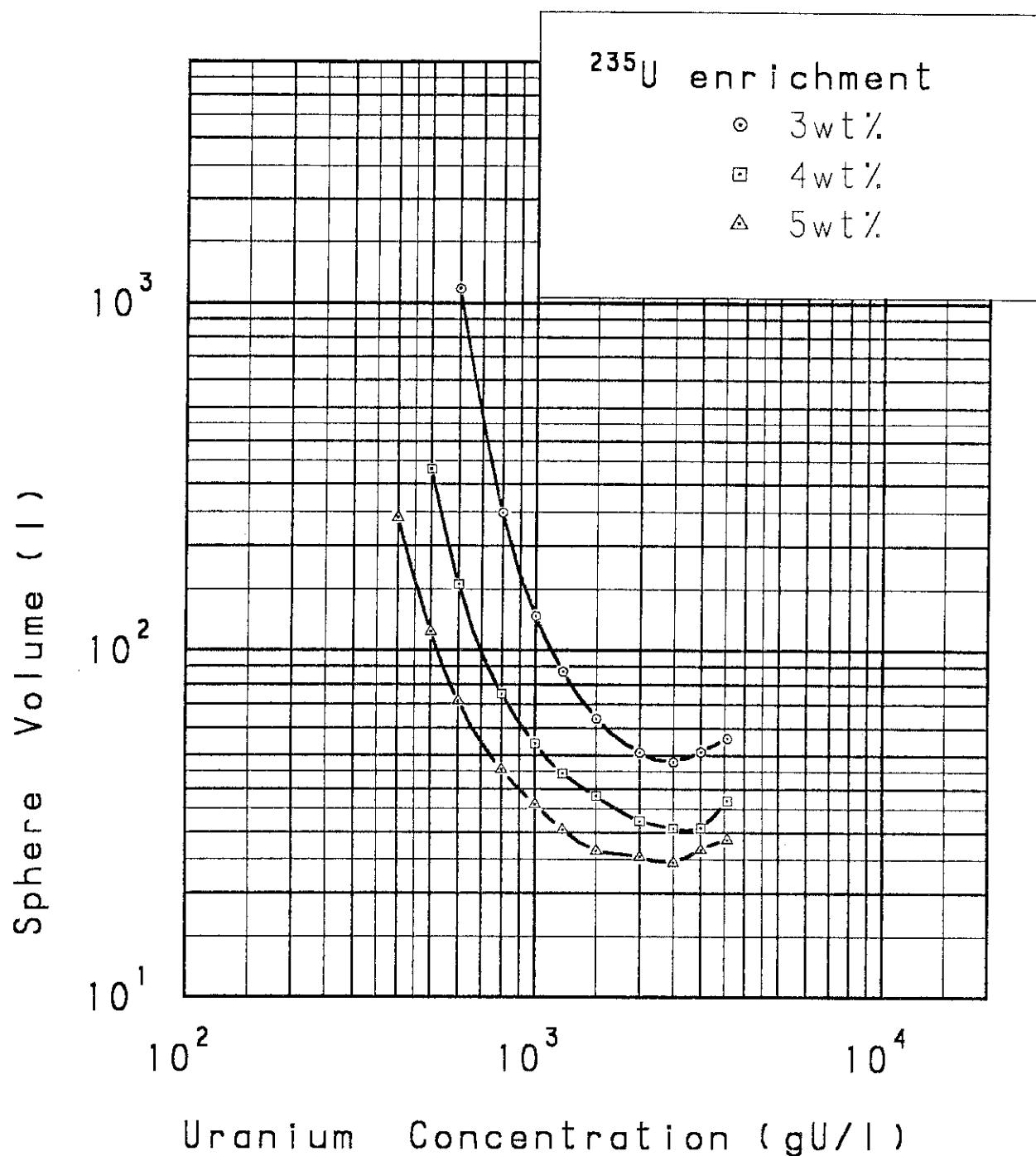


Fig. 3.4.2 Subcritical sphere volume limit of homogeneous water-reflected ADU(III)-H₂O

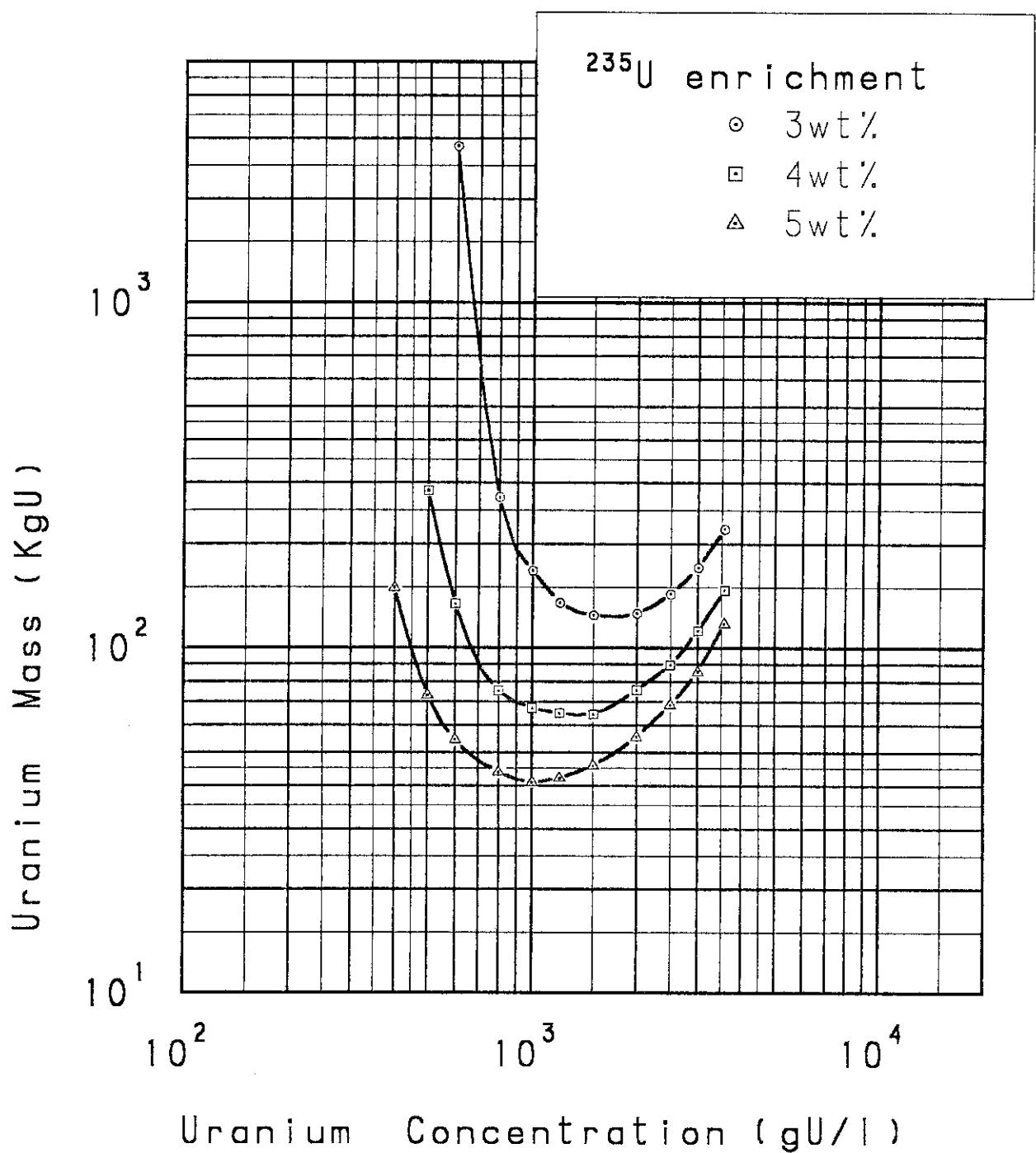


Fig. 3.5.1 Critical uranium mass of homogeneous water-reflected ADU(IV)-H₂O

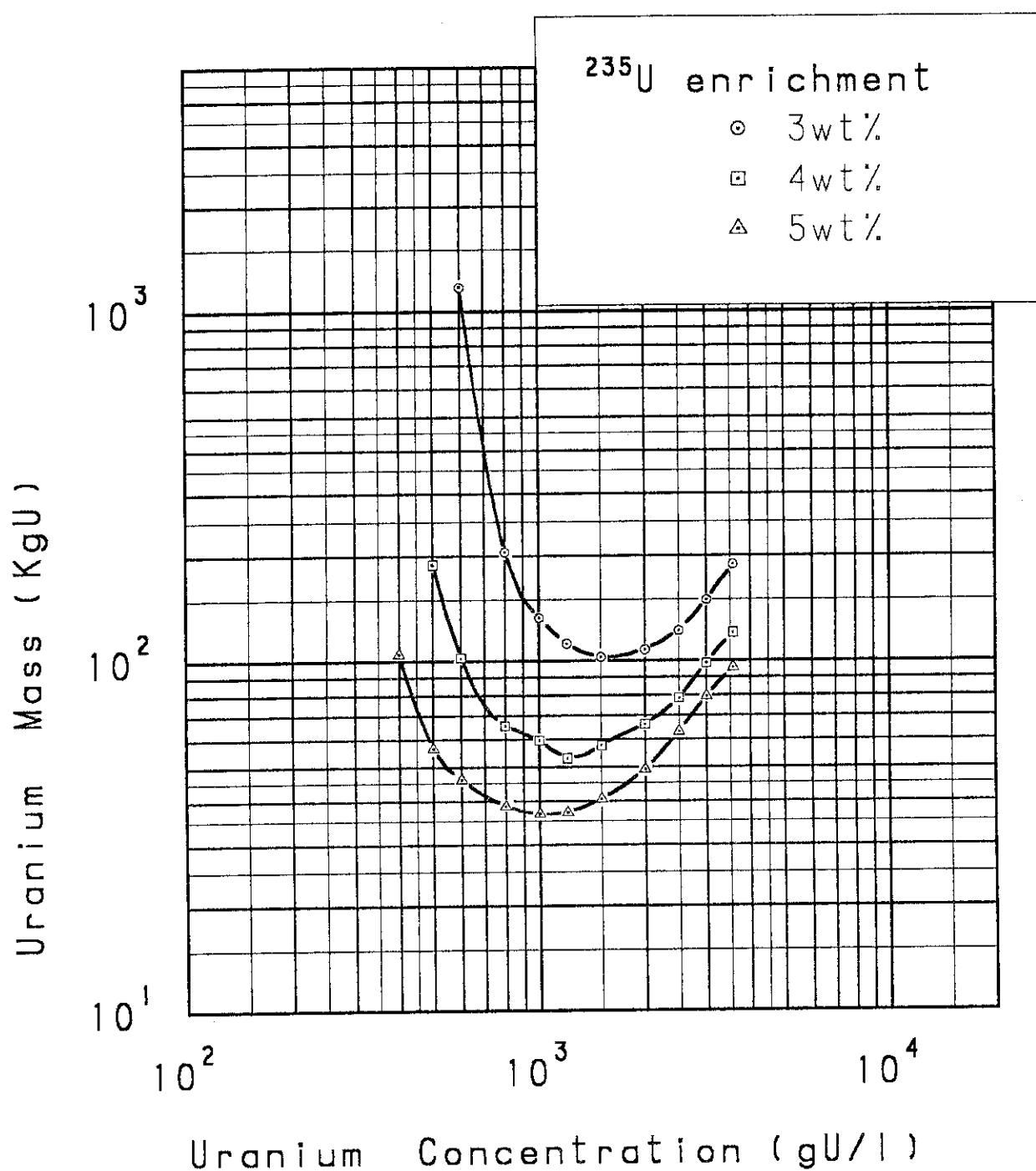


Fig. 3.5.2 Subcritical uranium mass limit of homogeneous water-reflected ADU(IV)- H_2O

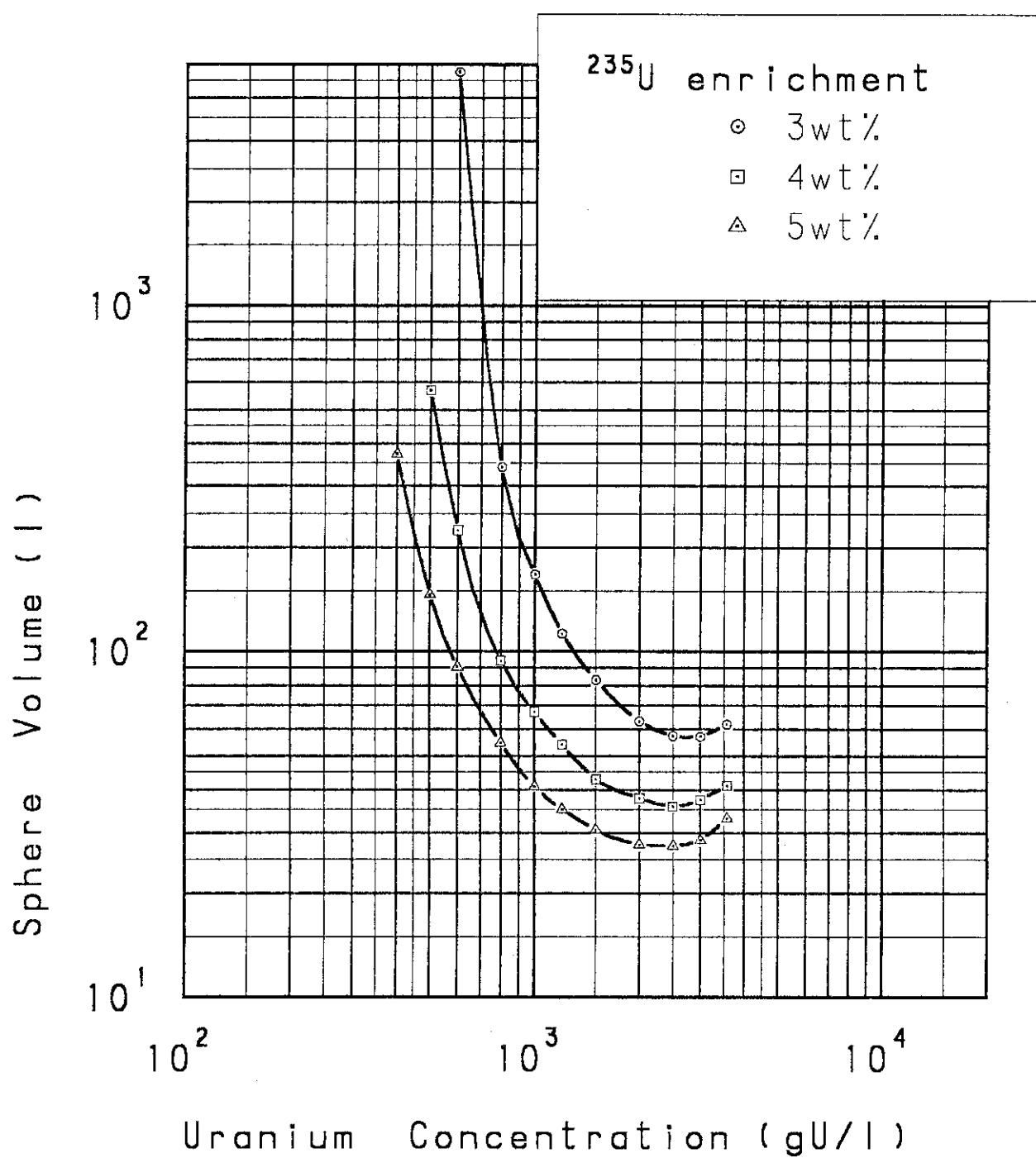


Fig. 3.6.1 Critical sphere volume of homogeneous
water-reflected ADU(IV)-H₂O

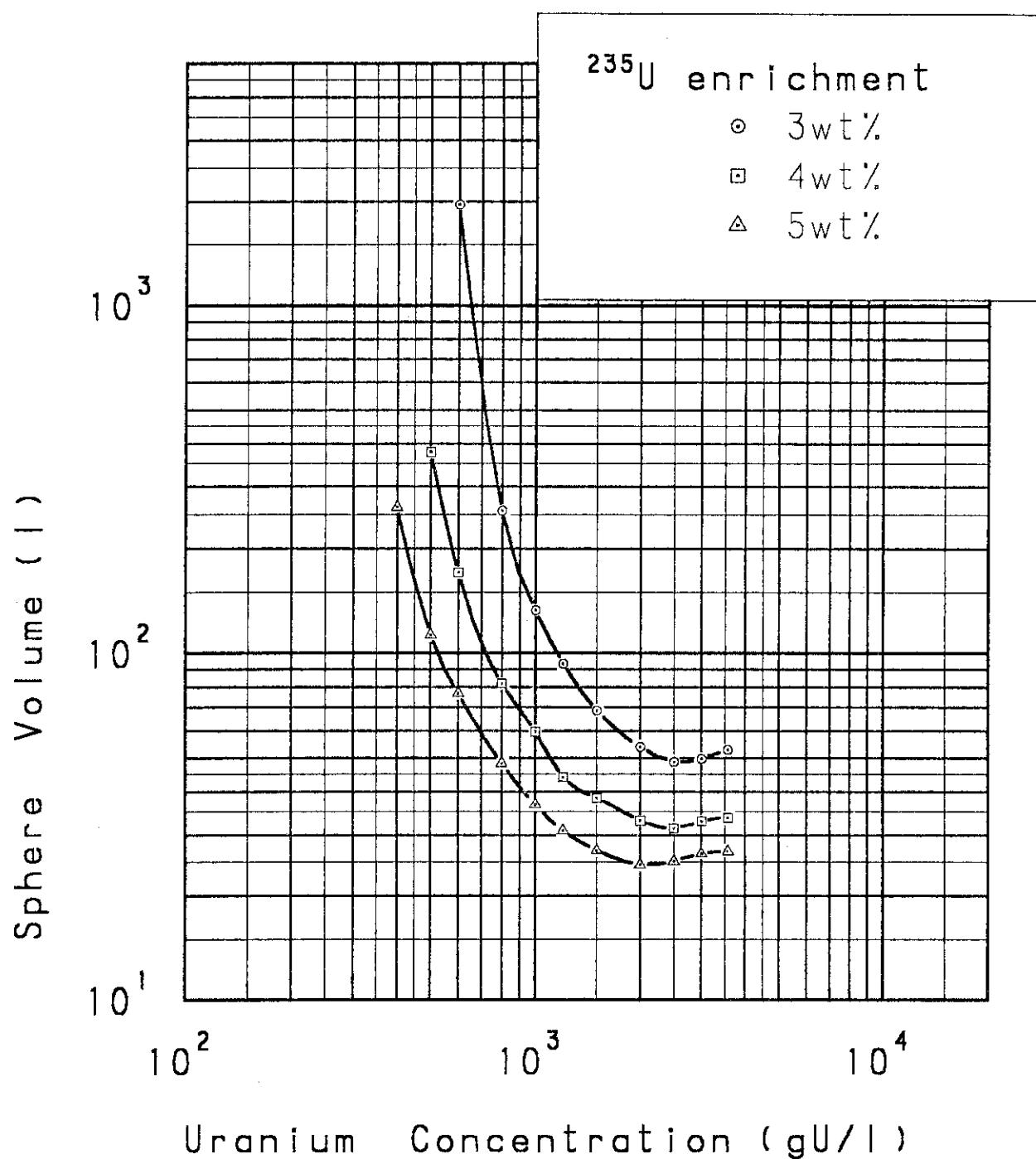


Fig. 3.6.2 Subcritical sphere volume limit of homogeneous water-reflected ADU(IV)-H₂O

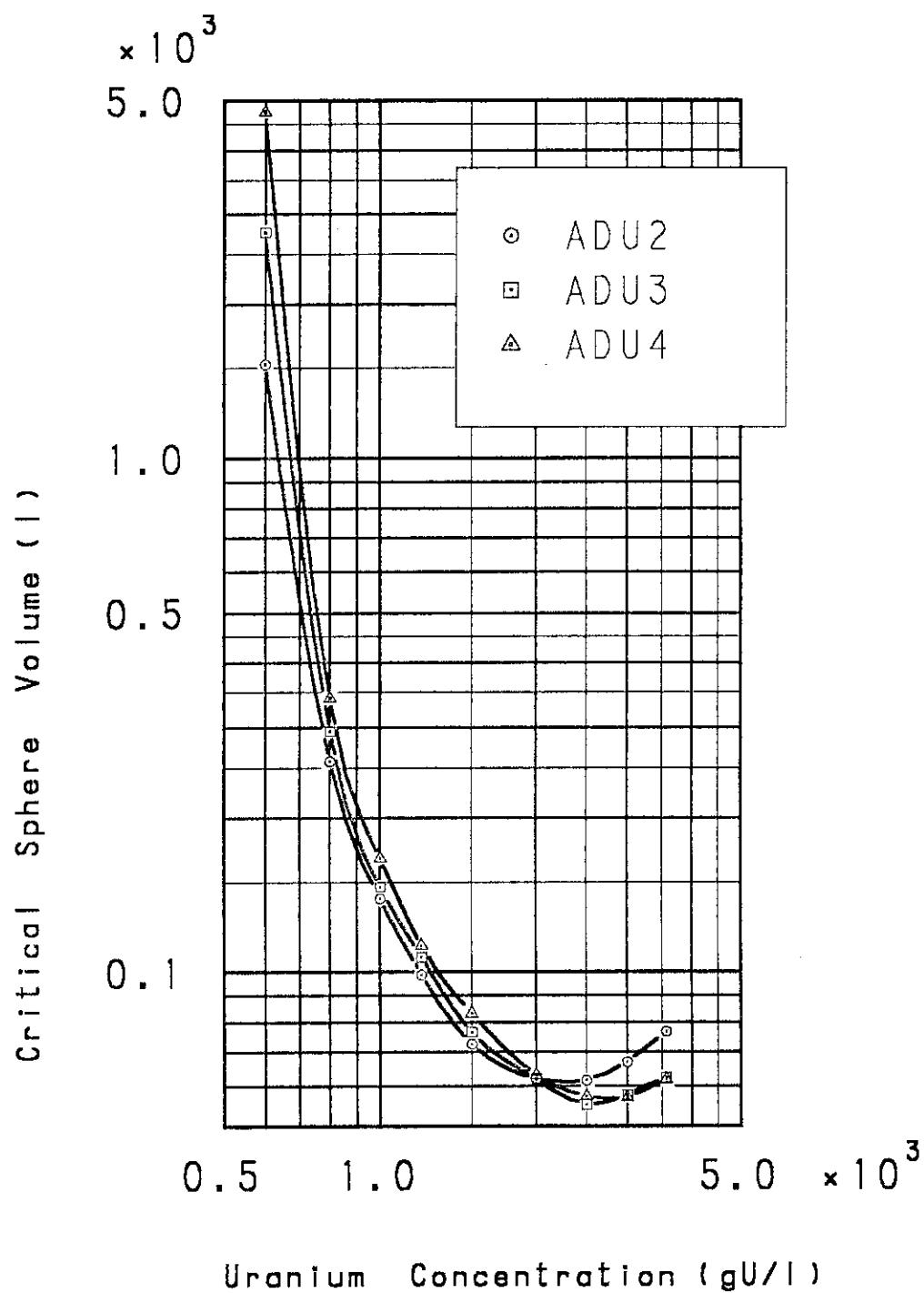


Fig. 3.7 Comparison of critical sphere volume among water-reflected 3 wt% enriched ADU(II)-H₂O, ADU(III)-H₂O and ADU(IV)-H₂O

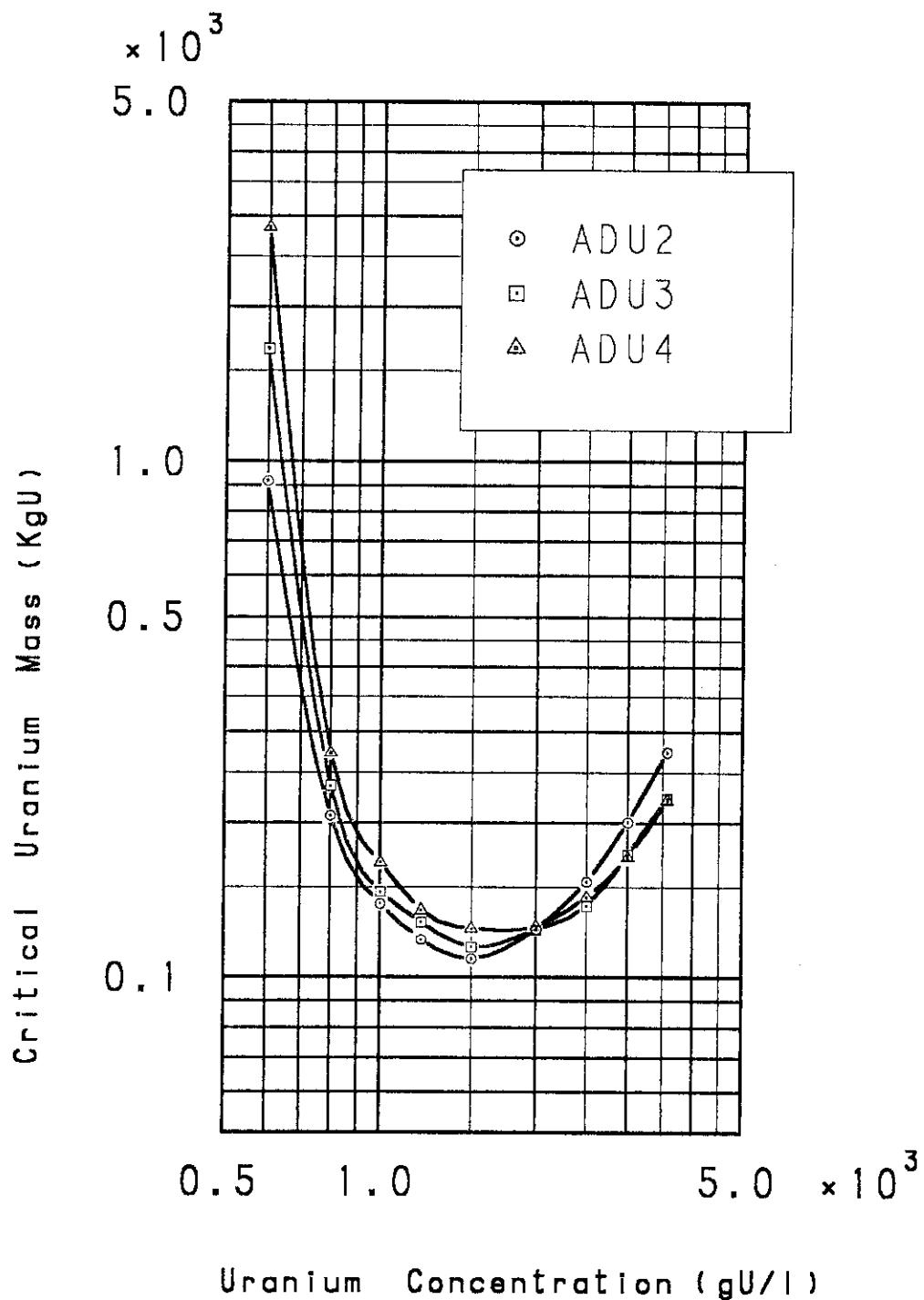


Fig. 3.8 Comparison of critical uranium mass among water-reflected 3 wt% enriched ADU(II)-H₂O, ADU(III)-H₂O and ADU(IV)-H₂O

Appendices

A.1 Composition of ADU

ADU is commonly produced in the ADU process of light water reactor fuel fabrication facility. Table A.1 shows a comparison of four kinds of ADUs reported as a results of a chemical analysis¹⁾. ADU is precipitated in a mixture of ammonium hydroxide and uranyl fluoride or uranyl nitrate. Composition of ADU produced depends on pH of the mixture as shown in Table A.2²⁾.

A.2 Atomic Number Densities of ADU-H₂O

MAIL program generates a region-wise macroscopic cross section set from number densities of each nuclide included in the region and the MGCL library. Atomic number densities of the nuclides in the ADU-H₂O having various ²³⁵U enrichments and uranium concentrations are lists in Table A.3. They were calculated with the AND program which can calculate atomic number densities of the nuclides included in many kinds of nuclear materials, that is, i.e. UO₂-H₂O, UO₂F₂ solution, ADU-H₂O, Pu(NO₃)₂ solution and so on. AND calculates the atomic number densities of the nuclides included in ADU-H₂O by the following manner.

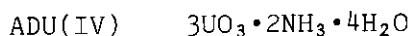
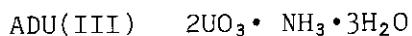
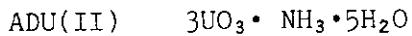
ADU-H₂O has four elements, U, N, O and H. If uranium concentration is given, then the number density of U can be calculated by the following equation.

$$N(U) = \{ C(U) \cdot N_A / A(U) \} (1/10^{24}) \quad (A.1)$$

where,

- N(i) [atoms/barn·cm] : number density of element i,
- C(i) [g/cm³] : concentration of element i,
- A(i) : atomic weight of element i,
- N_A [atoms/mol] : Avogadro number.

Once $N(U)$ has been calculated, atomic number densities of ^{235}U and ^{238}U , i.e., $N(^{235}U)$ and $N(^{238}U)$, can be obtained by using the value of ^{235}U enrichment. Further more $N(N)$ in each ADU can be calculated from the N/U atom ratio defined in the following chemical formulas.



Substituting $N(U)$ in the following equations, $N(H)$ in each ADU can be calculated.

ADU(II)-H₂O :

$$\begin{aligned} N(H)/N(U) = & 2 \cdot \rho(\text{H}_2\text{O})/\text{A}(\text{H}_2\text{O}) \cdot \{ A(\text{U})/\text{C}(\text{U}) - (1/3) \cdot A(\text{ADU(II)})/\rho(\text{ADU(II)}) \} \\ & + 13/3 \end{aligned} \quad (\text{A.2.1})$$

ADU(III)-H₂O :

$$\begin{aligned} N(H)/N(U) = & 2 \cdot \rho(\text{H}_2\text{O})/\text{A}(\text{H}_2\text{O}) \cdot \{ A(\text{U})/\text{C}(\text{U}) - (1/2) \cdot A(\text{ADU(III)})/\rho(\text{ADU(III)}) \} \\ & + 9/2 \end{aligned} \quad (\text{A.2.2})$$

ADU(IV)-H₂O :

$$\begin{aligned} N(H)/N(U) = & 2 \cdot \rho(\text{H}_2\text{O})/\text{A}(\text{H}_2\text{O}) \cdot \{ A(\text{U})/\text{C}(\text{U}) - (1/3) \cdot A(\text{ADU(IV)})/\rho(\text{ADU(IV)}) \} \\ & + 14/3 \end{aligned} \quad (\text{A.2.3})$$

where, $\rho(i)$ [g/cm³] is the density of element i.

Oxygen is included in both of ADU and H₂O. Substituting $N(U)$ and $N(H)$ in the following equation, $N(O)$ in each ADU-H₂O can be calculated.

$$\text{ADU(II)-H}_2\text{O} : N(O) = \{ (N(H)/N(U) - 13/3) \cdot (1/2) + 14/3 \} \cdot N(U) \quad (\text{A.3.1})$$

$$\text{ADU(III)-H}_2\text{O} : N(O) = \{ (N(H)/N(U) - 9/2) \cdot (1/2) + 9/2 \} \cdot N(U) \quad (\text{A.3.2})$$

$$\text{ADU(IV)-H}_2\text{O} : \text{N(O)} = \{ (\text{N(H)}/\text{N(U)} - 14/3) \cdot (1/2) + 13/3 \} \cdot \text{N(U)}$$

(A.3.3)

A.3 Atomic number Density of Water

Water reflected ADU-H₂O system consists fuel region and water reflector region. Temperature of the system is assumed to be 20°C so the density of the water in ADU-H₂O and reflector becomes 0.99820 g/cm³. The values of N(H) and N(O) in the reflector with this density are 0.066735[atoms/barn·cm], 0.033368[atoms/barn·cm].

A.4 Results of KENO-IV Calculation

Critical dimension searches on water-reflected ADU-H₂O were performed with KENO-IV program. KENO-IV calculated and printed out k_{eff}, standard deviation of k_{eff} and sphere radius. Table A.6.1 through Table A.8.6 lists these values.

A.5 Maximum Uranium Concentration of ADU-H₂O

ADU-H₂O with 0.0 of hydrogen/uranium atom ratio has the maximum uranium concentration. The maximum values calculated with AND program are listed in Table A.9. These values vary with uranium enrichment and composition of ADU.

References

- 1) E.H.P.Cordfunke, "On the Uranoates of Ammonium-II, X-ray Investigation of the Compounds in the System NH₃-UO₃-H₂O," J.Inorg.Nucl.Chem., Vol.25,pp.945 to 953 (1962)
- 2) Woolfrey,J.L., "The Effect of pH on the Properties of Ammonium Uranoate Precipitate with Gaseous Ammonia," AAEC/E397 (1977)

Table A.1 Composition of ADU(I), (II), (III) and (IV)

Type	Chemical formula	Theoretical density *1), g/cm ³	N / U atomic ratio	H / U atomic ratio
(I)	$\text{UO}_3 \cdot 2\text{H}_2\text{O}$	—	—	4.0
(II)	$3\text{UO}_3 \cdot \text{NH}_3 \cdot 5\text{H}_2\text{O}$	4.831	0.333	4.333
(III)	$2\text{UO}_3 \cdot \text{NH}_3 \cdot 3\text{H}_2\text{O}$	5.144	0.5	4.5
(IV)	$3\text{UO}_3 \cdot 2\text{NH}_3 \cdot 4\text{H}_2\text{O}$	5.201	0.667	4.667

* 1) Natural uranium (^{235}U enrichment 0.711 wt %)

Table A.2 Effect of pH precipitation on the types of ADU formed

p H	A D U Type *			
	I	II	III	IV
4.2		M	V M i	
4.6		M	V M i	
5.0		M	V M i	
5.9		M	V M i	
6.4		M	M	
6.9		M	M	M
7.1	M i	M	M	M
8.0	M i	M	M	M
8.6	M i	M	M	M
9.1			M	M
9.4			M	M
10.0			M	M

* Cordfunke's [1962] ADU compound

nomenclature is used

M = major, M i = minor

V M i = very minor

Table A.3.1 Atomic number densities of 3 wt% enriched ADU(II)-H₂O

10	137	2	
ADU2	235U:3(WT%)	, U:0.5(GU/CM**3)	
5	0	3	
4010010	4070140	4080160	49223350
6.28776E-02	4.21784E-04	3.46022E-02	3.84314E-05
ADU2	235U:3(WT%)	, U:0.6(GU/CM**3)	1.22692E-03
5	0	3	
4010010	4070140	4080160	49223380
6.21064E-02	5.06140E-04	3.48492E-02	4.61176E-05
ADU2	235U:3(WT%)	, U:0.8(GU/CM**3)	1.47230E-03
5	0	3	
4010010	4070140	4080160	49223350
6.05640E-02	6.74854E-04	3.53434E-02	6.14902E-05
ADU2	235U:3(WT%)	, U:1.0(GU/CM**3)	1.96307E-03
5	0	3	
4010010	4070140	4080160	49223380
5.90216E-02	8.43567E-04	3.58375E-02	7.68628E-05
ADU2	235U:3(WT%)	, U:1.2(GU/CM**3)	2.45384E-03
5	0	3	
4010010	4070140	4080160	49223350
5.74792E-02	1.01228E-03	3.63317E-02	9.22355E-05
ADU2	235U:3(WT%)	, U:1.5(GU/CM**3)	2.94461E-03
5	0	3	
4010010	4070140	4080160	49223380
5.51656E-02	1.26535E-03	3.70729E-02	1.15224E-04
ADU2	235U:3(WT%)	, U:2.0(GU/CM**3)	3.68076E-03
5	0	3	
4010010	4070140	4080160	49223350
5.13095E-02	1.68713E-03	3.83082E-02	1.53724E-04
ADU2	235U:3(WT%)	, U:2.5(GU/CM**3)	4.90768E-03
5	0	3	
4010010	4070140	4080160	49223380
4.74534E-02	2.10892E-03	3.95436E-02	1.92157E-04
ADU2	235U:3(WT%)	, U:3.0(GU/CM**3)	6.13459E-03
5	0	3	
4010010	4070140	4080160	49223350
4.35974E-02	2.53070E-03	4.07789E-02	2.30588E-04
ADU2	235U:3(WT%)	, U:3.57(GU/CM**3)	7.36151E-03
5	0	3	
4010010	4070140	4080160	49223380
3.92015E-02	3.01153E-03	4.21877E-02	2.74400E-04
			8.76020E-03

Units are all in atom/barn·cm

Nuclide ID numbers are as follows,

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
49223350	²³⁵ U
49223380	²³⁸ U

Units are all in atom/barn·cm

Nuclide ID numbers are as follows,

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
49223350	²³⁵ U
49223380	²³⁸ U

Table A.3.2 Atomic number densities of 4 wt% enriched ADU(II)-H₂O

10	137	2	
ADU2	235U:4(WT%)	, U:0.5(GU/CM**3)	
5	0	3	
4010010	4070140	4080160	49223350
6.28776E-02	4.21784E-04	3.46022E-02	3.84314E-05
ADU2	235U:3(WT%)	, U:0.6(GU/CM**3)	1.22692E-03
5	0	3	
4010010	4070140	4080160	49223380
6.21064E-02	5.06140E-04	3.48492E-02	4.61176E-05
ADU2	235U:3(WT%)	, U:0.8(GU/CM**3)	1.47230E-03
5	0	3	
4010010	4070140	4080160	49223350
6.05640E-02	6.74854E-04	3.53434E-02	6.14902E-05
ADU2	235U:3(WT%)	, U:1.0(GU/CM**3)	1.96307E-03
5	0	3	
4010010	4070140	4080160	49223380
5.90216E-02	8.43567E-04	3.58375E-02	7.68628E-05
ADU2	235U:3(WT%)	, U:1.2(GU/CM**3)	2.45384E-03
5	0	3	
4010010	4070140	4080160	49223350
5.74792E-02	1.01228E-03	3.63317E-02	9.22355E-05
ADU2	235U:3(WT%)	, U:1.5(GU/CM**3)	2.94461E-03
5	0	3	
4010010	4070140	4080160	49223380
5.51656E-02	1.26535E-03	3.70729E-02	1.15224E-04
ADU2	235U:3(WT%)	, U:2.0(GU/CM**3)	3.68076E-03
5	0	3	
4010010	4070140	4080160	49223350
5.13095E-02	1.68713E-03	3.83082E-02	1.53724E-04
ADU2	235U:3(WT%)	, U:2.5(GU/CM**3)	4.90768E-03
5	0	3	
4010010	4070140	4080160	49223380
4.74534E-02	2.10892E-03	3.95436E-02	1.92157E-04
ADU2	235U:3(WT%)	, U:3.0(GU/CM**3)	6.13459E-03
5	0	3	
4010010	4070140	4080160	49223350
4.35974E-02	2.53070E-03	4.07789E-02	2.30588E-04
ADU2	235U:3(WT%)	, U:3.57(GU/CM**3)	7.36151E-03
5	0	3	
4010010	4070140	4080160	49223380
3.92015E-02	3.01153E-03	4.21877E-02	2.74400E-04
			8.76020E-03

Table A.3.3 Atomic number densities of 5 wt% enriched ADU(II)-H₂OTable A.4.1 Atomic number densities of 3 wt% enriched ADU(III)-H₂O

10	137	2	235U:5(WT%) , U:0.5(GU/CM**3)		10	137	2	235U:3(WT%) , U:0.5(GU/CM**3)	
ADU2	0	3			*ADU3*	5	0		
4.010010	4.070140	4.080160	4.922350		4.010010	5	0	4.080160	4.922350
6.28766E-02	4.21891E-04	3.46025E-02	6.40223E-05	1.20162E-03	6.36627E-02	6.32676E-04	3.46784E-02	3.84314E-05	1.22692E-03
ADU2	235U:5(WT%) , U:0.6(GU/CM**3)				*ADU3*	235U:3(WT%) , U:0.6(GU/CM**3)			
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		4.010010	4.070140	4.080160	4.922350	4.922380
6.21052E-02	5.06270E-04	3.48496E-02	7.686.8E-05	1.44195E-03	6.30485E-02	7.59211E-04	3.49497E-02	4.61176E-05	1.47230E-03
ADU2	235U:5(WT%) , U:0.8(GU/CM**3)				*ADU3*	235U:3(WT%) , U:0.8(GU/CM**3)			
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		4.010010	4.070140	4.080160	4.922350	4.922380
6.05624E-02	6.75026E-04	3.53439E-02	1.02484E-04	1.92260E-03	6.38202E-02	1.01228E-03	3.54653E-02	6.14925E-05	1.94307E-03
ADU2	235U:5(WT%) , U:1.0(GU/CM**3)				*ADU3*	235U:3(WT%) , U:1.0(GU/CM**3)			
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		6.05918E-02	1.26535E-03	3.59900E-02	7.68868E-05	2.45384E-03
5.90196E-02	8.43783E-04	3.58382E-02	1.28105E-04	2.40324E-03	*ADU3*	235U:3(WT%) , U:1.2(GU/CM**3)			
ADU2	235U:5(WT%) , U:1.2(GU/CM**3)				5	0	3		
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		5.93634E-02	1.51842E-03	3.65146E-02	9.23335E-05	2.94461E-03
5.74768E-02	1.01254E-03	3.63324E-02	1.55726E-04	2.88389E-03	*ADU3*	235U:3(WT%) , U:1.5(GU/CM**3)			
ADU2	235U:5(WT%) , U:1.5(GU/CM**3)				5	0	3		
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		5.4010010	4.070140	4.080160	4.922350	4.922380
5.51626E-02	1.26567E-03	3.70739E-02	1.92177E-04	3.60487E-03	5.75208E-02	1.89803E-03	3.73015E-02	1.15294E-04	3.68076E-03
ADU2	235U:5(WT%) , U:2.0(GU/CM**3)				*ADU3*	235U:3(WT%) , U:2.0(GU/CM**3)			
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		5.4010010	4.070140	4.080160	4.922350	4.922380
5.13055E-02	1.68756E-03	3.83095E-02	2.56219E-04	4.80649E-03	5.44499E-02	2.53070E-03	3.86131E-02	1.53725E-04	4.90768E-03
ADU2	235U:5(WT%) , U:2.5(GU/CM**3)				*ADU3*	235U:3(WT%) , U:2.5(GU/CM**3)			
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		5.13789E-02	3.163337E-03	3.99246E-02	1.92157E-04	6.13459E-03
4.74485E-02	2.10946E-03	3.95452E-02	3.20262E-04	6.008114E-03	*ADU3*	235U:3(WT%) , U:3.0(GU/CM**3)			
ADU2	235U:5(WT%) , U:3.0(GU/CM**3)				5	0	3		
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		4.010010	4.070140	4.080160	4.922350	4.922380
4.35915E-02	2.53135E-03	4.07808E-02	3.84314E-04	7.20973E-03	4.83079E-02	3.79605E-03	4.12362E-02	2.30588E-04	7.36151E-03
ADU2	235U:5(WT%) , U:3.57(GU/CM**3)				*ADU3*	235U:3(WT%) , U:3.57(GU/CM**3)			
5	0	3			5	0	3		
4.010010	4.070140	4.080160	4.922350		4.010010	4.070140	4.080160	4.922350	4.922380
3.91944E-02	3.01230E-03	4.21895E-02	4.57533E-04	8.57958E-03	4.48070E-02	4.51730E-03	4.27314E-02	2.74400E-04	8.76020E-03

Units are all in atom/barn·cm

Nuclide ID numbers are as follows,

- 4010010 hydrogen,
- 4070140 nitrogen,
- 4080160 oxygen,
- 4922350 ²³⁵U
- 4922380 ²³⁸U

Units are all in atom/barn·cm

Nuclide ID numbers are as follows,

- 4010010 hydrogen,
- 4070140 nitrogen,
- 4080160 oxygen,
- 4922350 ²³⁵U
- 4922380 ²³⁸U

Table A.4.2 Atomic number densities of 4 wt% enriched ADU(III)-H₂OTable A.4.3 Atomic number densities of 5 wt% enriched ADU(III)-H₂O

10	137	2	
ADU3	235U:4(WTx) , U:0.5(GU/CM**3)		
5	0	3	
■	4.010010 4.070140 4.080160 4.922380		
■	6.36623E-02 6.32756E-04 3.46786E-02 5.12428E-05 1.21427E-03		
ADU3	235U:4(WTx) , U:0.6(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
6.30480E-02 7.59308E-04 3.4949E-02 6.14020E-05 1.45713E-03			
ADU3	235U:4(WTx) , U:0.8(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
6.18195E-02 1.01241E-03 3.54656E-02 8.19870E-05 1.94283E-03			
ADU3	235U:4(WTx) , U:1.0(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
6.05910E-02 1.26551E-03 3.59903E-02 1.02464E-04 2.42854E-03			
ADU3	235U:4(WTx) , U:1.2(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
5.93624E-02 1.51862E-03 3.65150E-02 1.22990E-04 2.91425E-03			
ADU3	235U:4(WTx) , U:1.5(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
5.75197E-02 1.89827E-03 3.73020E-02 1.53726E-04 3.64281E-03			
ADU3	235U:4(WTx) , U:2.0(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
5.44483E-02 2.53102E-03 3.86137E-02 2.04967E-04 4.85708E-03			
ADU3	235U:4(WTx) , U:2.5(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
5.13769E-02 3.16378E-03 3.99254E-02 2.56209E-04 6.07135E-03			
ADU3	235U:4(WTx) , U:3.0(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
4.83056E-02 3.79654E-03 4.12372E-02 3.07451E-04 7.28562E-03			
ADU3	235U:4(WTx) , U:3.57(GU/CM**3)		
5	0	3	
4.010010 4.070140 4.080160 4.922380			
4.48042E-02 4.51788E-03 4.27325E-02 3.65867E-04 8.66989E-03			

Units are all in atom/barn·cm
Nuclide ID numbers are as follows,

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
4922350	²³⁵ U
4922380	²³⁸ U

Units are all in atom/barn·cm
Nuclide ID numbers are as follows,

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
4922350	²³⁵ U
4922380	²³⁸ U

Table A.5.1 Atomic number densities of 3 wt% enriched ADU(IV)-H₂O

10	137	2	10	137	2				
ADU4	235U:3(WTx)	, U:0.5(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:0.5(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4080160	4922380			
6.39743E-02	8.43567E-04	3.45178E-02	3.84314E-05	1.22269E-03	6.39739E-02	8.435675E-04	3.45180E-02	5.12418E-05	1.21427E-03
ADU4	235U:3(WTx)	, U:0.6(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:0.6(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
6.34224E-02	1.01228E-03	3.47480E-02	4.61176E-05	1.47230E-03	6.34219E-02	1.01241E-03	3.47482E-02	6.14902E-05	1.45713E-03
ADU4	235U:3(WTx)	, U:0.8(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:0.8(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
6.23187E-02	1.34971E-03	3.52085E-02	6.14902E-05	1.96307E-03	6.23181E-02	1.34988E-03	3.52087E-02	8.19870E-05	1.94283E-03
ADU4	235U:3(WTx)	, U:1.0(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:1.0(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
6.12150E-02	1.68713E-03	3.56689E-02	7.68628E-05	2.45384E-03	6.12142E-02	1.68735E-03	3.56692E-02	1.02484E-04	2.42854E-03
ADU4	235U:3(WTx)	, U:1.2(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:1.2(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
6.01112E-02	2.02456E-03	3.61293E-02	9.22353E-05	2.94461E-03	6.01104E-02	2.02482E-03	3.61297E-02	1.22980E-04	2.91425E-03
ADU4	235U:3(WTx)	, U:1.5(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:1.5(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
5.84557E-02	2.53070E-03	3.68199E-02	1.15294E-04	3.680765E-03	5.84546E-02	2.53103E-03	3.68204E-02	1.53726E-04	3.64281E-03
ADU4	235U:3(WTx)	, U:2.0(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:2.0(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
5.56763E-02	3.37427E-03	3.79709E-02	1.53726E-04	4.907688E-03	5.56948E-02	3.37470E-03	3.79715E-02	2.04967E-04	4.85708E-03
ADU4	235U:3(WTx)	, U:2.5(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:2.5(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
5.29359E-02	4.21783E-03	3.91219E-02	1.92157E-04	6.13459E-03	5.29351E-02	4.21837E-03	3.91227E-02	2.56209E-04	6.07135E-03
ADU4	235U:3(WTx)	, U:3.0(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:3.0(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
5.01775E-02	5.06140E-03	4.02730E-02	2.30588E-04	7.36151E-03	5.01754E-02	5.06205E-03	4.02738E-02	3.07451E-04	7.28562E-03
ADU4	235U:3(WTx)	, U:3.57(GU/CM**3)	*ADU4*	235U:4(WTx)	, U:3.57(GU/CM**3)				
5	0	3	5	0	3				
4010010	4070140	4080160	4922380	4010010	4070140	4080160	4922380		
4.70319E-02	6.02307E-03	4.15851E-02	2.74400E-04	8.76020E-03	4.70293E-02	6.02384E-03	4.15862E-02	3.65867E-04	8.66988E-03

Units are all in atom/barn·cm
Nuclide ID numbers are as follows,

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
4922350	235U
4922380	238U

Units are all in atom/barn·cm
Nuclide ID numbers are as follows,

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
4922350	235U
4922380	238U

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
4922350	235U
4922380	238U

4010010	hydrogen,
4070140	nitrogen,
4080160	oxygen,
4922350	235U
4922380	238U

Table A.5.3 Atomic number densities of 5 wt% enriched ADU(IV)-H₂O

10	137	2	235U:5(WT%), U:0.5(GU/CM**3)	
ADU4	0	3	4070140 4080160 4922350 4922380	
6.39735E-02	8.43783E-02	3	3.45181E-02 6.40523E-05 1.20162E-03	
ADU4	0	3	235U:5(WT%), U:0.6(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
6.34215E-02	1.01254E-02	3	3.47484E-02 7.68628E-05 1.44195E-03	
ADU4	0	3	235U:5(WT%), U:0.8(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
6.23176E-02	1.35005E-02	3	3.52089E-02 1.024684E-04 1.92260E-03	
ADU4	0	3	235U:5(WT%), U:1.0(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
6.12135E-02	1.68757E-02	3	3.56695E-02 1.28105E-04 2.40324E-03	
ADU4	0	3	235U:5(WT%), U:1.2(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
6.01095E-02	2.02508E-02	3	3.61300E-02 1.53726E-04 2.88389E-03	
ADU4	0	3	235U:5(WT%), U:1.5(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
5.84535E-02	2.53135E-02	3	3.68208E-02 1.92157E-04 3.60487E-03	
ADU4	0	3	235U:5(WT%), U:2.0(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
5.56934E-02	3.37513E-02	3	3.79721E-02 2.56209E-04 4.80649E-03	
ADU4	0	3	235U:5(WT%), U:2.5(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
5.29334E-02	4.21891E-02	3	3.91234E-02 3.20262E-04 6.00811E-03	
ADU4	0	3	235U:5(WT%), U:3.0(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
5.01733E-02	5.06270E-02	3	4.02747E-02 3.84314E-04 7.20973E-03	
ADU4	0	3	235U:5(WT%), U:3.57(GU/CM**3)	
5	0	3	4070140 4080160 4922350 4922380	
4.70269E-02	6.02461E-02	3	4.15872E-02 4.57333E-04 8.57958E-03	

Units are all in atom/barn·cm
Nuclide ID numbers are as follows,

- 4010010 hydrogen,
- 4070140 nitrogen,
- 4080160 oxygen,
- 4922350 ²³⁵U
- 4922380 ²³⁸U

Table A. 6.1 The result of dimension search with KENO-IV
 (water-reflected ADU(II)-H₂O sphere, critical)

Enrichment (wt %)	Uranium concentration (g U/l)	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius (cm)	Sphere volume (l)	Uranium mass (kg)
3	400	0.986	—	—	—	—	—
	500		—	—	—	—	—
	600		0.98481	0.00274	71.416	1526	915.4
	800		0.98459	0.00294	39.465	257.5	206.0
	1000		0.98279	0.00334	32.142	139.1	139.1
	1200		0.98544*)	0.00258	28.673	98.74	118.5
	1500		0.98751	0.00341	25.853	72.38	108.6
	2000		0.98372	0.00446	24.561	62.06	124.1
	2500		0.98164	0.00457	24.491	61.53	153.8
	3000		0.98899	0.00416	25.164	66.75	200.2
	3570		0.98624	0.00412	26.351	76.64	273.6

*) 60000 histories

Table A. 6.2 The result of dimension search with KENO-IV
 (water-reflected ADU(II)-H₂O sphere, subcritical limit)

Enrichment (wt %)	Uranium concentration (g U/l)	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius (cm)	Sphere volume (l)	Uranium mass (kg)
3	400	0.965	—	—	—	—	—
	500		—	—	—	—	—
	600		0.96516	0.00253	59.431	879.3	527.6
	800		0.96447	0.00312	36.564	204.8	163.8
	1000		0.96411	0.00317	29.818	111.1	111.1
	1200		0.96428*)	0.00223	26.875	81.31	97.57
	1500		0.96562	0.00389	24.678	62.95	94.43
	2000		0.96747*)	0.00269	23.527	54.55	109.1
	2500		0.96559	0.00420	23.070	51.43	128.6
	3000		0.96571	0.00378	24.198	59.35	178.1
	3570		0.96728	0.00436	25.079	66.07	235.9

*) 60000 histories

Table A. 6.3 The result of dimension search with KENO-IV
 (water-reflected ADU(II)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
4	400	0.986	—	—	—	—	—
	500		0.98567	0.00283	45.853	403.8	201.9
	600		0.98754	0.00322	34.868	177.6	106.5
	800		0.98373	0.00405	28.027	92.22	73.77
	1000		0.98487	0.00336	24.688	63.03	63.03
	1200		0.98610*)	0.00328	22.926	50.47	60.57
	1500		0.98511	0.00450	21.863	43.77	65.66
	2000		0.98870	0.00467	20.825	37.83	75.66
	2500		0.98860*)	0.00305	21.355	40.79	102.0
	3000		0.98755	0.00425	21.936	44.21	132.6
	3570		0.98798	0.00422	23.329	53.18	189.9

*) 60000 histories

Table A. 6.4 The result of dimension search with KENO-IV
 (water-reflected ADU(II)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
4	400	0.965	—	—	—	—	—
	500		0.96353	0.00306	40.000	268.1	134.0
	600		0.96710	0.00352	32.587	145.0	86.97
	800		0.96565	0.00377	25.705	71.14	56.92
	1000		0.96423*)	0.00268	23.499	54.35	54.35
	1200		0.96700*)	0.00292	21.872	43.83	52.59
	1500		0.96415*)	0.00318	20.851	37.97	56.96
	2000		0.96716*)	0.00323	20.265	34.86	69.72
	2500		0.96521	0.00464	20.585	36.54	91.34
	3000		0.96395	0.00403	21.054	39.09	117.3
	3570		0.96657	0.00441	22.380	46.95	167.6

*) 60000 histories

Table A. 6.5 The result of dimension search with KENO-IV
 (water-reflected ADU(II)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
5	400	0.986	0.98879	0.00291	41.586	301.3	120.5
	500		0.98755	0.00326	31.376	129.4	64.69
	600		0.98883	0.00415	27.002	82.45	49.48
	800		0.98584*)	0.00274	23.233	52.53	42.02
	1000		0.98886	0.00409	20.490	41.57	41.57
	1200		0.98576*)	0.00290	20.284	34.96	48.95
	1500		0.98431	0.00428	19.803	32.53	48.79
	2000		0.98592*)	0.00340	19.500	31.06	62.12
	2500		0.98390	0.00438	19.467	30.90	77.25
	3000		0.98435	0.00472	20.194	34.49	103.5
	3570		0.98849	0.00451	21.625	42.36	151.2

*) 60000 histories

Table A. 6.6 The result of dimension search with KENO-IV
 (water-reflected ADU(II)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
5	400	0.965	0.96266	0.00314	37.242	216.4	86.55
	500		0.96723	0.00354	39.531	107.9	53.94
	600		0.96218	0.00360	25.538	69.77	41.86
	800		0.96711	0.00380	22.372	46.90	37.52
	1000		0.96442*)	0.00324	20.187	34.46	34.46
	1200		0.96237*)	0.00275	19.307	30.15	36.18
	1500		0.96629	0.00468	18.644	27.15	40.72
	2000		0.96498*)	0.00323	18.510	26.56	53.13
	2500		0.96725	0.00457	18.804	27.85	69.63
	3000		0.96661*)	0.00303	19.653	31.80	95.39
	3570		0.96896	0.00416	20.967	38.61	137.8

*) 60000 histories

Table A. 7.1 The result of dimension search with KENO-IV
 (water-reflected ADU(III)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
3	400	0.986	—	—	—	—	—
	500		—	—	—	—	—
	600		0.98809	0.00244	87.025	2761	1656
	800		0.98601	0.00322	41.272	294.5	235.6
	1000		0.98604	0.00302	32.724	146.8	146.8
	1200		0.98788*)	0.00262	29.438	106.9	128.2
	1500		0.98824	0.00404	26.319	76.37	114.5
	2000		0.98815	0.00395	24.537	61.88	123.8
	2500		0.98722	0.00355	23.611	55.14	137.8
	3000		0.98721	0.00387	23.970	57.69	173.1
	3570		0.98825	0.00366	24.594	62.31	222.5

*) 60000 histories

Table A. 7.2 The result of dimension search with KENO-IV
 (water-reflected ADU(III)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
3	400	0.965	—	—	—	—	—
	500		—	—	—	—	—
	600		0.96335	0.00227	64.074	1102	661.1
	800		0.96524	0.00304	39.019	248.8	199.1
	1000		0.96590	0.00338	31.051	125.4	125.4
	1200		0.96640*)	0.00242	27.493	87.05	104.5
	1500		0.96507	0.00357	24.782	63.75	95.63
	2000		0.96594	0.00403	22.996	50.94	101.9
	2500		0.96095	0.00408	22.538	47.96	119.9
	3000		0.96663	0.00442	23.033	51.18	153.6
	3570		0.96391*)	0.00274	23.727	55.95	199.7

*) 60000 histories

Table A. 7.3 The result of dimension search with KENO-IV
 (water-reflected ADU(III)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius (cm)	Sphere volume (l)	Uranium mass (kg)
4	400	0.986	—	—	—	—	—
	500		0.98689	0.00275	47.880	459.8	229.9
	600		0.98405	0.00314	36.007	195.5	117.3
	800		0.98672*)	0.00239	28.070	92.64	74.11
	1000		0.98622*)	0.00250	24.739	63.42	63.42
	1200		0.98435*)	0.00301	23.090	51.57	61.88
	1500		0.98585	0.00390	21.607	42.25	63.38
	2000		0.98611**)	0.00195	20.644	36.85	73.71
	2500		0.98771**)	0.00227	20.585	36.54	91.34
	3000		0.98581**)	0.00221	20.758	37.47	112.4

*) 60000 histories

**) 120000 histories

Table A. 7.4 The result of dimension search with KENO-IV
 (water-reflected ADU(III)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius (cm)	Sphere volume (l)	Uranium mass (kg)
4	400	0.965	—	—	—	—	—
	500		0.96515	0.00305	42.937	331.6	165.8
	600		0.96410	0.00315	33.315	154.9	92.93
	800		0.96365*)	0.00244	26.157	74.96	59.97
	1000		0.96594	0.00411	23.450	54.02	54.02
	1200		0.96595*)	0.00296	21.969	44.41	53.30
	1500		0.96737*)	0.00291	20.844	38.21	57.3
	2000		0.96808	0.00454	19.756	32.30	64.60
	2500		0.96523	0.00435	19.442	30.78	76.96
	3000		0.96439	0.00438	19.460	30.87	92.61
	3570		0.96321	0.00436	20.679	37.04	132.2

*) 60000 histories

Table A. 7.5 The result of dimension search with KENO-IV
(water-reflected ADU(III)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
5	400		—	—	—	—	—
	500		—	—	—	—	—
	600	0.98438	0.98438	0.00376	27.630	88.36	53.01
	800		0.98628	0.00357	23.382	53.55	42.84
	1000	0.986	0.98913	0.00416	21.460	41.40	41.40
	1200		0.98849*)	0.00293	20.202	35.54	41.44
	1500		0.98298	0.00364	19.127	29.31	43.97
	2000		0.98612	0.00483	18.852	28.06	56.13
	2500		0.98541	0.00422	18.883	28.20	70.51
	3000		0.98571	0.00456	19.195	29.62	88.87
	3570		0.98155	0.00445	19.889	32.96	117.65

*) 60000 histories

Table A. 7.6 The result of dimension search with KENO-IV
(water-reflected ADU(III)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
5	400		0.96252	0.00307	38.568	240.3	96.12
	500		0.96430	0.00784	30.009	113.2	56.60
	600	0.96427	0.96427	0.00368	25.745	71.48	42.89
	800		0.96756	0.00398	22.156	45.56	36.45
	1000	0.965	0.96360*)	0.00292	20.512	36.15	36.15
	1200		0.96583*)	0.00282	19.373	30.46	36.55
	1500		0.96495*)	0.00280	18.499	26.52	39.78
	2000		0.96603*)	0.00300	18.244	25.44	50.87
	2500		0.96838	0.00527	18.019	24.51	61.27
	3000		0.96469	0.00429	18.537	26.68	80.04
	3570		0.96406	0.00406	18.960	28.55	101.9

*) 60000 histories

Table A. 8.1 The result of dimension search with KENO-IV
 (water-reflected ADU(IV)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
3	400	0.986	—	—	—	—	—
	500		—	—	—	—	—
	600		0.98724	0.00185	104.31	4754	2852
	800		0.98755	0.00258	43.326	340.7	272.5
	1000		0.98667	0.00317	34.190	167.4	167.4
	1200		0.98692*)	0.00243	29.962	112.7	135.2
	1500		0.98731	0.00354	27.066	83.05	124.6
	2000		0.98803*)	0.00254	24.683	62.99	126.0
	2500		0.98602**)	0.00209	23.915	57.29	143.2
	3000		0.98554**)	0.00194	23.878	57.03	171.1
	3570		0.98651**)	0.00192	24.533	61.85	220.8

*) 60000 histories

**) 120000 histories

Table A. 8.2 The result of dimension search with KENO-IV
 (water-reflected ADU(IV)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
3	400	0.965	—	—	—	—	—
	500		—	—	—	—	—
	600		0.96574	0.00197	77.617	1959	1175
	800		0.96607	0.00300	39.424	256.7	205.3
	1000		0.96508*)	0.00244	31.650	132.8	132.8
	1200		0.96494*)	0.00242	28.150	93.44	112.1
	1500		0.96580*)	0.00240	25.378	68.46	102.7
	2000		0.96709*)	0.00282	23.435	53.84	107.7
	2500		0.96527**)	0.00195	22.664	48.76	121.9
	3000		0.96523**)	0.00215	22.819	49.77	149.3
	3570		0.96573**)	0.00192	23.279	52.84	188.6

*) 60000 histories

**) 120000 histories

Table A. 8.3 The result of dimension search with KENO-IV
 (water-reflected ADU(IV)-H₂O sphere, critical)

Enrichment (wt %)	Uranium concentration (g U/l)	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius (cm)	Sphere volume (l)	Uranium mass (kg)
4	400	0.986	—	—	—	—	—
	500		0.98710	0.00301	51.400	568.8	284.4
	600		0.98532	0.00330	37.679	224.1	134.4
	800		0.98268	0.00333	28.218	94.12	75.29
	1000		0.98285	0.00378	25.206	67.08	67.08
	1200		0.98463*)	0.00275	23.461	54.091	64.91
	1500		0.98760*)	0.00309	21.716	42.90	64.35
	2000		0.98727	0.00458	20.819	37.80	75.60
	2500		0.98805	0.00458	20.449	35.82	89.55
	3000		0.98612	0.00353	20.748	37.41	112.2
	3570		0.98528	0.00434	21.411	41.11	146.8

*) 60000 histories

Table A. 8.4 The result of dimension search with KENO-IV
 (water-reflected ADU(IV)-H₂O sphere, subcritical limit)

Enrichment (wt %)	Uranium concentration (g U/l)	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius (cm)	Sphere volume (l)	Uranium mass (kg)
4	400	0.965	—	—	—	—	—
	500		0.96513	0.00260	44.835	377.5	188.8
	600		0.96297	0.00336	34.407	170.6	102.4
	800		0.96552	0.00305	26.936	81.86	65.49
	1000		0.96792	0.00336	24.220	59.51	59.51
	1200		0.96268	0.00263	21.920	44.12	52.94
	1500		0.96299	0.00414	20.913	38.31	57.47
	2000		0.96420**)	0.00222	19.898	33.00	66.00
	2500		0.96480**)	0.00206	19.555	31.32	78.31
	3000		0.96676	0.00430	19.870	32.86	98.58
	3570		0.96354*)	0.00310	20.029	33.66	120.2

*) 60000 histories

**) 120000 histories

Table A. 8.5 The result of dimension search with KENO-IV
 (water-reflected ADU(IV)-H₂O sphere, critical)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
5	400	0.986	0.98738	0.00268	44.641	372.6	149.1
	500		0.98316	0.00324	32.676	146.1	73.07
	600		0.98433	0.00378	27.858	90.56	54.34
	800		0.98190	0.00424	23.546	54.68	43.75
	1000		0.98387	0.00386	21.371	40.88	40.88
	1200		0.98400*)	0.00308	20.306	35.07	42.09
	1500		0.99096	0.00503	19.388	30.53	45.79
	2000		0.98785*)	0.00298	18.766	27.68	55.36
	2500		0.98859	0.00422	18.710	27.44	68.59
	3000		0.98617*)	0.00299	18.952	28.51	85.54
	3570		0.98863	0.00436	19.889	32.96	117.7

*) 60000 histories

Table A. 8.6 The result of dimension search with KENO-IV
 (water-reflected ADU(IV)-H₂O sphere, subcritical limit)

Enrichment [wt %]	Uranium concentration [g U/l]	Desired k_{eff}	k_{eff}	$\pm \sigma$	Sphere radius [cm]	Sphere volume [l]	Uranium mass [kg]
5	400	0.965	0.96274	0.00261	39.713	262.0	104.9
	500		0.96573	0.00322	29.988	113.0	56.48
	600		0.96369	0.00330	26.354	76.67	46.00
	800		0.96868	0.00376	22.585	48.26	38.60
	1000		0.96745	0.00389	20.620	36.72	36.72
	1200		0.96429*)	0.00271	19.461	30.87	37.05
	1500		0.96757	0.00477	18.615	27.02	40.53
	2000		0.96715*)	0.00292	18.033	24.56	49.13
	2500		0.96601*)	0.00314	18.169	25.12	62.81
	3000		0.96717*)	0.00331	18.482	26.44	79.33
	3570		0.96554*)	0.00302	18.570	26.82	95.76

*) 60000 histories

Table A.9 Maximum uranium concentration and minimum H/U atomic ratio of ADU-H₂O

Type	²³⁵ U enrichment wt %	Maximum uranium concentration gU/cm ³	Minimum H/U atomic ratio
(II)	3	3.5727	
	4	3.5723	4.3333
	5	3.5718	
(III)	3	3.8068	
	4	3.8063	4.5000
	5	3.8058	
(IV)	3	3.8510	
	4	3.8506	4.6667
	5	3.8501	