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PORTSMOUTH GASEOUS DIFFUSION PLANT

Estimated Critical Conditions for UF_4-Oil Systems in Fully Oil-Reflected Spherical Geometry

M. J. Plaster

May 1997

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Summary

Paraffinic oil has been exposed to UF_6 gas in seal exhaust pumps and cascade equipment at the Portsmouth Gaseous Diffusion Plant. The resulting mixture is more nuclearly reactive than mixtures of UO_2F_2 and H_2O and is not bounded by the subcritical mass limits presented in several nuclear criticality safety guides. The purpose of this analysis is to determine several critical parameters; specifically, 1) k_∞ and the critical mass for several enrichments and moderation levels and 2) the mass limits for these mixtures.

The estimated critical masses for the UF_4-oil systems are smaller than for the UO_2F_2-H_2O systems. The suggested mass limits for the UF_4-oil systems are 0.240, 0.280, 0.350, 0.430, 0.670, and 1.170 kg ^{235}U for enrichments of 100, 50, 20, 10, 5, and 3 wt. % ^{235}U respectively.

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1.0 Introduction

Paraffinic oil has been exposed to UF_6 gas in seal exhaust pumps and cascade equipment at the Portsmouth Gaseous Diffusion Plant.[1] When the UF_6 gas reacts with paraffinic oil, the resulting mixture is more nuclearly reactive than mixtures of UO_2F_2 and H_2O, due to the higher hydrogen density of the oil as compared to H_2O, which increases the uranium density at all moderation levels. Therefore, oily mixtures of uranium-bearing material are not bounded from a nuclear criticality safety perspective by the subcritical mass limits for mixtures of UO_2F_2 and H_2O presented in various nuclear criticality safety guides. Hence, the mass limits for these oily mixtures need to be determined.

The purpose of this analysis is to investigate several critical parameters for mixtures of UF_4 and oil; specifically, to 1) determine k_∞ and estimate the critical masses for several enrichments and moderation levels, and 2) determine mass limits for these mixtures.

Initial scoping calculations were performed with the unvalidated PC version of SCALE 4.3.[2] Final confirmation calculations were performed with a validated version of SCALE 4.3.[3]

2.0 Products of Reaction of UF_6 with Paraffinic Oil

UF_6 gas is reactive with liquid hydrocarbons, *e.g.*, paraffinic oil. At the operating temperatures and pressures of the cascade, most of the reactions between the liquid hydrocarbons and UF_6 gas produce UF_4, HF, and hydrofluorocarbons.[4] One of the theoretical reactions that produce UF_4 is the complete conversion of the paraffinic oil to the corresponding fluorocarbon, which is expressed as:

$$H\left[CH_2\right]_n H(l) + (2n+2)UF_6(g) \rightarrow F\left[CF_2\right]_n F(l) + (2n+2)HF(g) + (2n+2)UF_4(s). \qquad (2.0.1)$$

Another theoretical reaction is the complete reaction of UF_6 with the paraffinic oil, which is expressed as:

$$H\left[CH_2\right]_n H(l) + (3n+1)UF_6(g) \rightarrow nCF_4(g) + (2n+2)HF(g) + (3n+1)UF_4(s). \qquad (2.0.2)$$

If water vapor or oxidation products are present in the paraffinic oil, UO_2F_2 and HF may be formed.[5] UF_4 and UO_2F_2 are both essentially insoluble in liquid hydrocarbons;[5,6] therefore, the UF_4-oil systems will typically have higher uranium densities than compared to the UO_2F_2-oil systems at all moderation levels. In general, the UO_2F_2-oil systems are bounded by the UF_4-oil systems due to the higher uranium density of UF_4.

In this analysis the reaction product of UF_6 and paraffinic oil is assumed to be a mixture of the paraffinic oil and UF_4. This assumption provides the highest system hydrogen density, thus making the system more nuclearly reactive (See Section 2.2).

2.1 UF_4-Oil Mixture Density

The volume additive method for calculating densities for the UF_4-oil systems is applicable, because UF_4 is essentially insoluble in oil.[5,6] The material densities are calculated as a function of the H/U ratio. The H/U ratio for a mixture of UF_4 and oil is:

$$\frac{H}{U} = \frac{\gamma \; ND^{oil}}{ND^{UF_4}}, \tag{2.1.1}$$

where,

γ = number of hydrogen atoms per molecule of oil, and
ND^x = number density of material x.

The number densities for UF_4 and oil in molecules per cm^3 are calculated as:

$$ND^{oil} = \frac{v_f \, \rho_{oil} \, A_0}{MW_{oil}}, and \tag{2.1.2}$$

$$ND^{UF_4} = \frac{(1-v_f)\rho_{UF_4} A_0}{MW_{UF_4}}, \tag{2.1.3}$$

where,

v_f = oil density multiplier (volume fraction),
ρ_x = density of material x,
A_0 = Avogadro's Number ($6.0221367x10^{23}$ "entities"/mole),
MW_x = Molecular weight of material x.

Inserting Equations 2.1.2 and 2.1.3 into Equation 2.1.1, and upon simplification yields:

$$\frac{H}{U} = \frac{\gamma \nu_f \rho_{oil} MW_{UF_4}}{(1 - \nu_f) \rho_{UF_4} MW_{oil}}. \tag{2.1.4}$$

Solving the above equation for the oil density multiplier (ν_f) yields:

$$\nu_f = \frac{H}{U}\left[\gamma\left(\frac{\rho_{oil}}{\rho_{UF_4}}\right)\left(\frac{MW_{UF_4}}{MW_{oil}}\right) + \frac{H}{U}\right]^{-1}. \tag{2.1.5}$$

The oil density for a given H/U ratio is calculated by multiplying the oil density by the oil density multiplier. The UF_4 density for a given H/U ratio is calculated by multiplying the crystalline density of UF_4 (6.7 g/cm^3)[5,6] by the quantity one minus the oil density multiplier.

2.2 Selection of Hydrocarbon to Represent Oil

Oil is a mixture of relatively pure hydrocarbons with impurities of other organic compounds. Of all the organic molecules, paraffins have the highest H/C ratio. The moderation provided by each of the various organic compounds is dependent on this ratio and the density of the compound. As shown in Table-2.2.1 and Figure-2.2.1, the paraffin with the largest hydrogen density is $C_{17}H_{36}$. Also, as shown in Table-2.2.1 the density increases and the H/C ratio decreases as the carbon chains become longer.

The melting points of the paraffins increase as the carbon chains become longer. The longest carbon chain in Table-2.2.1, $C_{43}H_{88}$, has a melting point of approximately 85.5 °C.[7] Even though the paraffin densities increase as the carbon chains become longer, the use of the paraffins becomes less suitable as a lubricant due to the higher melting points, and are omitted from this analysis.

"The effective molecular weight of a typical vacuum pump oil is approximately 400, suggesting that the average material is $C_{29}H_{60}$."[5] A typical pump oil, *e.g.*, Rarus 929, has a density of 0.87 g/ml.[5] The hydrogen density for this typical oil is 0.076898 atoms per barn·cm, compared to 0.066856 atoms per barn·cm for H_2O. The hydrogen density for this oil is larger than for the pure paraffins presented in Table-2.2.1 because; 1) oils contain impurities which increase the density, and 2) the value for H/C is over predicted by assuming oil is a pure paraffin. Assuming oil is $C_{29}H_{60}$ with a density of 0.87 g/ml is conservative from a nuclear criticality safety perspective, because this assumed paraffinic oil will have a higher hydrogen density than the paraffins presented in Table-2.2.1.

The hydrogen density affects the minimum critical mass more than the carbon density, because hydrogen more effectively decreases the energy of neutrons than carbon. Carbon does have a smaller absorption cross section than hydrogen, but the downscatering properties of hydrogen outweigh the difference in absorption cross sections. This may be shown by comparing the critical radii of spheres reflected by 30 cm of $C_{29}H_{60}$ for a mixture of; 1) $^{235}UF_4$ and $C_{29}H_{60}$ at a C/X$\approx$222 (ρ_C=0.731867 g C/cm^3, H/X=460), and 2) $^{235}UF_4$ and C at the same carbon density. The calculated critical radius for the $^{235}UF_4$ and $C_{29}H_{60}$ mixture is approximately 12.9308 cm compared to approximately 100.873 cm for the $^{235}UF_4$ and C mixture.

The critical radii searches were performed with the unvalidated PC version of the SCALE 4.3 XSDRNPM code,[8] with cross section preprocessing by the CSASI Module.[9] The 27 group ENDF-B/IV cross section set was used for these calculations.[10] The input decks are presented in Appendix A.

Table-2.2.1: Density and Hydrogen Density of Various Paraffins.

Compound	Density[7,11] [g/cm^3]	H Density [H atoms per barn·cm]	Compound	Density[7,11] [g/cm^3]	H Density [H atoms per barn·cm]
C_5H_{12}	0.6262	0.062721	$C_{17}H_{36}$	0.7767	0.070023
C_6H_{14}	0.6594	0.064512	$C_{18}H_{38}$	0.7767	0.06984
C_7H_{16}	0.6838	0.065753	$C_{19}H_{40}$	0.7776	0.069756
C_8H_{18}	0.7025	0.066664	$C_{20}H_{42}$	0.7777	0.069617
C_9H_{20}	0.7176	0.067388	$C_{21}H_{44}$	0.7782	0.069527
$C_{10}H_{22}$	0.7301	0.067983	$C_{22}H_{46}$	0.7782	0.069405
$C_{11}H_{24}$	0.7402	0.068442	$C_{23}H_{48}$	0.7785	0.06932
$C_{12}H_{26}$	0.749	0.068849	$C_{24}H_{50}$	0.7786	0.069227
$C_{13}H_{28}$	0.7563	0.069171	$C_{26}H_{54}$	0.7783	0.069019
$C_{14}H_{30}$	0.7627	0.069455	$C_{30}H_{62}$	0.7795	0.068834
$C_{15}H_{32}$	0.7684	0.06971	$C_{36}H_{74}$	0.7795	0.068518
$C_{16}H_{34}$	0.7733	0.069922	$C_{43}H_{88}$	0.7812	0.06841

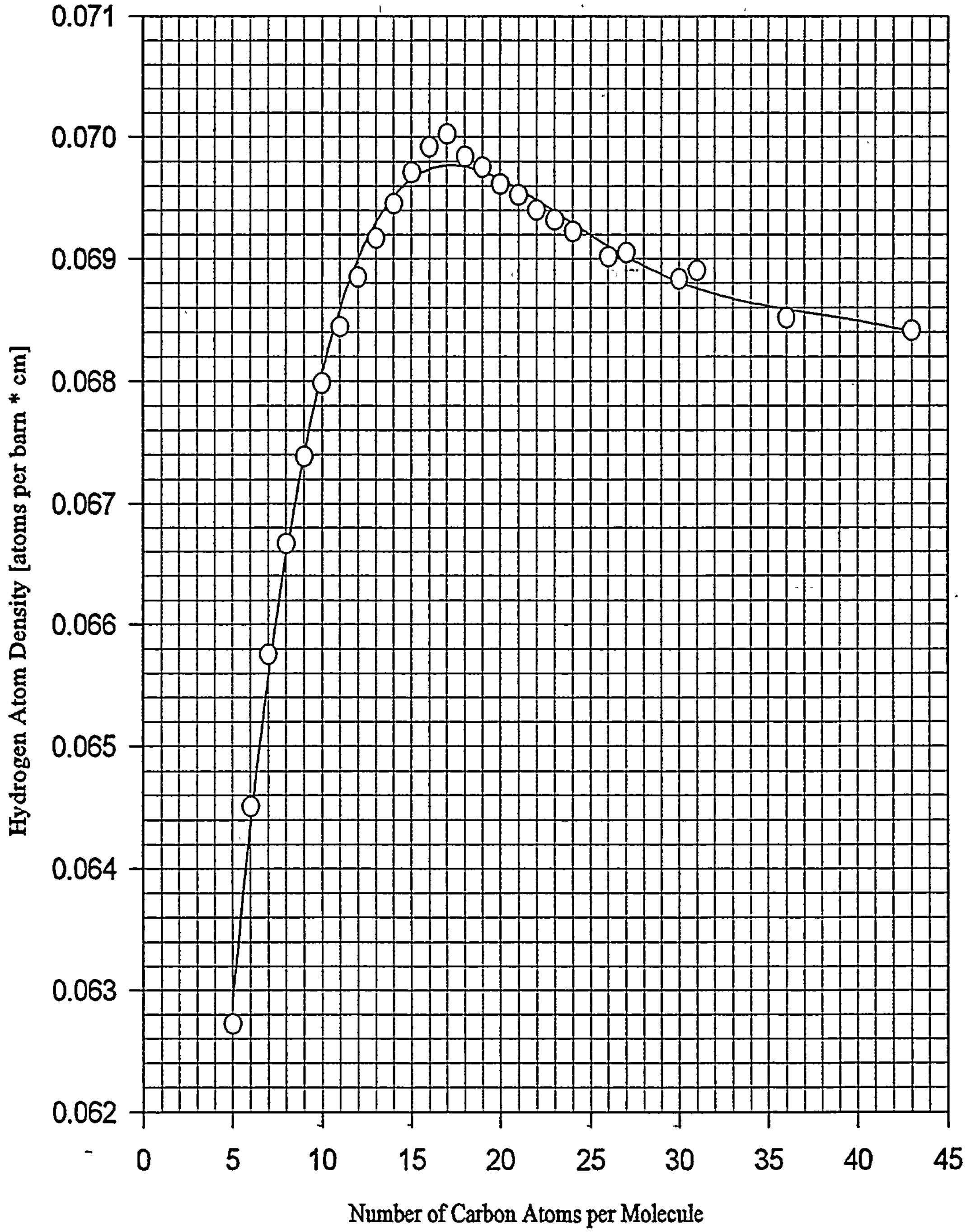

Figure-2.2.1: Hydrogen Density of Paraffins.

3.0 Infinite Multiplication Factor for UF_4-Oil Systems

The infinite multiplication factor, k_∞, yields important information about the reactivity of a system. It indicates 1) where criticality is possible, 2) the moderation region where peak reactivity occurs (minimum critical volume), and 3) the reactivity characteristics of under-moderated and over-moderated systems.

The k_∞ calculations were performed with the unvalidated version of the PC SCALE 4.3 CSAS1X Module.[9] The 27 group ENDF-B/IV cross section set was used for these calculations. The k_∞ values for the various H/X values and ^{235}U enrichments are presented in Table-3.0.1 and Figure-3.0.1. An example CSAS1X input deck is presented in Appendix A.

The k_∞ values calculated with the CSAS1X Module were compared to the values calculated using the validated version of the CSAS25 Module.[9] The CSAS25 Module does not have an option for calculating k_∞ values; therefore, an infinite system was approximated as a 10-meter mirror reflected cube. The CSAS25 results are in close agreement with the CSAS1X results as shown in Table-3.0.2. The 27 group ENDF-B/IV cross sections were used for the CSAS25 calculations. An example input deck is presented in Appendix A.

3.1 Estimated Critical Masses

A series of critical radius searches for $C_{29}H_{60}$ reflected spheres was performed to estimate the critical masses for the UF_4-oil system for various ^{235}U enrichments and moderation levels. The spheres were reflected by 30 cm of $C_{29}H_{60}$. The searches were performed with the unvalidated PC version of the SCALE 4.3 XSDRNPM code, with cross section preprocessing by the CSASI Module. The 27 group ENDF-B/IV cross section set was used for these calculations. The estimated minimum critical mass for the various enrichments occurs at an $H/X \approx 500$ as shown in Table-3.1.1, Figure-3.1.1, and Tables-B.1-B.6 in Appendix B. Several of the estimated critical conditions were modeled using the validated SCALE 4.3 CSAS25 Module to confirm the XSDRNPM results. The confirmation results are presented in Table-3.1.2.

Table-3.0.1: K_∞ for Various H/X Ratios and ^{235}U Enrichments.

H/X	K_∞					
	^{235}U Enrichment					
	3	5	10	20	50	100
5	0.6678	0.8648	1.1438	1.3893	1.6309	1.8030
10	0.7482	0.9528	1.2167	1.4317	1.6391	1.8066
20	0.8719	1.0774	1.3198	1.5063	1.6848	1.8420
50	1.0792	1.2683	1.4722	1.6210	1.7631	1.8916
100	1.2214	1.3871	1.5576	1.6785	1.7946	1.8938
200	1.3077	1.4454	1.5823	1.6774	1.7693	1.8384
300	1.3196	1.4400	1.5577	1.6390	1.7170	1.7700
400	1.3073	1.4150	1.5194	1.5912	1.6594	1.7022
450	1.2969	1.3994	1.4984	1.5664	1.6306	1.6695
500	1.2849	1.3827	1.4769	1.5416	1.6021	1.6378
600	1.2580	1.3476	1.4336	1.4925	1.5468	1.5772
700	1.2291	1.3119	1.3910	1.4450	1.4942	1.5205
1000	1.1417	1.2086	1.2722	1.3154	1.3531	1.3714
1500	1.0113	1.0612	1.1085	1.1400	1.1661	1.1777
2000	0.9042	0.9433	0.9801	1.0043	1.0235	1.0316

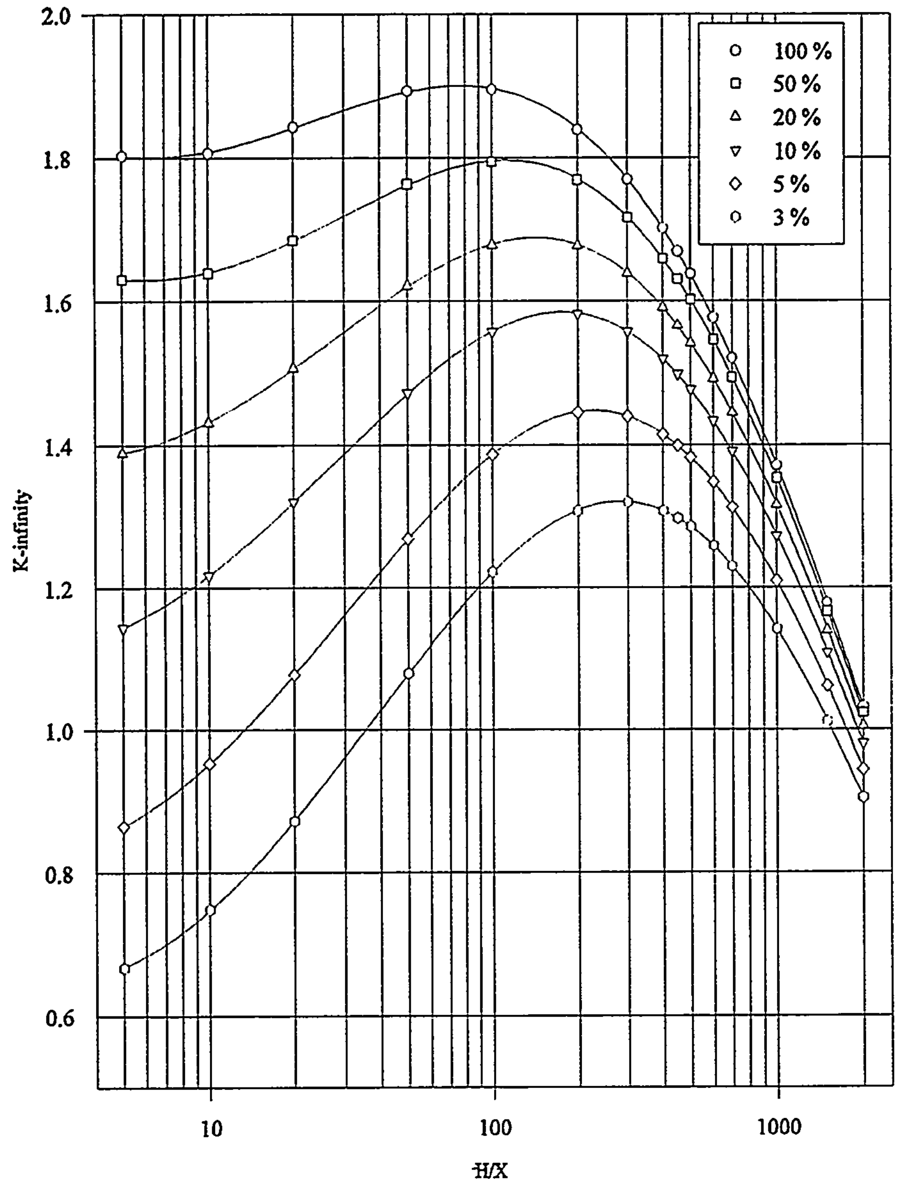

Figure-3.0.1: K_∞ as a Function of H/X for Various ^{235}U Enrichments.

Table-3.0.2: Comparison of k_∞ Calculated by the CSAS1X and CSAS25 Modules for Various Enrichments and H/X Ratios.

^{235}U Enrichment [wt. %]	Calculational Sequence	k_∞		
		H/X		
		10	100	1000
3	CSAS1X	0.7482	1.2214	1.1417
	CSAS25	0.7478 ± 0.0013	1.2219 ± 0.0017	1.1418 ± 0.0011
5	CSAS1X	0.9528	1.3871	1.2086
	CSAS25	0.9509 ± 0.0014	1.3892 ± 0.0017	1.2085 ± 0.0012
10	CSAS1X	1.2167	1.5576	1.2722
	CSAS25	1.2173 ± 0.0019	1.5573 ± 0.0017	1.2762 ± 0.0012
20	CSAS1X	1.4317	1.6785	1.3154
	CSAS25	1.4332 ± 0.0017	1.6791 ± 0.0018	1.3131 ± 0.0013
50	CSAS1X	1.6391	1.7946	1.3531
	CSAS25	1.6371 ± 0.0018	1.7928 ± 0.0016	1.3555 ± 0.0013
100	CSAS1X	1.8066	1.8938	1.3714
	CSAS25	1.8056 ± 0.0018	1.8935 ± 0.0019	1.3706 ± 0.0013

Table-3.1.1: H/X Ratio where Minimum Critical Mass Occurs and the Estimated Critical Mass for Various ^{235}U Enrichments.

Enrichment [wt. % ^{235}U]	H/X where Estimated Minimum Critical Mass Occurs	Estimated Critical Mass [Kg U]	Estimated Critical Mass [Kg ^{235}U]
100	470	0.583	0.583
50	480	1.29	0.645
20	475	3.95	0.790
10	500	10.1	1.01
5	535	31.0	1.55
3	520	90.2	2.71

Table-3.1.2: $K_{eff} \pm \sigma$ Calculated Using the Validated CSAS25 Module.

H/X	$k_{eff} \pm \sigma$	H/X	$k_{eff} \pm \sigma$
3 wt. % ^{235}U		5 wt. % ^{235}U	
100	0.9992 ± 0.0018	100	0.9946 ± 0.0019
520	0.9977 ± 0.0016	535	0.9989 ± 0.0018
1000	1.0004 ± 0.0014	1000	1.0016 ± 0.0015
10 wt. % ^{235}U		20 wt. % ^{235}U	
100	0.9975 ± 0.0021	100	0.9955 ± 0.0024
500	1.0032 ± 0.0021	475	1.0018 ± 0.0022
1000	0.9965 ± 0.0016	1000	1.0002 ± 0.0018
50 wt. % ^{235}U		100 wt. % ^{235}U	
100	0.9984 ± 0.0024	100	0.9955 ± 0.0024
480	0.9929 ± 0.0023	470	1.0003 ± 0.0022
1000	0.9975 ± 0.0017	1000	0.9987 ± 0.0018

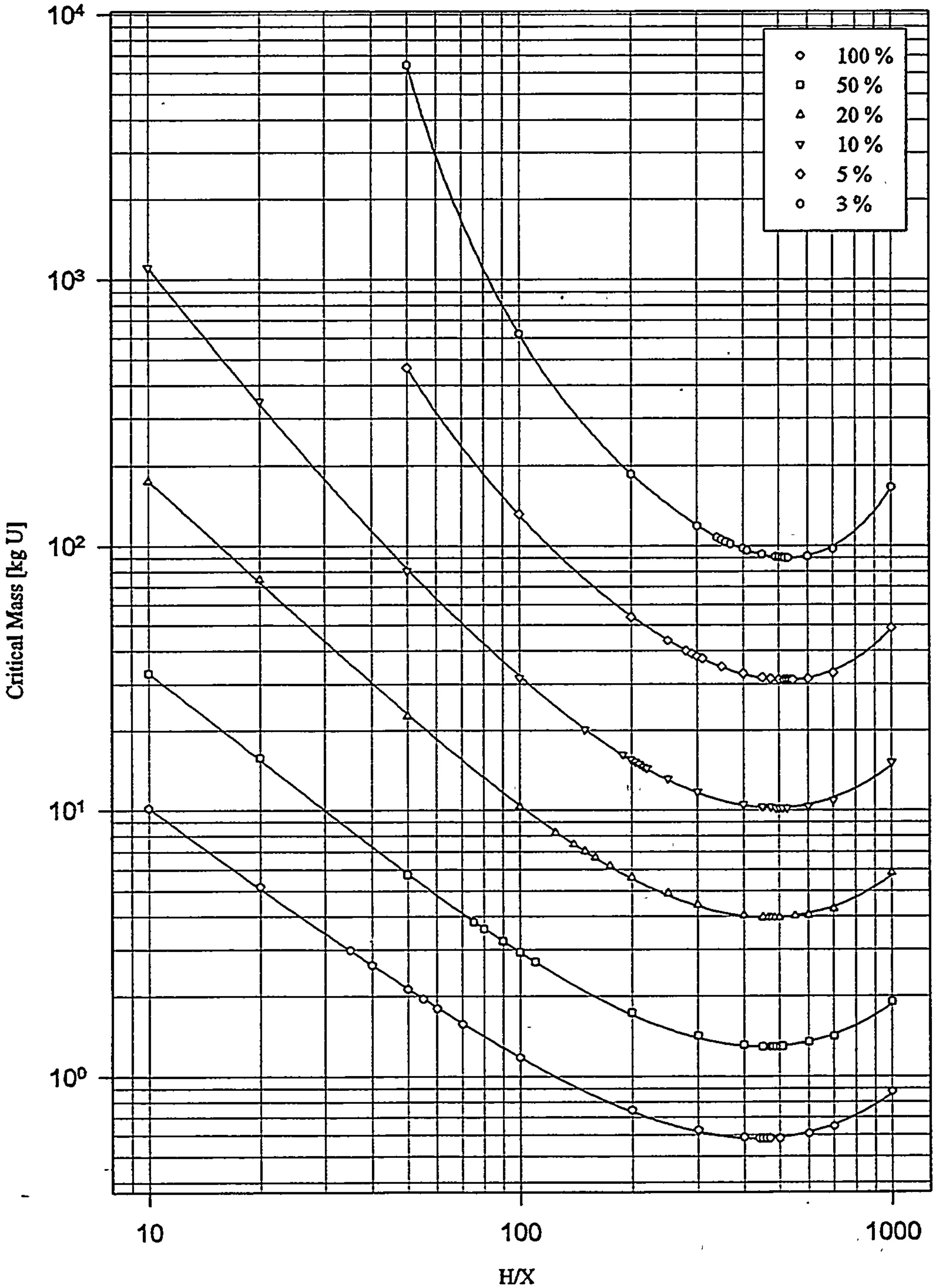

Figure-3.1.1: Estimated Critical Mass as a Function of H/X for Various ^{235}U Enrichments.

The critical masses for the UF_4-$C_{29}H_{60}$ system may also be calculated by reducing the estimated critical mass for the UO_2F_2-H_2O system by:[12,13]

$$\left(\frac{\rho_o}{\rho}\right)^2 \qquad (3.3.1)$$

where,

ρ_0 = uranium density at the moderation level where the critical mass occurs for the UO_2F_2-H_2O system, and

ρ = uranium density at the same moderation level for the UF_4-$C_{29}H_{60}$ system.

The minimum critical mass for all enrichments occurs at an $H/X \approx 500$ for the UO_2F_2-H_2O systems and other hydrogen moderated systems.[12,14] Therefore, the uranium density at an $H/X=500$ is used to determine the minimum critical masses for various ^{235}U enrichments. The calculated critical masses using this method for the UF_4-oil system are presented in Table-3.1.3.

Table-3.1.3: Uranium Densities for the UO_2F_2-H_2O and UF_4-$C_{29}H_{60}$ Systems, the Estimated Critical Mass for the UO_2F_2-H_2O System, and the Calculated Critical Mass for the UF_4-$C_{29}H_{60}$ System at an $H/X=500$ Using Reduction Factor 3.3.1.

Enrichment [wt. % ^{235}U]	Uranium Density for UO_2F_2-H_2O Mixture [g U/cm^3]	Uranium Density for UF_4-$C_{29}H_{60}$ Mixture [g U/cm^3]	Estimated Critical Mass for UO_2F_2-H_2O Mixture[14,15] [kg ^{235}U]	Calculated Critical Mass for UF_4-$C_{29}H_{60}$ Mixture [kg ^{235}U]
100	$5.1687x10^{-2}$	$5.9324x10^{-2}$	0.7751	0.588
50	$1.0256x10^{-1}$	$1.1728x10^{-1}$	0.8522	0.651
20	$2.5054x10^{-1}$	$2.8338x10^{-1}$	1.0209	0.798
10	$4.8269x10^{-1}$	$5.3680x10^{-1}$	1.27471	1.030
5	$8.9889x10^{-1}$	$9.7098x10^{-1}$	1.851	1.586
3	1.3734	1.4353	3.07734	2.817

4.0 Suggested Mass Limits for the UF_4-Oil Systems

The minimum critical masses for the various enrichments presented in Tables-3.1.1 and 3.1.3 are in good agreement. The masses calculated using XSDRNPM (Table-3.1.1) are slightly smaller than the masses calculated using the square of the uranium densities (Table-3.1.3). Therefore, the critical masses presented in Table-3.1.1 are used to determine the mass limits for mixtures of UF_4 and oil presented in Table-4.0.1.

A safety factor of approximately 2.3 is used to determine the mass limits. This factor ensures that a container filled under these limits will remain subcritical.

Table-4.0.1: Suggested Mass Limits for Various Enrichments and the Corresponding Approximate Safety Factors.

Enrichment [wt % ^{235}U]	Mass Limit [Kg ^{235}U]	Approximate Safety Factor
100	0.240	2.43
50	0.280	2.30
20	0.350	2.25
10	0.430	2.33
5	0.670	2.32
3	1.170	2.32

5.0 Applicability of the CSAS25 Validation

The principal moderator for the UF_4-$C_{29}H_{60}$ system is hydrogen (See Section 2.2). The validation contains many hydrogen moderated experiments over a wide range of moderation levels. Also, the validation contains many experiments containing uranium, oxygen, and fluorine and some contain carbon.

The average energy group causing fission for the k_∞ confirmation calculations presented in Table-5.0.1 and the critical mass confirmation calculations presented in Table-5.0.2 are within the energy range of the validation.[3] Therefore, the validation is applicable to the results presented in this analysis.

Figure-5.0.1: Average Energy Group Causing Fission (AEGCF) for the k_∞ Confirmation Calculations.

^{235}U Enrichment [wt. %]	AEGCF		
	H/X		
	10	100	1000
3	11.6811	21.2007	24.6337
5	12.5069	21.7490	24.7587
10	13.3236	22.2115	24.8518
20	13.8639	22.4867	24.8963
50	14.3396	22.6731	24.9271
100	14.7349	22.7646	24.9369

Table-5.0.2: Average Energy Group Causing Fission (AEGCF) for the Critical Mass Confirmation Calculations.

H/X	AEGCF	H/X	AEGCF
3 wt. % ^{235}U		5 wt. % ^{235}U	
100	21.4406	100	22.0545
520	24.1941	535	24.4151
1000	24.6315	1000	24.7584
10 wt. % ^{235}U		20 wt. % ^{235}U	
100	22.5513	100	22.8248
500	24.5259	475	24.5773
1000	24.8501	1000	24.8980
50 wt. % ^{235}U		100 wt. % ^{235}U	
100	23.0047	100	23.0981
480	24.6310	470	24.6420
1000	24.9267	1000	24.9346

6.0 Conclusions

The estimated critical masses for UF_4-oil systems are smaller than for the UO_2F_2-H_2O systems. Therefore, the resulting mixture are more nuclearly reactive than mixtures of UO_2F_2 and H_2O, and are not bounded by the subcritical limits presented in several nuclear criticality safety guides. The suggested mass limits for UF_4-oil systems are 0.240, 0.280, 0.350, 0.430, 0.670, and 1.170 kg ^{235}U for enrichments of 100, 50, 20, 10, 5, and 3 wt. % ^{235}U respectively.

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Appendix A

Example Input Decks

Example Input Decks for Section 2.2

```
=csasi
uf4-oil (c only) mixture, min crit mass calcs, ench=100%, c460
27groupndf4                  infhommedium
uf4                 1  0.0127229 293 92235 100.0          end
c                   1 den=0.731867 1.0 293                end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 2 1.0 293          end
end comp
end
=xsdrn
minimum mass req for criticality series
0$$ a3 2 e
1$$ 3 2 80 1 0 2 2 8 3 4 a12 400 e
2$$ -2 0 e
3$$ a12 1 e
5** a4 0 -1 a10 1.00 e            1t
13$$ 1 2
14$$ 1 2 15** f1.              2t
33## f1.                       4t
35** 49i0. 29i4.0 34.0
36$$ 50r1 30r2
39$$   1    2
41**  .8    0                  5t
end


=csasi
uf4-oil mixture, min crit mass calcs, ench=100%, cm290460
27groupndf4                  infhommedium
uf4                 1  0.0127229 293 92235 100.0          end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 1 0.9872771 293    end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 2 1.0 293          end
end comp
end
=xsdrn
minimum mass req for criticality series
0$$ a3 2 e
1$$ 3 2 80 1 0 2 2 8 3 4 a12 400 e
2$$ -2 0 e
3$$ a12 1 e
5** a4 0 -1 a10 1.00 e            1t
13$$ 1 2
14$$ 1 2 15** f1.              2t
33## f1.                       4t
35** 49i0. 29i4.0 34.0
36$$ 50r1 30r2
39$$   1    2
41**  .8    0                  5t
end
```

Example Input Decks for Section 3.1

```
#csas1x
uf4-oil mixture, kinf calcs, ench=100%, k000100
27groupndf4                  infhommedium
uf4           1  0.0559622 293 92235 100.0          end
arbm-oil 0.87 2 0 1 0 6012 29 1001 60 1  0.9440378 293 end
arbm-oil 0.87 2 0 1 0 6012 29 1001 60 2 1.0 293        end
end comp
cellmix       1
more data szf=0.8 end
end

#csas25
uf4-oil mixture, csas25 k-inf comparison, ki000100
27groupndf4                  infhommedium
uf4             1  0.0559622 293 92235 100.0 end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 1 0.9440378 293  end
end comp
uf-oil mixture, csas25 k-inf comparison,
read parm gen=210 npg=500 nsk=10 run=yes plt=yes nub=yes end parm
read geom
unit 1
com=!cuboid, 10m x 10m x 10m!
cuboid     1 1     500 -500 500 -500 500 -500
end geom
read bnds +xb=reflect -xb=reflect +yb=reflect -yb=reflect
+zb=reflect
 -zb=reflect end bnds
end data
end
```

Example Input Decks for Section 3.2

```
=csasi
uf4-oil mixture, min crit mass calcs, ench=100%, cm290470
27groupndf4                  infhommedium
uf4               1  0.0124556 293 92235 100.0            end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 1 0.9875444 293  end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 2 1.0 293        end
end comp
end
=xsdrn
minimum mass req for criticality series
0$$ a3 2 e
1$$ 3 2 80 1 0 2 2 8 3 4 a12 400 e
2$$ -2 0 e
3$$ a12 1 e
5** a4 0 -1 a10 1.00 e           1t
13$$ 1 2
14$$ 1 2 15** f1.             2t
33## f1.                      4t
35** 49i0. 29i4.0 34.0
36$$ 50r1 30r2
39$$   1    2
41**  .8    0                 5t
end
```

```
=csas25
uf4-oil mixture, confirmation calcs, ench=100%, c000470
27groupndf4                  infhommedium
uf4               1  0.0124556 293 92235 100.0            end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 1 0.9875444 293  end
arbm-oil  0.87 2 0 1 0 6012 29 1001 60 2 1.0 293        end
end comp
confirmation calcs
read parm tme=1000 gen=310 npg=500 nsk=10 nub=yes run=yes
end parm
read geom
global unit 1
sphere 1 1 13.0231
sphere 2 1 43.0231
end geom
end data
end
```

Appendix B

Estimated Critical Conditions

Table-B.1: H/U Ratio, UF_4 and $C_{29}H_{60}$ Volume Fractions, Critical Radius, and Critical Mass of Uranium for Various H/X Ratios for an Enrichment of 100 wt. % ^{235}U.

H/U	H/X	Volume Fraction UF_4	Volume Fraction $C_{29}H_{60}$	Radius [cm]	Mass U [kg]
5	5	0.5424579	0.4575421	11.6626	18.250
10	10	0.3721731	0.6278269	10.8782	10.161
20	20	0.2286319	0.7713681	10.2260	5.185
35	35	0.1448388	0.8551612	9.9052	2.985
40	40	0.1290708	0.8709292	9.8701	2.632
50	50	0.1059927	0.8940073	9.8227	2.130
55	55	0.0972945	0.9027055	9.8199	1.954
60	60	0.0899157	0.9100843	9.8201	1.806
70	70	0.0780734	0.9219266	9.8412	1.578
100	100	0.0559622	0.9440378	9.9805	1.180
200	200	0.0287866	0.9712134	10.6937	0.747
300	300	0.0193770	0.9806230	11.5135	0.627
400	400	0.0146035	0.9853965	12.3863	0.589
440	440	0.0132935	0.9867065	12.7454	0.584
450	450	0.0130020	0.9869980	12.8394	0.584
460	460	0.0127229	0.9872771	12.9308	0.583
470	470	0.0124556	0.9875444	13.0231	0.583
500	500	0.0117170	0.9882830	13.3042	0.585
600	600	0.0097833	0.9902167	14.3133	0.608
700	700	0.0083974	0.9916026	15.3818	0.648
1000	1000	0.0058930	0.9941070	19.1310	0.875
1500	1500	0.0039364	0.9960636	29.9239	2.237
2000	2000	0.0029552	0.9970448	99.7062	62.123

Table-B.2: H/U Ratio, UF_4 and $C_{29}H_{60}$ Volume Fractions, Critical Radius, and Critical Mass of Uranium for Various H/X Ratios for an Enrichment of 50 wt. % ^{235}U.

H/X	H/U	Volume Fraction UF_4	Volume Fraction $C_{29}H_{60}$	Radius [cm]	Mass U [kg]
5	2.516	0.7030459	0.2969541	15.8445	59.400
10	5.032	0.5420746	0.4579254	14.1887	32.889
20	10.06	0.3718123	0.6281877	12.5926	15.770
50	25.16	0.1914307	0.8085693	11.2177	5.740
75	37.74	0.1363190	0.8636810	10.9646	3.817
80	40.25	0.1288973	0.8711027	10.9412	3.586
90	45.29	0.1162401	0.8837599	10.9229	3.218
100	50.32	0.1058465	0.8941535	10.9232	2.930
110	55.35	0.0971590	0.9028410	10.9334	2.697
200	100.6	0.0558806	0.9441194	11.3622	1.741
300	151.0	0.0379608	0.9620392	12.0875	1.424
400	201.3	0.0287434	0.9712566	12.9099	1.314
450	226.4	0.0256316	0.9743684	13.3536	1.296
475	239.0	0.0243153	0.9756847	13.5796	1.293
480	241.5	0.0240681	0.9759319	13.6264	1.293
490	246.6	0.0235885	0.9764115	13.7204	1.294
500	251.6	0.0231277	0.9768723	13.8134	1.295
510	256.6	0.0226845	0.9773155	13.9096	1.297
600	301.9	0.0193476	0.9806524	14.8566	1.348
700	352.2	0.0166297	0.9833703	15.8954	1.419
1000	503.2	0.0116991	0.9883009	19.7225	1.906
1500	754.8	0.0078300	0.9921700	31.1835	5.043
2000	1006	0.0058840	0.9941160	125.8240	248.962

Table-B.3: H/U Ratio, UF_4 and $C_{29}H_{60}$ Volume Fractions, Critical Radius, and Critical Mass of Uranium for Various H/X Ratios for an Enrichment of 20 wt. % ^{235}U.

H/X	H/U	Volume Fraction UF_4	Volume Fraction $C_{29}H_{60}$	Radius [cm]	Mass U [kg]
5	1.0102	0.8553517	-0.1446483	26.4005	334.622
10	2.0204	0.7472616	0.2527384	22.2195	174.280
20	4.0408	0.5965026	0.4034974	18.0628	74.738
50	10.1021	0.3715957	0.6284043	14.2006	22.624
100	20.2042	0.2281962	0.7718038	12.8384	10.266
125	25.2552	0.1912872	0.8087128	12.657	8.246
140	28.2858	0.1743657	0.8256343	12.6184	7.448
150	30.3062	0.1646554	0.8353446	12.6122	7.023
160	32.3267	0.1559695	0.8440305	12.6147	6.656
175	35.3573	0.1445329	0.8554671	12.6366	6.201
200	40.4083	0.1287932	0.8712068	12.7082	5.620
250	50.5104	0.1057587	0.8942413	12.948	4.881
300	60.6125	0.0897136	0.9102864	13.2556	4.443
400	80.8166	0.0688289	0.9311711	14.0242	4.036
450	90.9187	0.0616528	0.9383472	14.4624	3.965
465	93.9494	0.0597829	0.9402171	14.6024	3.958
475	95.9698	0.0585980	0.9414020	14.6964	3.954
485	97.9902	0.0574592	0.9425408	14.7944	3.956
500	101.0208	0.0558317	0.9441683	14.9437	3.961
550	111.1229	0.0510150	0.9489850	15.4755	4.020
600	121.2250	0.0469634	0.9530366	15.9542	4.055
700	141.4291	0.0405263	0.9594737	17.0689	4.285
1000	202.0416	0.0287175	0.9712825	21.2195	5.833
1500	303.0624	0.0193301	0.9806699	34.7515	17.248

Table-B.4: H/U Ratio, UF_4 and $C_{29}H_{60}$ Volume Fractions, Critical Radius, and Critical Mass of Uranium for Various H/X Ratios for an Enrichment of 10 wt. % ^{235}U.

H/X	H/U	Volume Fraction UF_4	Volume Fraction $C_{29}H_{60}$	Radius [cm]	Mass U [kg]
5	0.5057	0.9220150	0.0779850	54.8851	3241.970
10	1.0115	0.8553134	0.1446866	39.3680	1109.846
20	2.0230	0.7472032	0.2527968	27.9952	348.656
50	5.0575	0.5417675	0.4582325	19.1259	80.609
100	10.1150	0.3715234	0.6284766	15.8547	31.490
150	15.1725	0.2826911	0.7173089	14.9607	20.131
190	19.2185	0.2372998	0.7627002	14.7452	16.179
200	20.2300	0.2281417	0.7718583	14.7230	15.485
205	20.7357	0.2238227	0.7761773	14.7222	15.189
210	21.2415	0.2196642	0.7803358	14.7196	14.899
215	21.7472	0.2156574	0.7843426	14.7191	14.626
220	22.2530	0.2117942	0.7882058	14.7195	14.365
250	25.2875	0.1912393	0.8087607	14.7671	13.097
300	30.3450	0.1646128	0.8353872	14.9552	11.710
400	40.4600	0.1287584	0.8712416	15.6306	10.457
450	45.5174	0.1161131	0.8838869	16.0798	10.267
475	48.0462	0.1106783	0.8893217	16.3285	10.247
490	49.5634	0.1076549	0.8923451	16.4304	10.155
500	50.5749	0.1057295	0.8942705	16.5178	10.134
510	51.5864	0.1038717	0.8961283	16.6204	10.142
525	53.1037	0.1012043	0.8987957	16.7649	10.142
600	60.6899	0.0896883	0.9103117	17.5444	10.301
700	70.8049	0.0778735	0.9221265	18.7306	10.883
1000	101.1499	0.0558154	0.9441846	23.3602	15.132
1500	151.7248	0.0379157	0.9620843	40.7182	54.437

Table-B.5: H/U Ratio, UF_4 and $C_{29}H_{60}$ Volume Fractions, Critical Radius, and Critical Mass of Uranium for Various H/X Ratios for an Enrichment of 5 wt. % ^{235}U.

H/X	H/U	Volume Fraction UF_4	Volume Fraction $C_{29}H_{60}$	Radius [cm]	Mass U [kg]
20	1.0121	0.8552943	0.1447057	75.5376	7841.152
50	2.5304	0.7027553	0.2972447	31.4780	466.230
100	5.0607	0.5417291	0.4582709	22.5001	131.253
200	10.1215	0.3714873	0.6285127	18.9527	53.794
250	12.6518	0.3210425	0.6789575	18.5783	43.788
280	14.1700	0.2968562	0.7031438	18.5196	40.107
290	14.6761	0.2895840	0.7104160	18.5138	39.087
300	15.1822	0.2826597	0.7173403	18.5176	38.176
310	15.6883	0.2760588	0.7239412	18.5381	37.409
350	17.7125	0.2524747	0.7475253	18.6488	34.829
400	20.2429	0.2281145	0.7718855	18.9077	32.798
450	22.7733	0.2080414	0.7919586	19.2648	31.639
475	24.0385	0.1992739	0.8007261	19.4721	31.294
500	25.3036	0.1912154	0.8087846	19.7008	31.099
515	26.0627	0.1866857	0.8133143	19.8438	31.028
525	26.5688	0.1837833	0.8162167	19.9433	31.008
535	27.0749	0.1809698	0.8190302	20.0455	31.005
545	27.5810	0.1782411	0.8217589	20.1500	31.018
600	30.3644	0.1645915	0.8354085	20.7615	31.330
700	35.4251	0.1444755	0.8555245	22.0613	32.996
1000	50.6073	0.1057148	0.8942852	27.9136	48.906
1500	75.9109	0.0730507	0.9269493	58.5148	311.313

Table-B.6: H/U Ratio, UF_4 and $C_{29}H_{60}$ Volume Fractions, Critical Radius, and Critical Mass of Uranium for Various H/X Ratios for an Enrichment of 3 wt. % ^{235}U.

H/X	H/U	Volume Fraction UF_4	Volume Fraction $C_{29}H_{60}$	Radius [cm]	Mass U [kg]
50	1.5186	0.7975766	0.2024234	72.378	6432.708
100	3.0372	0.6633077	0.3366923	35.3646	624.055
200	6.0744	0.4962306	0.5037694	26.0132	185.809
300	9.1116	0.3963868	0.6036132	24.1535	118.812
340	10.3265	0.3668612	0.6331388	23.9772	107.572
350	10.6302	0.3601545	0.6398455	23.9621	105.406
360	10.9340	0.3536886	0.6463114	23.9557	103.431
370	11.2377	0.3474508	0.6525492	23.9597	101.657
400	12.1489	0.3299912	0.6700088	24.0502	97.647
410	12.4526	0.3245548	0.6754452	24.0553	96.100
450	13.6675	0.3044898	0.6955102	24.3176	93.140
490	14.8823	0.2867613	0.7132387	24.618	91.008
500	15.1861	0.2826471	0.7173529	24.7171	90.790
510	15.4898	0.2786494	0.7213506	24.8048	90.462
520	15.7935	0.2747631	0.7252369	24.901	90.242
530	16.0972	0.2709837	0.7290163	25.017	90.251
600	18.2233	0.2471836	0.7528164	25.9041	91.396
700	21.2605	0.2196271	0.7803729	27.5292	97.469
1000	30.3721	0.1645830	0.8354170	36.1476	165.358
1500	45.5582	0.1160909	0.8839091	245.459	36520.496

Appendix C

Documentation of Peer Review

A-3548# (3/20/97)

NUCLEAR CRITICALITY SAFETY CALCULATION CHECK-OFF SHEET

Problem: Estimated Critical Conditions for UF_4-Oil Systems in Fully Oil-Reflected Spherical Geometry

Computer: PORTS NCS IBM RS/6000 Workstation Code: CSAS25

❑ **DESIGN CALCULATIONAL MODEL** (Attach Calculational Model Description)

The calculational model was designed by — 12 May 97 (analyst)

The calculational model was reviewed and found to be neither too conservative nor non-conservative. — Don D'Aquila 5/12/97 (technical reviewer)

❑ **PREPARE INPUT DATA** (Attach Input Data)

The computer input was prepared by — 12 May 97 (analyst)

The computer input was reviewed and found to be correct with proper selection of options. — Don D'Aquila 5/12/97 (technical reviewer)

❑ **COMPUTER CODE**

The computer code and cross sections have been validated and this is documented in — POEF-LMUS-13 (document)

The range of validated applicability is not exceeded in the calculations. — Don D'Aquila 5/12/97 (technical reviewer)

No changes have been authorized to the computer program or cross sections without subsequent retesting or validation. The job was run on the correct computer. — 5/12/97 (NCS Computer Systems Manager)

❑ **INTERPRET RESULTS** (Attach Sample Output and Results)

The assumptions, results, bias, and conclusions of the calculational study are documented in — POEF-LMUS-44 (retrievable document)

The assumptions, results, bias, and conclusions have been checked for logic and errors. The answers were not misread, the calculations converged, there was representative sampling for Monte Carlo calculations, and no conclusion is based on only one calculation. — Don D'Aquila 5/12/97 (technical reviewer)