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SIMPLE CRITICAL MASS CALCULATIONS

by
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ABSTRACT

This report gives (1) a simple empirical equation which should yield critical mass values of homogeneous, partially moderated, unreflected spherical assemblies with an accuracy of a factor two, and (2) critical mass estimates obtained from (1) for Oy-C-H and Oy-W-CH_2 systems.

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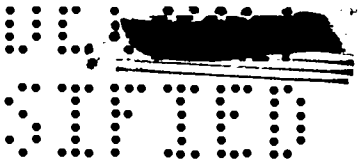

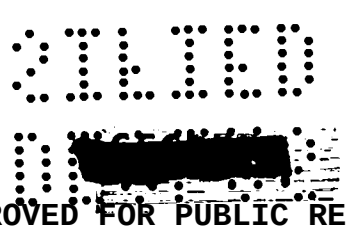

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1. A Simple Formula for Critical Masses of Partially Moderated Oralloy Assemblies

It appears that critical mass estimates with an accuracy of a factor two are useful for orientation in the nuclear aspects of rocket reactors, the reactors of interest containing anywhere from 2^1 to 2^7 kg of active material. With this tolerance in mind, the object here is to give a simple empirical equation for critical masses of spherical, unreflected, homogeneous assemblies of Oy containing moderator and poison. By including reflector savings (typically, a good reflector will reduce the bare M_c by a factor between two and three), core shape, and inhomogeneities, one may then proceed to critical mass estimates for the more specific families of preliminary reactor designs.

The empirical critical mass formula proposed is

$$M_c = \rho^{-1/2}(\text{U-235}) \left[\Sigma_{tr}(\nu - 1 - \alpha)\right]^{-3/2} f(\eta) \qquad (1.1)$$

$$\eta = \frac{\xi \Sigma_s}{\rho(\text{U-235}) \cdot (1+\alpha)} \qquad (1.2)$$

where

M_c = critical mass of U-235 in kilograms

ρ(U-235) = density of U-235 in grams per cubic centimeter

ν = 2.5 = number of neutrons per fission

Σ_{tr} = macroscopic transport cross section of the U-235 diluent (moderator plus poison) averaged over the fission spectrum

$\alpha = \Sigma_r / \Sigma_f$ = the ratio of macroscopic cross sections for radiative or parasitic captures and fission evaluated at thermal energy (except where otherwise indicated)

$f(\eta)$ = an empirical function graphed in Figure 1

$\xi\Sigma_s$ = slowing down power of moderator

A plausibility development of Equation 1.1 may go as follows: Let the macroscopic cross sections properly averaged over neutron flux spectrum be designated σ. The buckling, B, of the flux distribution is then given by

$$B^2 = 3(\nu - 1 - \alpha)\,\sigma_f\,\sigma_{tr} \tag{1.3}$$

Ignoring extrapolation lengths, the critical radius is given by

$$R_c = \frac{\pi}{B} \tag{1.4}$$

Hence the critical mass is given by

$$M_c = \frac{4\pi^4}{3}\,\rho(Oy)\left[3(\nu - 1 - \alpha)\,\sigma_f\,\sigma_{tr}\right]^{-3/2} \tag{1.5}$$

The value of σ_{tr} is very insensitive to spectral changes and

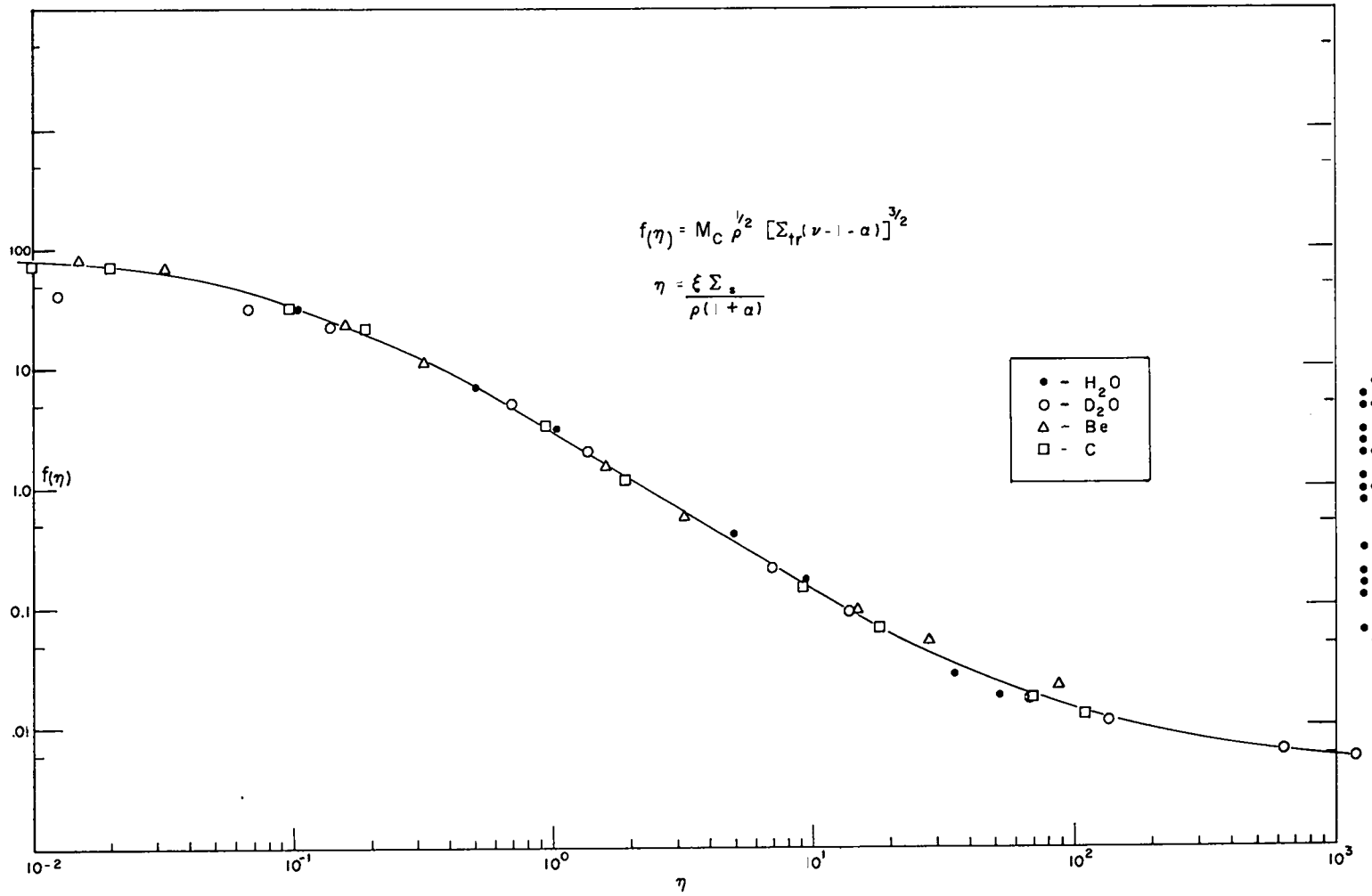


FIG. 1. Plot of $f(\eta)$.

may be put equal to Σ_{tr}. Barring poisons with epithermal resonances, α also is insensitive to neutron spectra and may be put equal to Σ_r / Σ_f evaluated at thermal energy. However, σ_f is extremely sensitive to spectral changes and we, therefore, place $\sigma_f = \Sigma_f\, g(\eta)$, where Σ_f = thermal macroscopic fission cross section and $g(\eta)$ is a function of the spectral index η. We thus obtain, since $\Sigma_f \sim \rho(Oy)$

$$M_c = \rho^{-1/2}(Oy) \left[\Sigma_{tr}(\nu - 1 - \alpha)\right]^{-3/2} \frac{4\pi^4}{9\sqrt{3}} \left[g(\eta)\right]^{-3/2} \qquad (1.6)$$

The ratio of fast to thermal neutron flux is equal to the rate at which neutrons are converted from fast to thermal divided by the rate at which thermal neutrons are absorbed. Qualitatively, the rate at which neutrons are thermalized is proportional to the slowing down power of the medium, $\xi \Sigma_s$, and hence, the ratio of fast to thermal neutron flux is proportional to $\xi\Sigma_s / \Sigma_f(1+\alpha)$. The parameter $\xi \Sigma_s / \Sigma_f(1+\alpha)$ is thus a spectral index, and indeed is an index for spectra which have no thermal neutron content at all. Quantitatively, a spectrum cannot, of course, be characterized by a single index, $\xi\Sigma_s / \Sigma_f(1+\alpha)$, as details depend on, say, whether the moderator is hydrogen, deuterium, carbon, etc. The suitability of $\xi\Sigma_s / \Sigma_f(1+\alpha)$, or what is equivalent

$$\frac{\xi \Sigma_s}{\rho(Oy)(1+\alpha)} = \eta$$

as a spectral index for critical mass estimates depends on the existence of a unique $g(\eta)$ in Equation 1.6 or better yet a unique $f(\eta)$ in Equation 1.1, since the latter may absorb some of the changes with spectrum of α, σ_{tr}, and extrapolation length. The function $f(\eta)$ was determined from Safonov's multigroup critical mass calculations on H_2O, D_2O, Be, and C moderated U-235 systems (RAND Corporation Report R-259, January 1954). That is

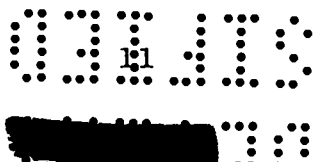
$$f(\eta) \equiv M_c(\text{Safonov})\ \rho^{1/2}\ \left[\Sigma_{tr}(\nu - 1 - \alpha)\right]^{3/2}$$

The various $f(\eta)$, η points obtained for the range

$$1 \leq (\text{moderator/uranium mole ratio}) < \infty$$

are plotted in Figure 1, and it is readily seen that, for this range, the function $f(\eta)$ is unique in so far as permitting critical mass estimates via Equation 1.1 to an accuracy within a factor two.

As the spectral index, η, goes from 0.1 to 100, the corresponding assembly spectrum goes from the typically fast Godiva or Topsy-like spectrum to the thermal pile type spectrum. For $\eta < 0.1$, the standard one-group treatments for critical mass are capable of high accuracy not only because



appropriate one-group cross sections are known, e.g., from replacement measurements (Los Alamos Scientific Laboratory Report LA-1708, July 1954), but also because of the possibility of normalization to critical mass values of known fast assemblies such as Topsy, Godiva, and Jemima. The macroscopic transport cross section, Σ_{tr}, appearing in Equation 1.1, was defined as an average over a fast spectrum partly with the hope that appropriate values could readily be obtained from the σ_{tr} tables of LA-1708. However, the high neutron energy transport cross sections of Be, C, O, H, and D employed by Safonov in R-259 imply σ_{tr} values considerably higher than those given in LA-1708, and, in our construction of $f(\eta)$, average transport cross sections were based on R-259 tables. A comparison is given in Table I.

TABLE I. VALUES OF σ_{tr}

Element	R-259* (barns)	LA-1708 (barns)
H	3.3	~ 2.0 (from LA-1525)
D	1.8	--
Be	3.3	2.2
C	3.0	2.2
O	3.1	2.2

*Used for $f(\eta)$ construction.

[redacted]

Because of these differences, transport cross sections for medium or large Z additives will be determined so as to force agreement between critical mass predictions of Equation 1.1 and one-group treatments (based on LA-1708 cross sections) for the limiting cases of no moderator.

A last remark concerns the quantity $\alpha = \Sigma_r / \Sigma_f$. This quantity is of importance in severely poisoned assemblies. Since the complete energy dependence of radiative capture cross sections is seldom known, the value of α averaged over an assembly spectrum can at best be guesstimated regardless of how accurately the assembly spectrum is computed (with the exception of the completely thermal system). Replacement measurements in Topsy Oy-Tu and Topsy Hydride can give approximate α values for fast and intermediate assemblies, respectively, and these, together with the known thermal values, should be adequate with the exception of poisons having epithermal capture resonances. Equation 1.1 is invalid for systems having epithermal capture resonances if α is evaluated from the above-mentioned sources. Validity can be regained, however, if the epithermal capture is computed and incorporated into α. The usefulness of Equation 1.1, of course, depends on the simplicity and accuracy of this computation.

[redacted]

It is intended to estimate in this way critical masses of the systems (a) Oy C_m H_n, and (b) Oy W_m $(CH_2)_n$.

2. Critical Mass Estimates of Oy-C-H Systems

These estimates, graphed in Figure 2, apply to normal density, homogeneous, unreflected, spherical assemblies of Oy C_m H_n mixtures, m and n denoting atomic ratios. Normal density is here defined as that density which results from additivity of volume of the mixture components. The normal density, ρ_o, and cross sections of these components are taken as:

ρ_o(Oy = 93% U-235) = 18.5 g/cm^3

ρ_o(C) = 1.67 g/cm^3, $\xi\sigma_s$(C) = 0.74 barn, σ_{tr}(C) = 3.0 barns

ρ_o(H) = 0.173 g/cm^3, $\xi\sigma_s$(H) = 20 barns, σ_{tr}(H) = 3.3 barns

σ_c(H) = 0.33 barn, σ_c(C) = 0.005 barn, $\dfrac{\sigma_c(\text{Oy})}{\sigma_f(\text{Oy})} = 0.20$

The values are calculated from the formula

$$M_c(\text{Oy}) = 1.1\ \rho^{-1/2}(\text{Oy})\ \left[\Sigma_{tr}(\nu - 1 - \alpha)\right]^{-3/2} f(\eta)$$

$$\eta = \frac{\xi\Sigma_s}{0.93(1+\alpha)\,\rho(\text{Oy})}$$

This formula differs slightly from that given in Section 1,

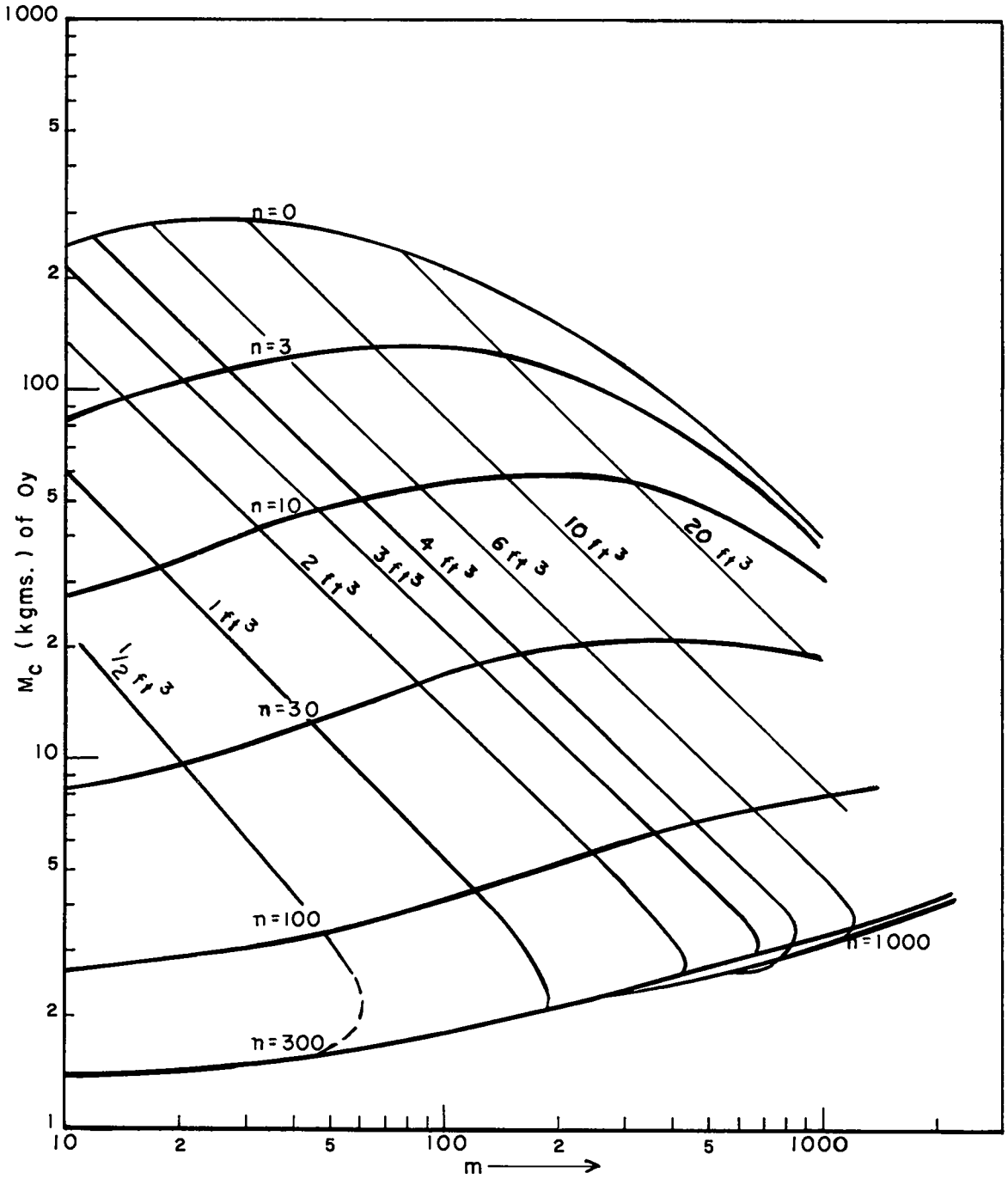


FIG. 2. Bare sphere critical mass estimates of Oy C_m H_n systems.

which applied to M_c(U-235).

3. Contribution of Resonance Capture to $\alpha = \Sigma_c / \Sigma_f$

It is desired here to develop (for use in treating Oy-W-CH_2 systems) a simple expression for the contribution of resonance capture to α and hence to critical mass via Equation 1.1

$$M_c = \rho^{-1/2} \left[\Sigma_{tr}(\nu - 1 - \alpha)\right]^{-3/2} f(\eta)$$

Such an expression must evidently be a function of the spectral index η .

Since the average energy decrement factor ξ of customary moderators is large compared to a capture resonance width, the flux equation in the vicinity of a resonance, $x_i \equiv \ell n\, E_i$, may be written approximately as

$$\left[\Sigma_c(x) + \Sigma_s\right] n(x) = \Sigma_s\, n(x + \xi) = \Sigma_s\, n_+$$

where n_+ is the flux density just above the resonance region. The resonance capture rate in the ith resonance is thus

$$(R.C.R.)_i = \int_i \Sigma_c(x)\, n(x)\, dx = \Sigma_s\, n_+ \int_i \frac{\Sigma_c(x)}{\Sigma_c(x) + \Sigma_s}\, dx \equiv \Sigma_s\, n_+ \frac{\gamma_i}{E_i} \qquad (3.1)$$

where the identically equal sign defines the effective resonance width, γ_i. The total resonance capture rate is then

$$(\text{R.C.R.}) = \Sigma_s \, n_+ \sum_i \frac{\gamma_i}{E_i} \tag{3.2}$$

Since the rate at which neutrons are slowed down past the resonance region is equal to the rate of thermal absorption (strictly, the rate of absorption below the resonance -- a distinction we shall not belabor), one has

$$n_+ \left[\Sigma_s - \sum_i \Sigma_s \frac{\gamma_i}{E_i}\right] \cong n_+ \, \xi \, \Sigma_s = \Sigma_a(\text{thermal}) \, \phi \, (\text{thermal}) \tag{3.3}$$

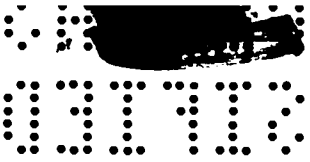
where ϕ (thermal) is the thermal flux. Eliminating n_+ between Equations 3.2 and 3.3, one has the standard expression

$$(\text{R.C.R.}) = \left(\frac{1}{\xi} \sum_i \frac{\gamma_i}{E_i}\right) \Sigma_a(\text{thermal}) \, \phi \, (\text{thermal}) \tag{3.4}$$

The contribution to α due to these resonances is then

$$\Delta \alpha = \frac{\left(\frac{1}{\xi} \sum_i \frac{\gamma_i}{E_i}\right) \Sigma_a(\text{thermal}) \, \phi \, (\text{thermal})}{\Sigma_f(\text{average}) \, \phi \, (\text{total})} \tag{3.5}$$

Adopting for the moment a two-group notation, Σ_f(fast),



Σ_f(thermal), etc., and letting

$$\Sigma_f(\text{average}) = \Sigma_f(\text{thermal})\, g(\eta) \tag{3.6}$$

where as usual η is the spectral index $\xi \Sigma_s/\rho(1+\alpha)$, one has

$$\Sigma_f(\text{average}) = \frac{\Sigma_f(\text{thermal})\, \phi(\text{thermal}) + \Sigma_f(\text{fast})\, \phi(\text{fast})}{\phi(\text{total})}$$

$$\phi(\text{total}) = \phi(\text{thermal}) + \phi(\text{fast})$$

From this follows

$$\frac{\phi(\text{thermal})}{\Sigma_f(\text{average})\, \phi(\text{total})} = \frac{1}{\Sigma_f(\text{thermal})} \left[\frac{1 - \Sigma_f(\text{fast})/\Sigma_f(\text{average})}{1 - \Sigma_f(\text{fast})/\Sigma_f(\text{thermal})}\right] \tag{3.7}$$

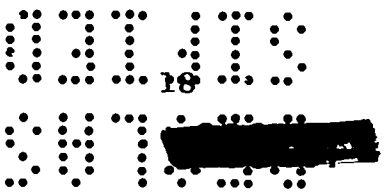
Because of the normal limitations of two-group treatments, the appropriate value of Σ_f(fast) depends on the assembly spectrum. Indeed, as Σ_f(average) changes over the factor ~ 400 from thermal ($\eta = \infty$) to fission spectrum ($\eta = 0$), Σ_f(fast) changes by approximately the factor 20. Thus

$$\frac{\Sigma_f(\text{fast})}{\Sigma_f(\text{thermal})} \cong \sqrt{g(o)\, g(\eta)} \tag{3.8}$$

and Equation 3.7 becomes

$$\frac{\phi(\text{thermal})}{\Sigma_f(\text{average})\, \phi(\text{total})} \cong \frac{1}{\Sigma_f(\text{thermal})} \frac{1 - \sqrt{g(o)/g(\eta)}}{1 - \sqrt{g(o)g(\eta)}}$$

$$\cong \frac{1 - \sqrt{g(o)/g(\eta)}}{\Sigma_f(\text{thermal})} \tag{3.9}$$



From the development of the critical mass formula, it follows that

$$\frac{f(\eta)}{f(o)} \cong \left[\frac{g(o)}{g(\eta)}\right]^{3/2} \tag{3.10}$$

so that, combining Equations 3.5, 3.9, and 3.10, one has

$$\Delta\alpha \cong \left(\frac{1}{\xi} \sum_i \frac{\gamma_i}{E_i}\right) [1 + \alpha(\text{thermal})] \left\{1 - \left[\frac{f(\eta)}{f(o)}\right]^{1/3}\right\} \tag{3.11}$$

which is the desired approximate expression giving the contribution to α due to resonance capture in terms of the resonance characteristics, γ_i/E_i, and the spectral index η. If the resonances follow the Breit-Wigner relation with peak Σ_o and width Γ, then

$$\gamma = \frac{\pi}{2} \Gamma \frac{\Sigma_o/\Sigma_s}{(1 + \Sigma_o/\Sigma_s)^{1/2}}$$

4. Critical Mass Estimates for OyO_2-W-CH_2 Systems

The results, graphed in Figures 3 and 4, apply to unreflected, homogeneous, normal density, spherical assemblies of $[(OyO_2)_x W]_y CH_2$, where x is the volume fraction of OyO_2 in the OyO_2-W "fuel", and y is the volume fraction of fuel in the fuel-moderator composite. These results follow from the "jam-handy" critical mass formula

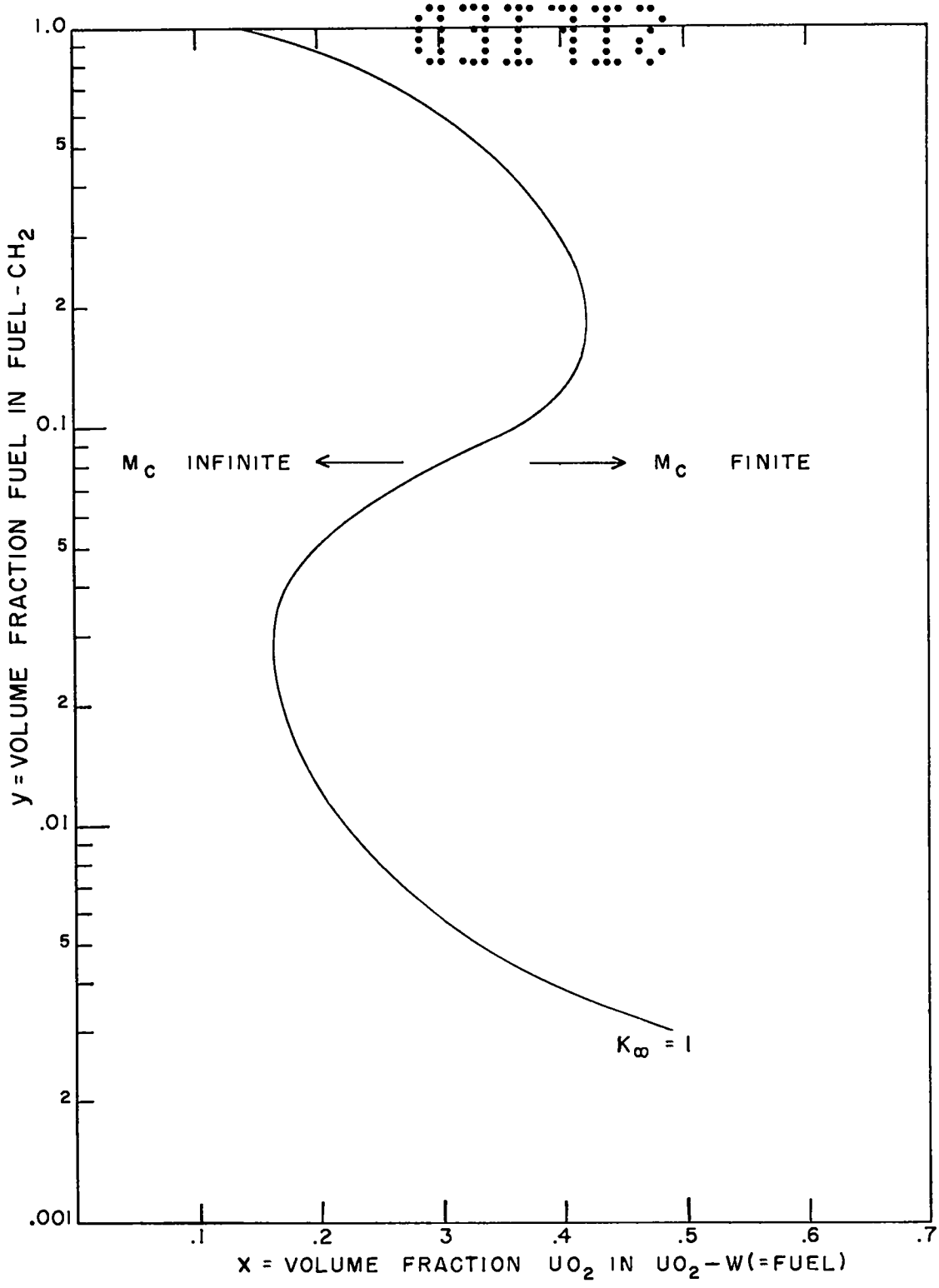


FIG. 3. Estimated $M_c = \infty$ contour for homogeneous UO_2-W-CH_2 mixtures.

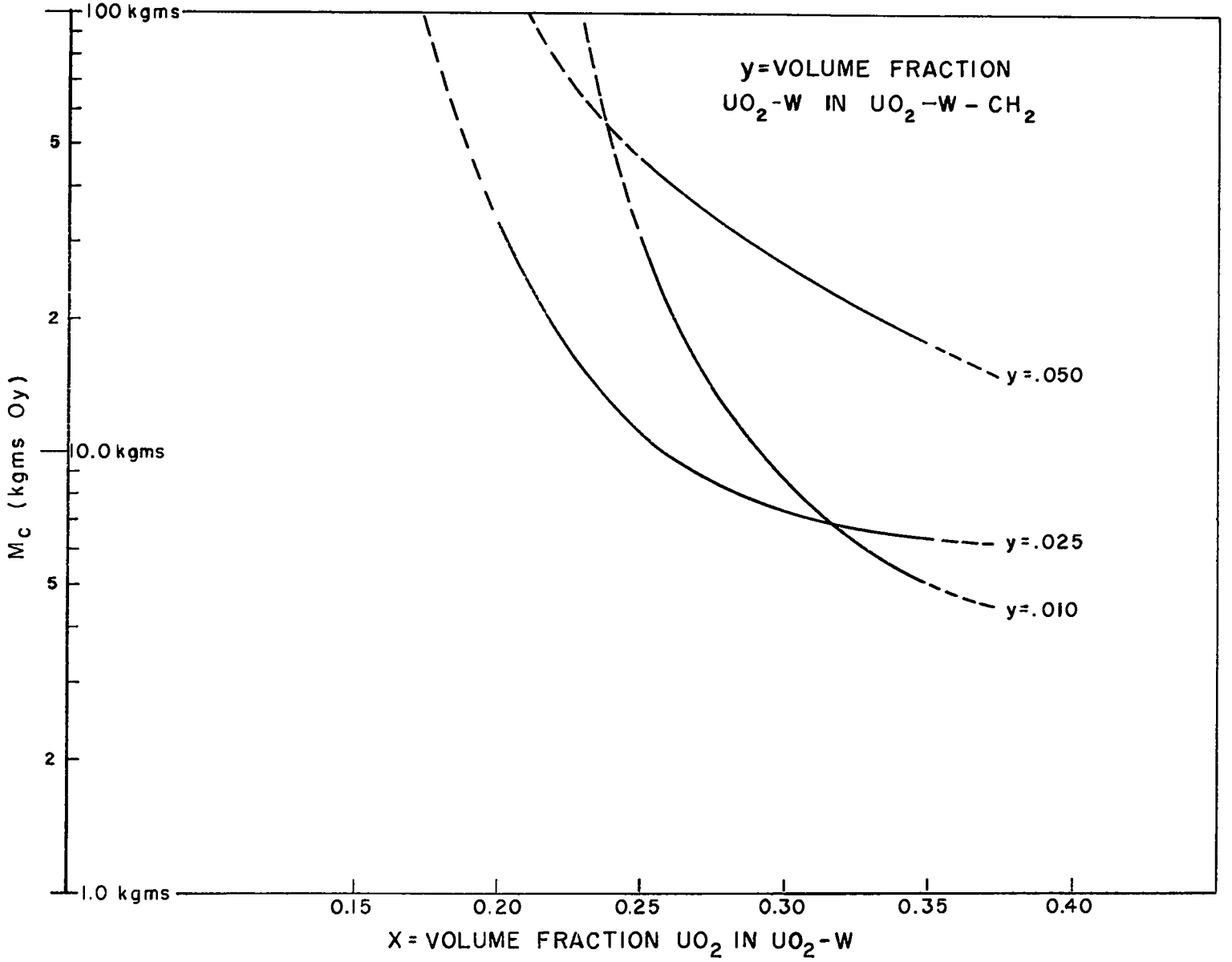


FIG. 4. Estimated critical masses of U(93.5%U-235) for UO_2-W-CH_2 mixtures.

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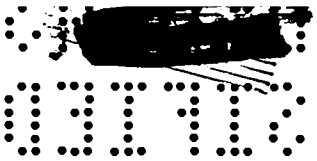


$$M_c = 1.1\ \rho^{-1/2}(Oy)\ \left[\Sigma_{tr}\ (\nu - 1 - \alpha)\right]^{-3/2} f(\eta)$$

and the nuclear data:

$\sigma_{tr}(CH_2)$ = 9.6 barns

$\xi\,\sigma_s(CH_2)$ = 40.7 barns, $\rho(CH_2)$ = 0.8 g/cm^3

$\sigma_{tr}(OyO_2)$ = 11.4 barns

$\xi\,\sigma_s(OyO_2)$ = 1.0 barn, $\rho(OyO_2)$ = 11.0 g/cm^3

$\sigma_{tr}(W)$ = 4.4 barns

$\xi\,\sigma_s(W)$ = 0, $\rho(W)$ = 18.8 g/cm^3

$\sigma_c(W)/\sigma_f(Oy) = 0.077 + (\sqrt{\eta} - 0.084\,\eta^2)/(3 + 2\,\eta^2)$, excluding resonance capture.

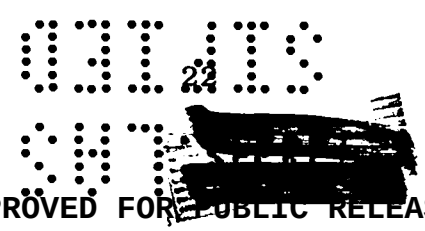
$\sigma_c(Oy)/\sigma_f(Oy) = 0.15$ for $\eta < 0.1$

$= 0.20$ for $\eta > 0.1$

The Breit-Wigner resonance capture parameters used for tungsten are:

E_{res}(ev)	Γ (ev)	σ_o(barns)
4.15	0.124	855
7.8	0.148	414
19.2	0.397	2810

These values of Γ and σ_o correspond approximately to the room temperature Doppler-broadened lines. The nonresonance capture cross sections in tungsten are not well known. The



The empirical equation given on the preceding page is consistent with the following values:

$\sigma_c(W)/\sigma_f(Oy)$ = 0.077 for Godiva (LA-1708)

= ~ 0.25 for Topsy-Hydride (LA-1159, May 1950)

= 0.035 at thermal (Brookhaven National Laboratory Report BNL-325, July 1955)

Since one is presumably interested in volume fractions of UO_2 in W less than ~ 30%, it is clear from Figure 3 that (aside from the UO_2-W metal system, i.e., y = 1) the fuel-moderator volume ratio is restricted to the range 0.006 to 0.08, of which Figure 4 covers only from y = 0.01 to 0.05.

In view of the uncertainty in nonresonance capture cross sections of W and the very nonrigorous treatment of resonance capture, one must certainly take the quantitative results in Figures 3 and 4 with a grain of salt. As an example of how the above uncertainties are reflected in critical mass estimates, we tabulate below the neutron fates for the y = 0.025, x = 0.25 case:

Fission in OyO_2	40.0%
Radiative capture in OyO_2	8.0%
Radiative capture in CH_2	10.4%
Nonresonance capture in W	14.3%
Resonance capture in W	11.4%
Remainder ≡ Leakage	15.9%

The critical mass is related to the inverse 3/2 power of the leakage probability so that a factor two uncertainty in critical mass results from an $\sim$ 60% uncertainty in leakage, or in the present example a 30% uncertainty in total W capture.

The tabulated numbers are somewhat artificial since the first two percentages are essentially defined constants not subject to error, the actual, or Safonov, spectral dependence of $\sigma_c(Oy)/\sigma_f(Oy)$ being included in the $f(\eta)$ calibration. This artificiality is more than compensated for by the ease with which replacement data on various poisons can be incorporated into M_c calculations; viz.,

$$\sigma_c(\text{poison})/\sigma_f(Oy) \cong 1.3 \frac{\Delta K(\text{poison})}{\Delta K(Oy)}$$