LETTERS TO THE EDITOR

COMMENTS ON "A SIMPLE RELATIONSHIP OF MAXIMUM Δk DUE TO COMPACTION OF UNMODERATED FISSILE MATERIALS" AND THE USE OF THE TROMBAY CRITICALITY FORMULA FOR THE SAME

Marotta[1] has proposed a simple heuristic formula to predict the increase in the effective multiplication factor resulting from compaction of a single, bare, spherical, unmoderated, homogeneous fissile system. The relation given by Marotta is

$$k_n = k_0 N^{2/3} \quad , \tag{1}$$

where k_0 and k_n are the effective multiplication factors before and after compaction, respectively, and N represents the core density compaction factor.

UNIVERSAL EMPIRICAL RELATION FOR k_{eff}

The problem of variation of k_{eff} of spherical small fast assemblies with core radius (R) and density (ρ) was investigated in detail by us in Ref. 2. It was shown that for both bare and reflected constant density, fixed reflector thickness, spherical hard fast systems, the variation of k_{eff} with core radius can be described by a universal empirical relation (UER) as follows[2]:

$$k_{eff} = k_\infty^*\left[1 - \exp\left(-\theta \frac{R}{R_c}\right)\right] = k_\infty^*\left[1 - \exp\left(-\theta \frac{\hat{l}}{\hat{l}_c}\right)\right] , \tag{2a}$$

or, equivalently,

$$k_{eff} = k_\infty^*[1 - \exp(-\theta f_{crit}^{1/3})] \quad , \tag{2b}$$

where k_∞^* is a constant that was shown to be quite close to k_∞ of the core material and θ is related to k_∞^* through

$$\theta = \ln[k_\infty^*/(k_\infty^* - 1)] \quad .$$

Here, R_c is critical core radius, and $\hat{l}$ is the mean-chord-length of the core given by $4V/S$, V and S being the volume and surface area of the core, respectively; f_{crit} is fractional critical mass at a given core density. The term in square brackets in Eqs. (2a) and (2b) represents the nonleakage probability of neutrons from the assembly. Note that the relation between θ and k_∞^* as given above follows from the normalization condition that at $R = R_c$, $k_{eff} = 1$.

The UER has been extended to be applicable to systems with varying core density, using the well-known inverse square relationship between critical mass and core density for bare assemblies. It was shown in the context of micro-fission systems [see Eq. (4) of Ref. 2] that

$$k_{eff} = k_\infty^*\left[1 - \exp\left(-\theta \frac{R\rho}{R_{c0}\rho_0}\right)\right] = k_\infty^*\left[1 - \exp\left(-\theta \frac{\sigma}{\sigma_c}\right)\right] \quad . \tag{3}$$

The product $R\rho$ is a measure of the surface mass density σ, i.e., mass per unit surface area of the core, R_{c0} is the critical core radius at density ρ_0, and σ_c pertains to the bare critical system and is a constant characteristic of the core composition and is independent of density. Thus $\sigma_c \simeq 324$ kg/m^2 for ^{239}Pu metal systems, 301 kg/m^2 for $^{239}PuO_2$ systems, and ~530 kg/m^2 for enriched ^{235}U assemblies.

The importance of $R\rho$ (or σ) as an index of reactivity was also noted by Marotta and, in fact, forms the basis of his Note. However, whereas Marotta assumed $k_{eff} \propto \rho R$, the actual relationship between k_{eff} and ρR is more correctly described by Eq. (3). The form of Eq. (3) ensures that whatever the value of $R\rho$ (or σ), k_{eff} can never exceed k_∞^*. This feature is responsible for the elimination of the limitations posed by neglect of what Marotta refers to as "surface leakage" term. Equation (3) is therefore free of any restrictions on density such as $(\eta/k_0)^{3/2}$ specified in Ref. 1.

When the mass of the system undergoing compaction is conserved,

$$\frac{R}{R_0} = \left(\frac{\rho_0}{\rho}\right)^{1/3} = \frac{1}{N^{1/3}} \quad , \tag{4}$$

where R_0 is initial core radius before compaction. Using relation (4), Eq. (3) can be written as

$$k_n = k_\infty^*\left[1 - \exp\left(-\theta \frac{R_0}{R_{c0}} N^{2/3}\right)\right] \equiv k_\infty^*\left[1 - \exp\left(-\theta \frac{\sigma_0}{\sigma_c} N^{2/3}\right)\right], \tag{5a}$$

or, equivalently,

$$k_n = k_\infty^*[1 - \exp(-\theta f_{crit}^{0\,1/3} N^{2/3})] \quad . \tag{5b}$$

Here, σ_0 and f_{crit}^0 are the surface mass density and fractional critical mass at the initial core density of ρ_0. Prior to compaction, since N is unity, we get from Eq. (5a)

$$k_0 = k_\infty^*\left[1 - \exp\left(-\theta \frac{R_0}{R_{c0}}\right)\right] \quad . \tag{6}$$

From Eqs. (5a) and (6), it follows that

$$k_n = k_0\left[\frac{1-\exp\left(-\theta\dfrac{R_0}{R_{c0}}N^{2/3}\right)}{1-\exp\left(-\theta\dfrac{R_c}{R_{c0}}\right)}\right] . \tag{7}$$

Equation (7) can be simplified if the arguments of exponentials in the numerator and denominator are assumed to be small compared to unity. Using Taylor series expansion and retaining only up to first-order terms, we obtain

$$k_n = k_0\left[\frac{1-\left(1-\theta\dfrac{R_0}{R_{c0}}N^{2/3}\right)}{1-\left(1-\theta\dfrac{R_c}{R_{c0}}\right)}\right] = k_0 N^{2/3} . \tag{8}$$

This is seen to be identical to Eq. (1), the relation derived by Marotta. Thus, Marotta's relation may be looked upon as a linear approximation to Eq. (7). The derivation of Eq. (8) from Eq. (7) clearly brings out the more general applicability of the UER propounded by the authors.

CRITICAL COMPRESSION FACTOR, N_{crit}

If one is interested in calculating the critical compression factor N_{crit} only, it may simply be obtained from the relation

$$M_0\rho^2 \equiv M_{c0}\rho_0^2$$

or

$$\frac{\rho}{\rho_0} = N_{crit} = \left(\frac{M_{c0}}{M_0}\right)^{1/2} = \left(\frac{1}{f_{crit}^{0}}\right)^{1/2} = \left[\frac{\sigma_c}{\sigma_0}\right]^{3/2} . \tag{9}$$

Here, M_0 is the mass of the assembly undergoing compaction, and M_{c0} is the critical mass at the initial density ρ_0. Equation (9) is an identity, since it follows directly from the inverse square variation of critical mass with density, which is often referred to as a basic law of criticality physics.[3] Since Eq. (5a) incorporates this law, it also reduces to Eq. (9) at critical, thus predicting the correct compression value.

RESULTS

The k_{eff} computed using the UER for the cases considered by Marotta are presented in Tables I, II, and III along with Marotta's results. Two approaches have been adopted for this: In approach A, the k_{eff}'s are computed using Eq. (5a) with R_{c0} deduced from published critical mass data. The k_∞^* values for the cores have been taken from Ref. 2. In approach B, k_{eff} is taken as equal to R/R_c, and Eq. (10) is used to compute k_n as a function of N. Details of this method are explained later. When the initial reference system is critical, approach B becomes identical to Marotta's method. The k_{eff} at which normalization is done either to transport theory results (KENO/ANISN/DTF-IV) or experimental critical data in each of the approaches is underlined in the tables. Wherever transport theory calculated critical compression is not available, N_{crit} has been obtained from Eq. (9).

It can be seen from Table I, which pertains to supercritical cases, that k_{eff}'s calculated by UER (approach A) are in most cases within KENO statistics and show better agreement with it than that given by Marotta's relation.

TABLE I

Variation of k_{eff} of an Initially Critical Bare 16.2-kg Plutonium Metal Sphere with Compaction

Compression, N[a]	KENO	A (UER)	B (Marotta)
1.00	1.002[b] ±0.007	<u>1.002</u>	<u>1.002</u>
1.05	1.031 ±0.009	1.028	1.035
1.10	1.051 ±0.008	1.054	1.068
1.25	1.114 ±0.009	1.126	1.163
1.50	1.250 ±0.009	1.235	1.313
1.75	1.340 ±0.008	1.332	1.455
2.00	1.452 ±0.009	1.419	1.590

[a]For convenience, we have considered the same values of compression, N, as Marotta.
[b]Jezebel system; radius = 0.0631 m, density = 1.54×10^4 kg/m^3, and σ_c = 324 kg/m^2.

TABLE II

The k_{eff}'s of Highly Subcritical Bare 2.0-kg PuO_2 Spheres at Different Densities

Compression, N[a]	KENO	A, Eq. (5a) (UER)	B, Eq. (10) (Linear)	Marotta, Eq. (1) (Linear)
1.00[b]	0.169 ±0.002	0.213	0.180	<u>0.169</u>
1.05	0.172 ±0.003	0.220	0.186	0.174
1.10	0.176 ±0.002	0.227	0.192	0.178
1.25	0.195 ±0.002	0.246	0.209	0.196
1.50	0.220 ±0.003	0.276	0.236	0.221
1.75	0.248 ±0.004	0.304	0.261	0.245
2.00	0.268 ±0.004	0.331	0.286	0.268
13.1[c] (N_{crit})	<u>(1.00)</u>	<u>1.000</u>[c]	<u>1.000</u>[c]	0.939

[a]For convenience, we have considered the same values of compression, N, as Marotta.
[b]Initial PuO_2 density = 3.0×10^3 kg/m^3.
[c]σ_c of PuO_2 = 301 kg/m^2.

TABLE III

The k_{eff} of Thinly Reflected PuO_2 Cylinders of Various Masses and Densities

Core Density, ($\times 10^{-3}$) (kg/m^3)	Core Mass, M (kg)	f_{crit} at Density ρ	KENO	A, Eq. (5a)[a] (UER)	B, Eq. (10) (Linear)	Marotta, Eq. (1) (Linear)
1.8	8.687	0.0091	0.226	0.246	0.209	0.226
2.0	8.687	0.0112	0.238	0.263	0.224	0.242
3.0	8.779	0.0255	0.318	0.340	0.294	0.318
3.45	8.779	0.0338	0.353	0.371	0.323	0.349
5.0	8.298	0.0670	0.438	0.459	0.406	0.438
5.8	8.298	0.0902	0.484	0.502	0.448	0.484
11.5	12.000	0.5130	0.833	0.834	0.801	0.833
12.0	12.000	0.5580	0.854	0.854	0.823	0.856
12.0	21.5[a]	1.0000	(1.000)	1.000[a]	1.000[a]	1.083 1.079 1.078 1.040

[a] σ_c = 235 kg/m^2 for a cylinder with an H/D ratio of 3.0 with a stainless-steel reflector 0.0127 m thick.

In Table II, it is seen that Marotta's relation gives results that are in reasonably good agreement with KENO in the highly subcritical region of $k_{eff} < 0.3$, since it is normalized to the initial KENO k_{eff} value of 0.169. However, k_{eff} at critical compression given by Marotta's relation is seen to be quite inaccurate.

Table III gives the k_{eff} values for the cylindrical PuO_2 cores of Marotta's Note having masses between 8 and 12 kg and densities varying from 1.8×10^3 to 1.2×10^4 kg/m^3. These subcritical cases were considered by Marotta in pairs differing by not more than 20% in density, since Eq. (1) has limited applicability only. It is presumed that the H/D ratio of the cylinder was maintained constant by Marotta during compaction.[a] It was demonstrated in Ref. 2 that UER is also valid for highly elongated or pancaked cylinders, provided the H/D ratio is maintained constant during density changes. We have deduced the k_{eff} of all the cases starting from a critical mass value of (21.5 ± 0.05) kg at a density of 1.2×10^4 kg/m^3. The critical σ_c value of 235 kg/m^2 was derived from KENO k_{eff} data by plotting $[k_\infty^*/(k_\infty^* - 1)]$ against σ on semilog paper, as suggested by Eq. (3), and extrapolating to $[k_\infty^*/(k_\infty^* - 1.0)]$. The value of k_∞^* was taken from Ref. 2 as 2.88 valid for hard fast plutonium cores. The deduced σ_c value of 235 kg/m^2 is lower than the standard PuO_2 figure of 301 kg/m^2 presumably because the system under consideration is not a bare sphere, but a cylinder having a 0.0127-m-thick stainless-steel reflector. The k_{eff}'s at the core density of 12.0 kg/m^2 corresponding to a critical mass of 21.5 kg given by Marotta's relation starting with k_0 values of 0.226, 0.318, 0.438, and 0.833 are also presented in the lower right corner of Table III.

[a] Incidentally, the inside height of 0.762 m quoted in Ref. 1 is inconsistent with the inside diameter of 0.127 m for the initial 8.687-kg system at density = 1.8×10^3 kg/m^3. It would seem that the actual height used in KENO computations was probably 0.381 m, which is half the quoted height. This will then yield a height-to-diameter (H/D) ratio of 3.0.

It may be observed that as the k_0 used for normalization approaches unity, the accuracy of k_{eff} at critical also improves. However, even starting with a k_0 of 0.833, Marotta's relation is seen to overpredict k_{eff} at critical by 40 mk.

The fact that UER consistently overpredicts k_{eff} in the highly subcritical region was also noted earlier.[2] The reason for this was discussed and possible remedies were sought in Ref. 2. Interestingly, in this context, it was observed that the ratio R/R_c, R and R_c being at the same core density, directly gives k_{eff} within 10% accuracy in the highly subcritical region for small hard fast systems σ. It so happens that a linear "approximation" gives reasonably accurate k_{eff} values in the far subcritical region in spite of the fact that neglect of higher order terms in the Taylor series expansion of Eq. (7) may not be valid from an algebraic point of view. This stems from an inherent drawback of UER, which is compensated for in the linear approximation. This is also the reason for the limited success of Marotta's relation in the highly subcritical region.

Linear representation of k_{eff} directly as R/R_c leads to the following relation for k_n in terms of N:

$$k_n \simeq \frac{R}{R_c} = \frac{R_0}{R_{c0}} N^{2/3} = [f_{crit}^0 \cdot N^2]^{1/3} \quad . \qquad (10)$$

The main difference between Eq. (10) and Marotta's relation Eq. (1), which is also a linear approximation, is that while the latter is normalized at the initial subcritical k_{eff} value of k_0, the former is normalized at critical. This ensures that Eq. (10) would also reduce to Eq. (9), the identity giving the correct critical compression (N_{crit}) value. For the same reason, close to critical, Eq. (10) also gives k_{eff} more accurately than that given by Marotta's relation. The advantages of normalization at critical therefore cannot be overemphasized.

Thus, in summary, just as Marotta's relation [Eq. (1)] is a linear approximation of Eq. (7), Eq. (10) is a linear version of the UER [Eq. (5a)]. It is recommended that, in general, Eq. (5a) may be used confidently for purposes of estimation of reactivity increase due to uniform compaction of unmoderated fissile materials, since it is based on critical mass data (either experimental or accurately computed) and is valid for large density changes. In the highly subcritical region, however, even Eq. (10) may be reasonably accurate. Both Eqs. (5a) and (10) give correct N_{crit} values.

WIGNER RATIONAL APPROXIMATION FOR LEAKAGE PROBABILITY

The Wigner rational (WR) approximation is often used[4] for computing fast-neutron leakage probability from systems having a uniformly distributed neutron source. Since source distribution may not be far from uniform in small hard fast systems whose dimensions are on the order of a neutron mean-free-path, it is tempting to apply the WR approximation to such systems owing to its inherent simplicity. In this approximation, leakage probability, p_L^{WR}, can be represented by

$$p_L^{WR} = \frac{1}{1 + \gamma \hat{l}} \quad , \tag{11}$$

where γ is a constant that is characteristic of the neutron energy spectrum in the system and $\hat{l}$ is mean-chord-length of the system. The k_{eff} of the system can then be expressed by

$$k_{eff}^{WR} = k_\infty^*(1 - p_L^{WR}) = \frac{k_\infty^*}{1 + (k_\infty^* - 1)\left(\frac{\hat{l}}{\hat{l}_c}\right)^{-1}} \quad ,$$

or, equivalently,

$$k_{eff}^{WR} = \frac{k_\infty^*}{1 + (k_\infty^* - 1)(f_{crit}^0 N^2)^{-1/3}} \quad . \tag{12}$$

In the above derivation, $[(k_\infty^* - 1)\hat{l}_c]^{-1}$ may be identified with γ and determined from the condition that at $\hat{l} = \hat{l}_c$, $k_{eff} = 1$, under the assumption that neutron energy spectrum does not change significantly when the system size is altered. We have studied the validity of the WR approximation for small hard fast systems.[5] The k_{eff}'s for all the cases of Tables I, II, and III were computed using Eq. (12). It was observed that the WR approximation also gives k_{eff}'s that are overpredicted in the subcritical region and underpredicted in the supercritical region similar to UER, but the discrepancies are, on the whole, much larger in all cases studied. The k_0^* values used in these computations were the same as for the corresponding UER calculations.

TROMBAY CRITICALITY FORMULA

Thus far, the discussion has been confined to bare systems only. However, it was demonstrated in Ref. 2 that the empirical relation and its variations are valid as such for reflected systems as well, provided the reflector thickness measured in units of neutron mean-free-path is maintained constant whenever reflector density is varied. If this condition is satisfied, then all the formulas given in the Letter may be applied to reflected systems, also under the stipulation that both core and reflector densities are changed simultaneously by the same factor N. These concepts have since been extended to the case of reflected small fast systems whose *core and reflector* densities are changed by large and unequal amounts through the use of an integrated version of Los Alamos density exponent formula[6] (ILADEF) derived by the authors. Situations wherein core shape changes to any arbitrary nonreentrant geometry are treated in Ref. 7, which gives appropriate formulas to compute shape factors and k_{eff}'s therefrom. Thus, the cylindrical cores of Table III could be dealt with even if their H/D ratio were to vary arbitrarily during compaction.

In fact, it has recently been shown by us that Eqs. (3) and (5a) are special cases of an even more general criticality relation referred to as the Trombay Criticality Formula[8] (TCF). The underlying physical basis of this formula is the postulate that mean-chord-length of the core ($\hat{l}$), measured in units of neutron mean-free-paths relative to its value for the corresponding critical system ($\hat{l}_c$), essentially determines net neutron leakage and hence system k_{eff}. The TCF combines the basic concepts developed in Refs. 2, 5, 6, and 7 to give a very general and useful criticality formula that enables calculation of k_{eff} of small fast reflected assemblies having cores of any uniform density and nonreentrant shape, the only input data requirement being spherical critical surface mass density σ_c along with the system geometrical parameters.

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