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LIMITING SURFACE DENSITY METHOD ADAPTED TO LARGE ARRAYS OF HETEROGENEOUS SHIPPING PACKAGES WITH NONLINEAR RESPONSES

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ABSTRACT

The classic Limiting Surface Density (LSD) method is an empirical calculation technique for analyzing and setting mass limits for fissile items in storage arrays. LSD is a desirable method because it can reduce or eliminate the need for lengthy detailed Monte Carlo models of the storage arrays. The original (or "classic") method was developed based on idealized arrays of bare spherical metal items in air-spaced cubic units in a water-reflected cubic array. In this case, the geometric and material based surface densities were acceptably correlated by linear functions. Later updates to the method were made to allow for concrete reflection rather than water, cylindrical masses rather than spheres, different material forms, and non-cubic arrays. However, in the intervening four decades since those updates, little work has been done to update the method, especially for use with contemporary highly heterogeneous shipping packages that are non-cubic and stored in non-cubic arrays.

In this work, the LSD method is reevaluated for application to highly heterogeneous shipping packages for fissile material. The package modeled is the 9975 shipping package, currently the primary package used to store fissile material at Savannah River Site's K-Area Complex. The package is neither cubic nor rectangular, but resembles nested cylinders of stainless steel, lead, aluminum, and Celotex. The fissile content is assumed to be a cylinder of plutonium metal. The packages may be arranged in arrays with both an equal number of packages per side (package-cubic) and an unequal number of packages per side (non-cubic).

The cubic arrangements are used to derive the 9975-specific material and geometry constants for the classic linear form LSD method. The linear form of the LSD, with non-cubic array adjustment, is applied and evaluated against computational models for these packages to determine the critical unit fissile mass. Sensitivity equations are derived from the classic method and these are also used to make projections of the critical unit fissile mass. It was discovered

that the heterogeneous packages have a non-linear surface density versus critical mass relationship, compared to acceptably linear response of bare spherical fissile masses. Methodology is developed to address the non-linear response. In so doing, the solution to the non-linear LSD method becomes decoupled from the critical mass of a single unit, adding to its flexibility. The ability of the method to predict changes in neutron multiplication due to perturbations in a parameter is examined to provide a basis for analyzing upset conditions.

A full re-derivation of the classic LSD method from diffusion theory is also included as this was found to be lacking in the available literature.

Keywords: surface density, material storage, arrays

I. INTRODUCTION

In recent years, the former K-Reactor facility at the Savannah River Site has taken on a stewardship mission. The reactor building, a hardened and defensible structure, was modified and converted from its original purpose to safely store large quantities of special nuclear materials. The layout of the K-Area facilities was also modified to support the increased security necessary for this new mission. The K-Area Complex (KAC), as it is now known, is currently able to store many shipping packages. These containers are mostly of uniform design, and mostly contain the same material – plutonium in metal or oxide form. This means that within this facility, there are large arrays of heterogeneous shipping packages each containing up to some limit of fissile material.

Because KAC has the capability to store many packages, the storage arrays analyzed must be very large, but not infinite. In practice they are bound to a finite number of units high, limited by operational safety rather than criticality concerns. The arrays in practice may also be only a few units wide to allow aisles for moving and inspecting packages. They may be many units long though.

Criticality safety analyses of the storage arrays develop in the same manner as any criticality safety evaluation. Normal conditions and credible abnormal conditions (upsets) are defined. The array is then analyzed in the normal condition and with the various upsets to ensure no normal condition or credible abnormal condition leads to an inadvertent criticality. Since the inception of the KAC's new mission, this problem has been approached computationally. While this approach yields results, the burden on criticality safety engineering is great. Many man-years of time have been used to develop acceptable simplifications of the package geometry, create and verify computational models of the normal and credible abnormal conditions, execute computer calculations with long run times due to the package geometry and array size, and then

post process and document that data. Until recently, the basic package geometry itself had to be recreated each time there was a new analysis because there was no common pedigreed model.

While it is the tendency of many engineers today to turn to computational models, when the modeling becomes extensive enough to affect the economic operation of the facility, it is advantageous to at least explore other possibilities. The KAC storage arrays were qualitatively found to be a good candidate for hand calculations, supported/verified by limited computational analysis. The packages are mostly of one uniform design, the 9975 shipping package. The packages are limited to a pre-determined mass of plutonium or fissile equivalent (although overmass of a package is a credible abnormal condition). The packages are stored in uniform arrangement with fixed spacing. In practice, four 9975 drums are stored on a uniform design pallet and bound in place with fixed spacing between the drums. The pallets are then arranged into arrays. Externally, the array looks very simple and well defined, though the internal components of each package are highly heterogeneous.

The Limiting Surface Density (LSD) method was selected as a possible means of analyzing the storage arrays using a hand calculation. It was developed in the 1970s, primarily by Joseph Thomas through work at Oak Ridge National Laboratory ([1][2][3]). It was eventually published for the criticality safety community at large ([4]). As can be seen in the development, there was some effort around that time to extend the method to non-cubic arrays and to allow for shapes of fissile material other than perfect spheres, in this case cylinders. There has been little to no significant update to the method in the intervening four decades. Despite that fact, the method has found its way into common use ([5]) and into the criticality safety standards ([6]) themselves. Only recently has work been done to examine the method's ability to handle highly heterogeneous packages in more realistic arrays ([7][8]).

In general, the classic form of the LSD method ([5]) equates two competing definitions of surface density for a *critical* array of packages. One definition is based on the geometry (spacing and number of packages) accounting for neutron leakage but conservatively assuming reflective boundary conditions. The second definition is based entirely on the relationship between critical mass of the given material and surface density. The intersection of the two expressions is the limiting mass of the array; keep each package at or below that fissile mass and the array is subcritical. This simplistic approach then avoids many lengthy computational calculations, requiring only the constants necessary for the method to be computed. The simple linear forms of the classic method even lend toward easy sensitivity studies to assess the impacts of abnormal conditions (upsets in spacing or mass for example).

The classic LSD method has limitations, especially when examined in light of a practical array of heterogeneous packages. The classic method was derived for a water-reflected cubic array of bare air-filled/air-spaced cubic units. While the fissile material may be any shape, the individual unit was an air-filled cube. The first issue was the cubic geometry of the array. Early in the development of the method, a shaping factor adjustment was developed to apply to non-cubic arrays. The second issue was the geometry of the individual package. Few practical packages are cubic, and even height-to-diameter-ratio (H/D) equal to one cylinder in a square pitch is a special case rarely seen in reality ([7]). The third issue is the intervening material. Practical packages like the 9975 have substantial amounts of intervening materials separating the fissile material. These change the neutron interaction of the packages substantially compared to bare fissile metals separated only by air. A fourth, though somewhat less impactful, issue is that the arrays are usually surrounded, with some additional spacing, by thick concrete walls and

floors rather than water reflection. Both provide neutron reflection, but the effect will be different.

This work addressed the package geometry issue. A real array does not store air-spaced bare spheres of metal. At KAC, real arrays store fissile material inside packaging that has many layers between the fissile material and the outside world. The 9975 package has multiple nested containers and dunnage for insulation and shock absorption. The package itself is not a cube; the 9975 is a cylindrical drum with a H/D near 2. Uniform bare fissile materials in cubic storage have significant, easily estimated, and symmetric neutronic interaction between them. Fissile materials in the 9975 are off-center axially and the radial and axial distances between materials are different, making the neutronic coupling between materials radially and axially asymmetric. Based on the inherent spacing provided by the package and the many layers of packaging material, the fissile units may be nearly neutronically decoupled. It would not be an unexpected outcome if even the linear assumptions of the LSD method require modification because these heterogeneities result in non-linear array responses.

The LSD method is examined and developed in detail in this work to apply to large arrays of heterogeneous packages that are neither cubic themselves nor stored in cubic arrays. Initial work established that modern computational methods acceptably reproduce the original data used to derive the classic LSD method ([7]). This initial work also established that the LSD method may be applicable to arrays of heterogeneous packages but that work relied on a simplified cubic model of the 9975 that had been axially compressed to have an H/D=1. The methods developed in this work are applicable to non-cubic heterogeneous packages. Work has already been done to demonstrate a verification pathway toward implementation of the method in practical application ([8]). Methodology is developed herein to address situations where the

packages result in non-linear array responses. For these situations, classic LSD method predictions are compared to predictions from the non-linear LSD method developed in this work. The non-linear results are also compared to predictions based on postulated sensitivities derived from the classic LSD.

Terminology in the remainder of this document abbreviates the methods. The classic LSD method wherein the material-based expression of surface density is based on a linear relationship between package mass and critical surface density is called L-LSD, for linear LSD method. Non-linear responses required the development of a new expression for material based surface density and the method including this non-linear modification is called N-LSD. Comparative calculations based on sensitivities (partial derivatives) derived from the L-LSD are called S-LSD results.

II. 9975 PACKAGE MODEL

The KENO-VI code, using the 238-group ENDF/B-VI.1 cross sections, within the SCALE 6.1 code package is used exclusively for calculations in this analysis.

A highly-detailed model of the 9975 shipping package based on the actual documented geometry has been created for consistent use in KAC criticality safety analyses. Only minor simplifications, which were assessed to have negligible neutronic impact, are made between the modeled geometry and the engineered design. This pedigreed model is used in this work for the a priori calculations necessary to establish L-LSD and N-LSD array constants and for comparative calculations of real geometry arrays. The fissile content is assumed to be a cylinder of plutonium metal at theoretical density, with H/D = 1.

The key 9975 dimensions are presented in Table I, and Figure 1 shows the difference between the 9975 engineering drawing and its pedigreed KENO model. The pedigreed KENO

model is based upon "Safety Analysis Report for Packaging Model 9975, Revision 4" ([9]) and is retained for further use because it is generically applicable to KAC analyses beyond this work. The dimension of specific interest to the L-LSD and N-LSD methods is the diameter of 46.6 cm. This is the minimum radial spacing for the shipping package arrays. Axial spacing is based on the actual height of the drums. In practice up to four drums sit on a pallet, which is about 4 inches thick. The pallet is conservatively ignored in these calculations and array spacing varied from edge-to-edge up to arbitrarily large.

III. METHODOLOGY DEVELOPMENT

III.A L-LSD Method Application

The L-LSD method is documented in the literature so only a brief explanation is given here to familiarize the reader with its application. The specific form used to compute package fissile mass, which would make the array critical, is shown. It is also from this form the S-LSD expressions are derived. The development of the array constants is discussed because these constants are application specific. Use of the shaping factor is also addressed.

The L-LSD method begins with the definition that the number of units in the array, N, times the array buckling, B_N^2, is equal to:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \sqrt{\frac{4\lambda_{array}^2 NB_N^2}{N3\pi^2}}\right)^2 \qquad (1)$$

Note that $2a_n$ equals the center-to-center package pitch, n is the smallest dimension number of units in the array (typically the vertical stacking), and λ_{array} is the extrapolation distance for the array as a whole (not an individual package). The method then asserts that $\sqrt{\frac{4\lambda_{array}^2 NB_N^2}{3\pi^2}}$ is a

constant, c. This constant by nature depends only on the geometry of the array so therefore it is called the geometric array constant, yielding the formula:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 \qquad (2)$$

Surface density, generically, is mass divided by area. The limiting surface density is that which results in a critical configuration of the array. The dimensions of the critical array must include the array extrapolation distance, λ_{array}. The surface density, σ, of a cubic array of packages each of mass m is (see derivation in the Appendix leading to Equation A.37):

$$\sigma(m) = \frac{mass}{area} = \frac{mn^3}{(n2a_n + 2\lambda_{array})^2} = \frac{mNB_N^2}{3\pi^2} = \left(\frac{mn}{(2a_n)^2}\right)\left(1 - \frac{c}{\sqrt{N}}\right)^2 \qquad (3)$$

This defines surface density based on geometry. A competing definition is based on material properties. Thomas' papers ([1]-[4]) state that, in the plot of surface density versus m_c, the slope of the linear fit of the data is a constant called c_2. Let m_o = critical fissile mass of a single unreflected unit and m_c = the fissile mass of a single unreflected unit in an array of identical units which is critical. Therefore a surface density relationship exists, which is:

$$\sigma(m_c) = c_2(m_c - m_o) \qquad (4)$$

As defined, c_2 will be negative because, mathematically, $m_c \leq m_o$ and surface density is a positive number. Also, physically, as as m_c increases the surface density of an exactly critical array will necessarily decrease due to the need for greater spacing. A line fitted to the surface density versus m_c trend will have a negative slope, so c_2 is negative.

This however requires the array response in terms of mass per package versus critical surface density to be linear in nature, extending to m_o. Non-linear array responses may lose accuracy if they deviate significantly from this relationship. It should also be noted that the user must determine m_o either through calculation or experimentation.

Equating the two forms of the surface density, exemplified in Figure 2 (which graphically is a negative sloping line and positive sloping lines with some intersection point at m_c), yields the classic application of the L-LSD method for cubic arrays:

$$\frac{m_c n}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2 = c_2(m_c - m_o) \quad (5)$$

This is in turn solved for m_c:

$$m_c = \left[1-\frac{1}{c_2}\frac{n}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2\right]^{-1} m_o \quad (6)$$

III.B N-LSD Method Development

Evaluation of the KENO results for the cubic dimension arrays of 9975s revealed that the mass versus critical surface density did not have a linear trend (Figure 3). The heterogeneities of the packages have potentially invalidated that portion of the L-LSD method basis so that a new form of the material based surface density expression must be derived. This non-linear relationship was partially evident in early work; however, approximated linear projections of the relationship were able to still give acceptable results ([7]) for certain cases.

Examination of this relationship reveals that the results clearly show that there is an exponential relationship, instead of a linear one. The non-linear behavior is most likely attributable to the nested interstitial layers of dissimilar attenuating materials (i.e. the 9975 package itself, Figure 1) between the fissile masses since radiation attenuation is naturally a non-linear exponential relationship. The data are well represented by the power fit:

$$\sigma(m_c) = c_3 e^{c_4 m_c} \quad (7)$$

The fact that this is a power fit instead of a linear function is a variation from Thomas' original derivation. The resulting changes to the relationships establish a new non-linear Limiting Surface Density formulation, the N-LSD.

It should not be overlooked that this material based surface density relationship is a function only of m_c. Addressing the non-linear response in this manner eliminates coupling the N-LSD method to the critical mass of a bare unreflected package, m_o. In practice, no facility is going to fill a package to critical mass just to set a package and material specific m_o. This eliminates the need to estimate m_o (computationally or otherwise), which removes that calculation and its uncertainty from the method.

Applying the method often involves calculating critical mass for some variation in the geometric or material parameters. To do this, we revisit the L-LSD formula equating the two definitions of surface density:

$$\frac{m_c n}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2 = c_2(m_c - m_o) \tag{8}$$

For these arrays of shipping packages, the right hand side (or material based definition) of the L-LSD method is replaced with the new material-based non-linear exponential relationship, so that the equation becomes:

$$\frac{m_c n}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2 = c_3 e^{c_4 m_c} \tag{9}$$

Rearranging the terms in a manner similar to directly solving the L-LSD method yields:

$$m_c = \frac{(2a_n)^2 c_3 e^{c_4 m_c}}{n\left(1-\frac{c}{\sqrt{N}}\right)^2} \tag{10}$$

The nature of the N-LSD form requires iteration to solve, but numerous methods and computational algorithms are available to handle this. Unfortunately this form also does not easily lend itself to partial differentiation to arrive at simple closed form sensitivities as does the L-LSD method (see Section III.C).

III.C. S-LSD Estimations

The equated surface densities definitions in the L-LSD method yield a readily solvable algebraic equation:

$$\frac{n}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2 = c_2\left(1-\frac{m_o}{m_c}\right) \tag{11}$$

It is rare that a practical application is well represented by a closed form algebraic equation. The form lends itself well to both direct solution and closed form sensitivity analysis.

The engineer typically wants the most storage capacity available and will set an arbitrarily large N to satisfy their needs. The objective then becomes to set the array spacing or the fissile mass limit that yields the desired array. If the spacing a_n is set, one can solve for a package fissile mass m_c as was shown earlier. If the package fissile mass is set, one can solve for spacing:

$$a_n = \frac{1}{2}\sqrt{\left[c_2\left(1-\frac{m_o}{m_c}\right)\left(1-\frac{c}{\sqrt{N}}\right)^{-2}\right]^{-1} n} \tag{12}$$

One may wonder at this point how sensitive is the maximum allowed mass to spacing or vice versa. To derive the sensitivity of package spacing to package fissile mass, $\frac{\partial a_n}{\partial m_c}$, let $x = c_2\left(1-\frac{c}{\sqrt{N}}\right)^{-2}$, which as defined will always be a negative value:

$$a_n = \frac{1}{2}\sqrt{\left[\left(1-\frac{m_o}{m_c}\right)x\right]^{-1} n} \tag{13}$$

The constants are collected:

$$a_n = \frac{1}{2}\sqrt{n}\left(\sqrt{x}\right)^{-1}\sqrt{\left[\left(1-\frac{m_o}{m_c}\right)\right]^{-1}} \tag{14}$$

The expression rewritten:

$$a_n = \frac{1}{2}\sqrt{n}\left(\sqrt{x}\right)^{-1}\frac{\sqrt{1}}{\sqrt{1-\frac{m_o}{m_c}}} \tag{15}$$

Let $x' = \frac{1}{2}\sqrt{n}\left(\sqrt{x}\right)^{-1}$ and $x'' = \frac{m_o}{m_c}$:

$$a_n = x'\frac{1}{\sqrt{1-x''}} \tag{16}$$

Since the result sought is $\frac{\partial a_n}{\partial m_c}$ then compute $\frac{\partial a_n}{\partial x''}$ and $\frac{\partial x''}{\partial m_c}$ and multiply them to get $\frac{\partial a_n}{\partial m_c}$:

$$\frac{\partial x''}{\partial m_c} = -\frac{m_o}{m_c^2} \text{ and } \frac{\partial a_n}{\partial x''} = x'\frac{1}{2(1-x'')^{3/2}} \tag{17}$$

Multiplying the results:

$$\frac{\partial a_n}{\partial m_c} = \frac{\partial a_n}{\partial x''}\frac{\partial x''}{\partial m_c} = x'\frac{1}{2(1-x'')^{3/2}} * \frac{-m_o}{m_c^2} \tag{18}$$

Expanding to remove x' and x'':

$$\frac{\partial a_n}{\partial m_c} = \frac{1}{2}\sqrt{n}\left(\sqrt{x}\right)^{-1}\frac{-m_o}{2\left(1-\frac{m_o}{m_c}\right)^{3/2}m_c^2} \tag{19}$$

Rearrange, replace x with $c_2\left(1-\frac{c}{\sqrt{N}}\right)^{-2}$ and collect terms:

$$\frac{\partial a_n}{\partial m_c} = \left(\frac{1}{4}\sqrt{n}\right)\left(\frac{1}{\sqrt{c_2\left(1-\frac{c}{\sqrt{N}}\right)^{-2}}}\right)\left(\frac{-m_o}{\left(1-\frac{m_o}{m_c}\right)^{3/2}m_c^2}\right) \tag{20}$$

However the following form may be a little more manageable:

$$\frac{\partial a_n}{\partial m_c} = \frac{-m_o\sqrt{n}}{4\sqrt{x}(m_c-m_o)^2\sqrt{\frac{m_c}{(m_c-m_o)}}} \tag{21}$$

To derive the sensitivity of package fissile mass to package spacing, $\frac{\partial m_c}{\partial a_n}$, let $y = \frac{1}{c_2}\left(1-\frac{c}{\sqrt{N}}\right)^2$, which as defined is also always a negative value:

$$m_c = \left[1 - y\frac{n}{(2a_n)^2}\right]^{-1} m_o \tag{22}$$

This derivation follows a similar approach and is left to the reader. The resulting sensitivity is:

$$\frac{\partial m_c}{\partial a_n} = \frac{-8a_n y n m_o}{(4a_n{}^2 - ny)^2} \quad (23)$$

Both of these show, as expected, a direct relationship of m_c and a_n such that if one increases the other must also increase to balance the array to critical conditions. These are the more useful expressions as they allow the user to directly see the sensitivity of the two most easily engineered parameters to each other. The caveat is that if the array response is non-linear, as has been seen to be the case with the heterogeneous 9975 packages, these expressions are only locally accurate. The expressions are expected to yield results increasing farther from the expected (i.e. KENO calculated) values as the m_c or a_n of interest become significantly different than the reference m_c or a_n. The S-LSD predictions would be expected to be more accurate if the array response was linear and the L-LSD method could be used.

It should be clear that it is also possible to derive relatively simple S-LSD forms with respect to c, c_2, or m_o. However, these forms tend to be of less practical use because an engineer would have much less control over these parameters than over m_c or a_n.

III.D. Shaping Factor Corrections

The methods discussed so far have been derived assuming that the arrays are cubic. In Thomas' original derivation, the arrays were spheres of material in the center of cubic volumes of air. The array was then assumed to be water reflected beyond these air-filled volumes. In practice, such as with the heterogeneous packages examined in this work, they are neither air filled nor cubic. However, the derivation is the same so long as the array is made up of a cubic *number* of units. The non-cubic nature of each individual unit and how this affects array leakage is implicitly accounted for in deriving the array constants, specifically it contributes to the numerical value of λ_{array}. It should be noted that Thomas established the validity of the method

down to a minimum number of 64 units in the array. This work evaluated established the validity down to a minimum number of 40 units.

Cubic arrays are preferential to analyze but are rarely implemented in practical situations. Especially in the KAC, arrays are typically only a few units wide and high but many units long. Different array shapes have different neutron leakage characteristics. Changing the arrangement of the array will change the neutron leakage out of it. Three options are available to the engineer. The engineer could choose to continue to use the derived constants for a cubic array, recognizing there would be a leakage error and then introduce additional margin to account for it. This defeats the purpose of having a reasonably precise method for setting the limiting mass per package. The engineer could choose to re-derive the geometry and material array constants for the specific situation, which would tune these values to the specific case being evaluated. This defeats the purpose of having a simple hand method involving few additional calculations. The remaining option is to make a leakage adjustment, a posteriori, to the array constant(s).

The adjustment is usually based on a scalar quantity known commonly as a shape factor, R. For the L-LSD method, this is a well-defined process put forth in "Generic Array Criticality: An Analytic Representation of Reflected Arrays of Fissile Units" ([3]) and illustrated for use in "Hand Calculation Methods for Criticality Safety – A Primer" ([5]). The leakage differences for this method may be compared using the shape factor defined as:

$$\mathrm{R} = \frac{\sqrt[3]{\mathrm{N}}}{3}\left(\frac{1}{\mathrm{n_x}} + \frac{1}{\mathrm{n_y}} + \frac{1}{\mathrm{n_z}}\right) \tag{24}$$

This shape factor is then used to adjust the value of c_2 compared to a cubic array. The adjustment is made using the empirical formula:

$$c_2' = \frac{4n_z'}{\sqrt[3]{N}}\left(\frac{c_2}{5R^{-0.672}-1}\right) \tag{25}$$

where c_2 is the previously determined material array constant and n_z' is the number of vertical units in the non-cubic array. The vertical dimension is used here because it is the limiting dimension (i.e. the one with the fewest units). The value c_2' is then used in place of c_2 in evaluating the L-LSD equation.

For the L-LSD method, this adjustment was originally derived for an idealized array of bare U(93.2) metal spheres with eight units per side. A similar approach was taken here in an attempt to develop an adjustment for non-cubic arrays of the heterogeneous package. Unlike the results for air-spaced arrays, these critical masses are poorly correlated with the R value. This is understandable based on the low neutron interaction between units. The 9975 package is low neutron leakage and thus any array of them, cubic or otherwise, also has minimal leakage. Any shape factor adjustment for shipping package arrays would be much smaller than that for air spaced arrays. This evaluation found no generally applicable adjustment factor based on R that improves the LSD method results. Most shipping package arrays of interest have $R < 2$, and arrays with higher R values may be evaluated using arrays with $R < 2$, without excessive conservatism. Therefore, no correction for shape will be applied to shipping package arrays, but this application is limited to $R < 2$, pending further study. For perspective, an example of an array with an $R \geq 2$ is a long row of packages, one wide and one tall.

III.E. Multiplication Factor Perturbations

The methodology developed so far is applicable to evaluating the normal or expected conditions of the storage array. However, criticality safety evaluations must also show the storage array will be safely subcritical under credible abnormal conditions due to upsets. The final portion of this work was to gauge the method's applicability for estimating the perturbation

to the multiplication factor that is introduced by a perturbation to the array using a simple approximation.

The criticality safety hand calculation primer LA-14244-M ([5]) shows that k-effective of the array can be estimated from:

$$k_{eff} = (\frac{m}{m_c})^{1/3} \quad (26)$$

Where the value of m_c is determined from the L-LSD or N-LSD method, whichever is used. With this relationship, the multiplication and reactivity (Δk/k) effect of increasing and decreasing the fissile mass loading in each unit can be estimated.

IV. PRACTICAL APPLICATION AND TESTING

Early work for the KAC problem demonstrated the feasibility of extending the L-LSD method to arrays of highly heterogeneous packages, such as the 9975 ([7]). For that early work, a special model of the 9975 was constructed which eliminated a portion of the axial geometry not occupied by fissile material while retaining the radial geometry. This resulted in a H/D=1 package which fit the cubic unit assumption of the original method development. Results were promising so further work was completed. As discussed earlier, this work employs a detailed model of the 9975 package, which retains both the axial and radial geometry near to the actual as-built package such that H/D is close to 2. This pedigreed model is used for demonstration of the methods developed herein.

First, models are constructed of arrays of 9975 packages. The arrays are cubic in the number of units per side, but not cubic in actual geometry. Cubic arrays of between 4 and 10 packages per side (i.e. 4x4x4, 5x5x5, etc.) and center-to-center package spacing of 46.6, 60, 70, 80, 90, 120, and 150 cm are evaluated. The minimum spacing is 46.6 cm as this is the diameter of the 9975 package, while 150 cm is chosen as it is arbitrarily large compared to actual array

spacing options (equate to about 1 meter of edge-to-edge spacing). These cubic arrays are modeled in SCALE with the same fissile mass in each unit and 30-cm thick concrete reflection beyond the air space boundary on all sides rather than water reflection. The mass is assumed to be 100% ^{239}Pu at 19.84 g/cm^3. For each combination of spacing and array dimension, the fissile mass per package that would make the array critical is computed in SCALE and shown in Table II. This data is then used to derive the constants c, c_2, c_3, and c_4.

A plot of surface density versus critical mass is found to have an exponential, non-linear, decay trend that is well represented by the $\sigma(m_c) = c_3 e^{c_4 m_c}$ formulation (Figure 3). For the 9975-specific application $c_3 = 1.03723\times10^{16}$ and $c_4 = -5.26423$. Five decimal places are retained here because of the strong variation in the final value of $\sigma(m_c)$ based on the exact value of the coefficients. The non-linearity of the data, as expected, did not yield a highly satisfactory value of c_2 for $\sigma(m_c) = c_2(m_c - m_o)$. The best judgement value is concluded to be -0.04839 based on trials deriving c_2 from various portions of the linear region of the data to minimize the mismatch between L-LSD results and those computed by SCALE. The critical mass of a single 9975 was determined a priori using a single unit, bare, vacuum boundary condition version of the pedigreed model: $m_o = 8385$ grams ^{239}Pu.

Although the values of NB_N^2 and $\lambda_{array}{}^2$ vary widely for different arrays, the product $NB_N^2\,\lambda_{array}{}^2$ is much less variable. Figure 4 shows a scatter plot of the results. Array pitch was arbitrarily chosen for the x-axis. The values of $NB_N^2\,\lambda_{array}{}^2$ are not clearly correlated to any single geometry parameter. The plot simply shows that most of the values are less than 10. For these shipping package arrays, that average of all the data is about 3.3. However, there are a few large values that skew this average. Since most of the data is less than 10, the outliers above 10 were discarded, and the resulting average value of $NB_N^2\,\lambda_{array}{}^2$ is 1.41. [Recall that

approximating $NB_N^2\ {\lambda_{array}}^2$ as a constant is a basic assumption for the method. Attempts to reproduce Thomas' original work indicate that he also would have discarded some outliers in the $NB_N^2\ {\lambda_{array}}^2$ values that he computed.] This results in the following geometric constant, c:

$$c = \sqrt{\frac{4 * 1.41}{3\pi^2}} = 0.44$$

This value is consistent with the value of 0.55± 0.18 recommended by Thomas.

The ability of the L-LSD and N-LSD methods to reproduce the SCALE computed critical masses for each configuration are shown in Table III and Table IV, as a percent error with respect to the values in Table II. Additionally, the S-LSD estimation technique was attempted, evaluating the sensitivity at spacing of 46.6, 90, and 150 cm with varying success as shown in Table V. The values on these tables were solved mathematically with the sensitivity equations being evaluated at the three points using the SCALE values for m_c at those points. Traditionally the method could also be solved graphically by plotting the geometric and material based formulations for surface density and citing where the curves intersected. This approach is still possible with both N-LSD as well as the L-LSD method as shown by example in Figure 2, which is for a center-to-center spacing of 46.6 cm and a cubic array of 8 packages per side. The non-linear curve in Figure 2 is the same as shown in Figure 3. It can be observed that the intersecting points of the geometry and two competing material formulas correspond to the limiting masses calculated for each method which can be derived by the reader by using the errors in Tables III and IV and the respective gram value from Table II.

Next, non-cubic arrays of 9975 packages were modeled in SCALE and the mass per package resulting in a critical array determined. The arrays are chosen to reflect practical arrangements in KAC and have (x,y,z) dimensions of 2x20x1, 2x30x1, 2x20x2, 2x20x3, 4x20x3,

and 5x5x3. Table VI shows the SCALE results for masses. Three attempts were made to reproduce the values from SCALE, which included the unmodified L-LSD method, the unmodified N-LSD method, and the shape factor corrected L-LSD method. The relative error between these predictions and the SCALE values are shown in Table VII, Table VIII, and Table IX, respectively. The reader is reminded to view these results with the knowledge that, by design, the 9975 is a low neutron leakage package in and of itself so there is little coupling between the packages regardless of array dimensions.

Finally, the ability of the method to predict perturbations in the multiplication factor, by appropriately predicting changes in mass, is evaluated. There is typically some spacing between each shipping package based on how they are palletized. But for this example that spacing is ignored and the horizontal pitch is assumed to be 46.6 cm. The N-LSD equation for critical mass is applied with a_n = 46.6, c = 0.44, $c_3 = 1.03723 \times 10^{16}$, $c_4 = -5.26423$, N = 10×14×3 = 420, and $n = \sqrt[3]{420}$. The first mass permutation considered is for the current loading limit of 4.4 kg ^{239}Pu in the 9975. Using this input, the method returns an array critical mass per unit of m_c = 7.703 kg.

$$k_{eff} = \left(\frac{m}{m_c}\right)^{\frac{1}{3}} = \left(\frac{4.4\ kg}{7.703\ kg}\right)^{\frac{1}{3}} = 0.830$$

Computing the changes in reactivity as Δk/k for several changes in mass is shown in Table X compared with the same scenario modeled in SCALE. The values in Table X are rounded to three decimal places.

Next, the reactivity effect of spacing changes are examined. Suppose that the base case array pitch is increased by 5 cm or 10 cm. These changes result in k_{eff} values of 0.828 and 0.827, respectively. This may also be expressed as Δk/k of -0.002, and -0.003.

Then, the reactivity effect of stacking changes is examined. Suppose that an additional layer of identical shipping packages is placed on the base case array. At KAC, adding a full fourth layer is not credible, but this is done as a bounding estimate. The calculations use N = $10\times14\times4$ = 560, and $n = \sqrt[3]{560}$. The results are m_c = 7.685 kg and k_{eff} = 0.830. The change in multiplication is only seen in the 4th significant figure, and is a trivial change in safety margin.

Finally, the reactivity effect of varying array size is examined. Suppose that different sizes of separate storage arrays are used in a facility. Consider arrays that are 6x6x3 and 20x30x3. The calculations are repeated with:

- $N = 6\times6\times3$ = 108, and $n = \sqrt[3]{108}$
- $N = 20\times30\times3$ = 1800, and $n = \sqrt[3]{1800}$

Resulting critical mass and multiplication values are:

- 6x6x3: m_c = 7.795 kg and k_{eff} = 0.826
- 20x30x3: m_c = 7.609 kg and k_{eff} = 0.833

These substantial differences in array size have a modest reactivity effect, with Δk/k of -0.005 and 0.004, respectively, compared to the 10x14x3 base case. This shows that there is little penalty in safety margin due to over estimating the array size.

Although not explicitly presented here, except in Table X, these calculations are in reasonably good agreement with the SCALE results for the same perturbations.

V. CONCLUSIONS AND FUTURE WORK

The LSD method is found to be acceptable for evaluating arrays of heterogeneous 9975 shipping packages containing plutonium metal (or equivalent) fissile mass. Of the three methods evaluated herein, the N-LSD method provides results closest to the computational models. This

is to be expected since it accounts for the non-linear response of the packages within the array. The L-LSD method provides acceptable results but would require some additional engineering margin. For non-cubic arrays, the L-LSD method shaping adjustment to account for leakage results in marginal improvements in agreement with computational models, but still does not surpass the N-LSD method without adjustment. The S-LSD method provides various degrees of disagreement with the computational models, depending upon which conditions are used for evaluation. In general, disagreement with computational models is more severe as spacing became increasingly different than the conditions where the sensitivity was evaluated. The S-LSD method may then be better for only localized or scoping predictions for arrays that are already modestly spaced.

No practical adjustment correlating shape factor to array neutron leakage was determined for the N-LSD method. The 9975 is a low leakage package so any adjustment would be minimal anyway. The N-LSD method was thus qualitatively restricted to cubic arrays and non-cubic arrays of $R < 2$.

The N-LSD method also provides very good predictions for changes in reactivity due to changes in package mass, spacing, stacking, and array size. This indicates the method is acceptable for examining certain array perturbations due to credible abnormal events. Being applicable to both normal and credible abnormal events would make this method viable for performing criticality safety evaluations without using other methods.

Future work will continue to examine the development of the method for reactivity perturbations induced by credible abnormal events. There is also interest in examining the response of the system if the fissile mass is assumed to be oxide rather than metal.

Finally, the reader will find in the Appendix a re-derivation of the classic L-LSD method from diffusion theory, specifically from cuboid buckling, and the first principle's definition of surface density. A full derivation was found to be lacking in the original literature and may be a useful reference for future method development.

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REFERENCES

[1] J.T. Thomas, "Uranium Metal Criticality, Monte Carlo Calculations and Nuclear Criticality Safety", *Y-CDC-7*, Union Carbide Corporation, Oak Ridge Y-12 Plant, Nuclear Division, September 1970.

[2] J.T. Thomas, "The Criticality of Cubic Arrays of Fissile Material", *Y-CDC-10*, Union Carbide Corporation, Oak Ridge Y-12 Plant, Nuclear Division, November 1971.

[3] J.T. Thomas, "Generic Array Criticality: An Analytic Representation of Reflected Arrays of Fissile Units", *Y-CDC-13*, Union Carbide Corporation, Oak Ridge Y-12 Plant, Nuclear Division, August 1973.

[4] J.T. Thomas, "Surface Density and Density Analog Models for Criticality in Arrays of Fissile Materials", *Nuclear Science and Engineering*, Vol. 62, 1977.

[5] D. Bowen and R. Busch, "Hand Calculation Methods for Criticality Safety – A Primer", *LA-14244-M,* Los Alamos National Laboratory, 2006.

[6] "Nuclear Criticality Safety in the Storage of Fissile Materials", *ANS/ANSI 8.7-1998*, Reaffirmed 2007, American Nuclear Society, La Grange Park, IL, 2007.

[7] T. Stover, J. Baker, M. Ratliff, "Limiting Surface Density Method Application to Large Arrays of Highly Heterogeneous Shipping Packages," *Trans. Amer. Nucl. Soc.*, Vol. 114, June 2016.

[8] J. Baker, M. Ratliff, T. Stover, G. Mitschelen, "Verification Suite for the Application of the Limiting Surface Density Method to Arrays of 9975 Packages", *Proceedings of the ANS 2017 Nuclear Criticality Safety Division Topical*, September 2017.

[9] J. Bellamy, J. McEvoy, R. Watkins, "Safety Analysis Report for Packaging Model 9975, Revision 4", *S-SARP-G-00003*, Savannah River Nuclear Solutions, Aiken, SC, December 2015.

APPENDIX: LINEAR LSD METHOD RE-DERIVATION

For a number of years engineers implementing the classic L-LSD method have dealt with rather spartan literature regarding Thomas' original method development. Effort was made in this work to re-derive Thomas' method for documentation purposes, and a derivation of the basic relationships is included here to provide complete documentation of the method development.. Much of the detail given here was omitted from Thomas' papers ([1]-[4]). The LSD method is based on the number of units in the array, N, and the array buckling, B_N^2. From basic nuclear physics, the geometric buckling of a parallelepiped is:

$$B_g^2 = \frac{\pi^2}{(d_x+2\lambda_x)^2} + \frac{\pi^2}{(d_y+2\lambda_y)^2} + \frac{\pi^2}{(d_z+2\lambda_z)^2} \quad \text{(A.1)}$$

Here the dimensions in the x, y, and z directions are denoted by d_x, d_y and d_z and extrapolation distances λ_x, λ_y, and λ_z are determined by the geometry along each direction. Thomas worked with air filled, material centric cubic geometry which results in relatively simple reduced expressions, beginning first by considering symmetry: $d_x = d_y = d_z = d = 2a_n$ and $\lambda_x = \lambda_y = \lambda_z = \lambda$

Note that a_n is the half dimension of the cubic cell, and λ is the extrapolation distance of the unit cell, not of the array. Substituting this back into the preceding form reduces the geometric buckling of the unit cell to:

$$B_g^2 = \frac{3\pi^2}{(2a_n+2\lambda)^2} \quad \text{(A.2)}$$

The extension of the cubic unit is the cubic array of N units that is n x n x n units in dimension. The array buckling is then:

$$B_N^2 = \frac{3\pi^2}{(n2a_n+2\lambda_{array})^2} \quad \text{(A.3)}$$

The form of NB_N^2 developed for Thomas's method is as follows:

$$NB_N^2 = \frac{N3\pi^2}{(n2a_n+2\lambda_{array})^2} = \frac{n^3 3\pi^2}{(n2a_n+2\lambda_{array})^2} \tag{A.4}$$

Expanding the denominator gives:

$$NB_N^2 = \frac{n^3 3\pi^2}{(4\lambda_{array}^2+4n^2a_n^2+8na_n\lambda_{array})} \tag{A.5}$$

Next, divide both the numerator and denominator by the quantity $(4n^2a_n^2)$:

$$NB_N^2 \frac{(4n^2a_n^2)}{(4n^2a_n^2)} = \frac{n^3 3\pi^2/(4n^2a_n^2)}{\left(\frac{4\lambda_{array}^2}{(4n^2a_n^2)}+\frac{4n^2a_n^2}{(4n^2a_n^2)}+\frac{8na_n\lambda_{array}}{(4n^2a_n^2)}\right)} \tag{A.6}$$

Reducing this as appropriate:

$$NB_N^2 = \frac{n3\pi^2/(4a_n^2)}{\left(\frac{\lambda_{array}^2}{n^2a_n^2}+1+\frac{2\lambda_{array}}{na_n}\right)} = \frac{n3\pi^2/(2a_n)^2}{\left(\frac{\lambda_{array}^2}{n^2a_n^2}+1+\frac{2\lambda_{array}}{na_n}\right)} \tag{A.7}$$

Because it will be used in algebraic manipulations, write the numerator into a separate quantity:

$$NB_N^2 = \left(\frac{n3\pi^2}{(2a_n)^2}\right)\frac{1}{\left(\frac{\lambda_{array}^2}{n^2a_n^2}+1+\frac{2\lambda_{array}}{na_n}\right)} \tag{A.8}$$

However, it is observed now that the denominator of the second term is itself a perfect square:

$$\left(\frac{\lambda_{array}^2}{n^2a_n^2}+1+\frac{2\lambda_{array}}{na_n}\right) = \left[\left(\frac{\lambda_{array}}{na_n}\right)\left(\frac{\lambda_{array}}{na_n}\right)+1+\left(\frac{\lambda_{array}}{na_n}\right)+\left(\frac{\lambda_{array}}{na_n}\right)\right] = \left(1+\left(\frac{\lambda_{array}}{na_n}\right)\right)^2$$

(A.9)

Then NB_N^2 is written:

$$NB_N^2 = \left(\frac{n3\pi^2}{(2a_n)^2}\right)\frac{1}{\left(1+\frac{\lambda_{array}}{na_n}\right)^2} \tag{A.10}$$

Next, the second term on the right is manipulated using the mathematical relationship:

$$\frac{1}{(1+x)^2} = \left(1-\frac{1}{1+1/x}\right)^2 \tag{A.11}$$

Conceding that $1^2=1$:

$$\frac{1}{(1+x)^2} = \left(1 - \frac{1}{1+1/x}\right)^2 \tag{A.12}$$

This is just an identity property the same as $1^2=1$.

Begin by considering $\frac{1}{(1+x)^2} = \left(\frac{1}{1+x}\right)^2$ because 1*1 = 1:

$$\left(\frac{1}{1+x}\right)\left(\frac{1}{1+x}\right) = \left(\frac{1*1}{(1+x)(1+x)}\right) = \frac{1^2}{(1+x)^2} = \left(\frac{1}{1+x}\right)^2 \tag{A.13}$$

Dividing both the numerator and denominator by x has no effect because $\frac{x}{x} = \frac{x^{-1}}{x^{-1}} = 1$:

$$\left(\frac{1}{1+x}\right)^2\left(\frac{x^{-1}}{x^{-1}}\right) = \left(\frac{1/x}{1/x+x/x}\right)^2 = \left(\frac{1/x}{1/x+1}\right)^2 \tag{A.14}$$

Adding and subtracting 1 from the numerator has no effect on the value because -1 + 1 = 0:

$$\left(\frac{\frac{1}{x}+1-1}{1/x+1}\right)^2 \tag{A.15}$$

But this does allow separation into two fractions:

$$\left(\frac{\frac{1}{x}+1-1}{1/x+1}\right)^2 = \left(\frac{\frac{1}{x}+1}{1/x+1} - \frac{1}{1/x+1}\right)^2 \tag{A.16}$$

Which reduces to:

$$\left(\frac{\frac{1}{x}+1}{1/x+1} - \frac{1}{1/x+1}\right)^2 = \left(1 - \frac{1}{1+1/x}\right)^2 \tag{A.17}$$

So:

$$\frac{1}{(1+x)^2} = \left(\frac{1}{1+x}\right)^2 = \left(\frac{1/x}{1+1/x}\right)^2 = \left(\frac{\frac{1}{x}+1-1}{1+1/x}\right)^2 = \left(\frac{1+1/x}{1+1/x} - \frac{1}{1+1/x}\right)^2 = \left(1 - \frac{1}{1+1/x}\right)^2 \tag{A.18}$$

Let $x = \frac{\lambda_{array}}{na_n}$:

$$\frac{1}{\left(1+\frac{\lambda_{array}}{na_n}\right)^2} = \left(1 - \frac{1}{1+1/\left(\frac{\lambda_{array}}{na_n}\right)}\right)^2 \tag{A.19}$$

But since $\frac{1}{\left(\frac{\lambda_{array}}{na_n}\right)} = \frac{na_n}{\lambda_{array}}$ it follows that:

$$\frac{1}{\left(1+\frac{\lambda_{array}}{na_n}\right)^2} = \left(1 - \frac{1}{1+\frac{na_n}{\lambda_{array}}}\right)^2 \quad \text{(A.20)}$$

Inserting the relationship back into the expression forNB_N^2:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \frac{1}{1+\frac{na_n}{\lambda_{array}}}\right)^2 \quad \text{(A.21)}$$

Consider the quantity $1 + \frac{na_n}{\lambda_{array}}$, which if it is squared looks like:

$$\left(1 + \frac{na_n}{\lambda_{array}}\right)\left(1 + \frac{na_n}{\lambda_{array}}\right) = 1 + \left(\frac{na_n}{\lambda_{array}}\right) + \left(\frac{na_n}{\lambda_{array}}\right) + \left(\frac{na_n}{\lambda_{array}}\right)\left(\frac{na_n}{\lambda_{array}}\right) = 1 + 2\left(\frac{na_n}{\lambda_{array}}\right) + \left(\frac{na_n}{\lambda_{array}}\right)^2 \quad \text{(A.22)}$$

It was stated earlier that:

$$B_N^2 = \frac{3\pi^2}{(4\lambda_{array}^2 + 4n^2a_n^2 + 8na_n\lambda_{array})} \quad \text{(A.23)}$$

If this quantity was inverted:

$$\frac{1}{B_N^2} = \frac{(4\lambda_{array}^2 + 4n^2a_n^2 + 8na_n\lambda_{array})}{3\pi^2} \quad \text{(A.24)}$$

And then it was multiplied by $3\pi^2$:

$$\frac{3\pi^2}{B_N^2} = \left(4\lambda_{array}^2 + 4n^2a_n^2 + 8na_n\lambda_{array}\right) \quad \text{(A.25)}$$

And then it was divided by $4\lambda_{array}^2$:

$$\frac{3\pi^2}{4\lambda_{array}^2 B_N^2} = \left(\frac{4\lambda_{array}^2}{4\lambda_{array}^2} + \frac{4n^2a_n^2}{4\lambda_{array}^2} + \frac{8na_n\lambda_{array}}{4\lambda_{array}^2}\right) \quad \text{(A.26)}$$

$$\frac{3\pi^2}{4\lambda_{array}^2 B_N^2} = \left(1 + \frac{n^2 a_n^2}{\lambda_{array}^2} + \frac{2na_n}{\lambda_{array}}\right) \tag{A.27}$$

However, we just established another form of this right hand side:

$$\frac{3\pi^2}{4\lambda_{array}^2 B_N^2} = \left(1 + \frac{na_n}{\lambda_{array}}\right)^2 \tag{A.28}$$

Taking the square root of the right hand side takes us back to our starting quantity of $1 + \frac{na_n}{\lambda_{array}}$

so that means:

$$\sqrt{\frac{3\pi^2}{4\lambda_{array}^2 B_N^2}} = \sqrt{\left(1 + \frac{na_n}{\lambda_{array}}\right)^2} = 1 + \frac{na_n}{\lambda_{array}} \tag{A.29}$$

Now substitute back into the equation for NB_N^2:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \frac{1}{\sqrt{\frac{3\pi^2}{4\lambda_{array}^2 B_N^2}}}\right)^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \sqrt{\frac{4\lambda_{array}^2 B_N^2}{3\pi^2}}\right)^2 \tag{A.30}$$

Multiply the fraction under the radical by 1 and change nothing so we multiply it by 1 = N/N:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \sqrt{\frac{4\lambda_{array}^2 B_N^2}{3\pi^2} * 1}\right)^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \sqrt{\frac{4\lambda_{array}^2 NB_N^2}{N3\pi^2}}\right)^2 \tag{A.31}$$

Which is the Thomas form of NB_N^2. Using Thomas' assertion that $\sqrt{\frac{4\lambda_{array}^2 NB_N^2}{3\pi^2}}$ is a constant, c:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 \tag{A.32}$$

The problem now is to relate this to surface density. Surface density, generically, is mass divided by area. The array mass is projected onto a plane and that plane is chosen to be the surface area the array occupies. The limiting surface density is that which results in a critical configuration of the array. The dimensions of the critical array must include the array extrapolation distance, λ_{array}. The surface density, σ, of an array of packages each of mass m is:

$$\sigma(m) = \frac{mass}{area} = \frac{mN}{(n2a_n+2\lambda_{array})^2} = \frac{mn^3}{(n2a_n+2\lambda_{array})^2} \quad (A.33)$$

Recall our earliest definition of NB_N^2:

$$NB_N^2 = \frac{n^3 3\pi^2}{(n2a_n+2\lambda_{array})^2} \quad (A.34)$$

Divide both sides by $3\pi^2$ and then multiply both sides by m:

$$\frac{mNB_N^2}{3\pi^2} = \frac{n^3 3\pi^2 m}{3\pi^2(n2a_n+2\lambda_{array})^2} = \frac{mn^3}{(n2a_n+2\lambda_{array})^2} \quad (A.35)$$

Then the right hand side now matches the definition of surface density so:

$$\sigma(m) = \frac{mn^3}{(n2a_n+2\lambda_{array})^2} = \frac{mNB_N^2}{3\pi^2} \quad (A.36)$$

At this point, substitute in the final definition of $NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2$ and reduce:

$$\sigma(m) = \left(\frac{m}{3\pi^2}\right)\left(\frac{n3\pi^2}{(2a_n)^2}\right)\left(1-\frac{c}{\sqrt{N}}\right)^2 = \left(\frac{mn}{(2a_n)^2}\right)\left(1-\frac{c}{\sqrt{N}}\right)^2 \quad (A.37)$$

The form $\sigma(m) = \left(\frac{mn}{(2a_n)^2}\right)\left(1-\frac{c}{\sqrt{N}}\right)^2$ is the definition of surface density from the classic limiting surface density method that Thomas developed.

Let m_o = critical fissile mass of a single unreflected unit and m_c = the fissile mass of a single unit in an array of identical units which is critical. When Thomas derived the method, m_o was the mass of a bare sphere and m_c was the mass of air spaced spheres in a water reflected array.

Everything derived up to this point is geometry based. One may also define surface density based on material properties. One may define many combinations of N and a_n of an array and then calculate the m_c for each combination. The surface density can then be determined by calculating mass/area of the critical array. The plot of surface density versus m_c may be linear, nearly linear, or as we see in the body of this work, non-linear. For the classic LSD

method however, it is assumed to be linear and will thus always cross the x-axis at $m_c = m_o$. Physically, this means that as mass of each unit approaches m_o, the surface density approaches zero because the surface area becomes infinite.

In this manner, by directly calculating m_c which makes the array exactly critical, the geometry of the fissile material, spacing of the units, and number of units are pre-set by the user. This means approximations of physical behaviors that have been made, specifically λ_{array}, are implicitly included because the user manually tunes m_c so the array is critical with N and a_n specified.

Thomas' papers state that, in the plot of surface density versus m_c, the slope of the linear fit of the data is a constant called c_2. c_2 is negative because as fissile mass per unit goes up surface density of the critical array must go down. Therefore a surface density relationship exists, which is:

$$\sigma(m_c) = c_2(m_c - m_o) \tag{A.38}$$

The right hand side is as defined above because the slope of surface density versus m_c is c_2 and that value is always negative. Because $(m_c - m_o)$ is also always negative, the product of this and c_2 must always be positive. We could just as easily have defined c_2 as the absolute value of the slope and just reverse the order to $(m_o - m_c)$ to get the same result. The original formulation is retained here for consistency with the previously referenced material.

Equating the two forms of the surface density (which graphically are a negative sloping line and positive sloping line with some intersection point at m_c) yields the classic application of the limiting surface density method for cubic arrays:

$$\frac{m_c n}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = c_2(m_c - m_o) \tag{A.39}$$

This form has many parameters, so it is good for study but not yet for practical application. The material specific array constant, c_2, cannot be manipulated by the user since it is a property of the fissile material and its packaging. The geometry specific array constant, c, cannot be directly manipulated by the user because it is a constant value. This single unit critical mass, m_o, cannot be manipulated by the user because it is also a property of the fissile material and its packaging. What the user can control is number of packages N, spacing a_n, and mass per package. In practice, the engineer will have $\{c,c_2,m_o\}$ as fixed properties, set two of the three variables $\{N,a_n,m_c\}$ and solve for the remaining one. The engineer may do a parametric search to find some optimal solution, but the equation can have only one unknown to get a numerical solution. The equated surface densities above are divided through by m_c and this is the final form of the classic limiting surface density method commonly seen in textbooks and primers:

$$\frac{n}{(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2 = c_2\left(1-\frac{m_o}{m_c}\right) \qquad \text{(A.40)}$$

It is rare that a practical application is well represented by a closed form algebraic equation. The form lends itself well to both direct solution and closed form sensitivity analysis.

As discussed earlier, Thomas asserts that $c = \sqrt{\frac{4\lambda_{array}{}^2}{3\pi^2}NB_N^2}$ is a constant independent of material and dependent only on geometry. "The Criticality of Cubic Arrays of Fissile Material" ([2]) gives c = 0.312 ± 0.001, however later work ([1],[3]) gives c = 0.55 ± 0.18. The relatively large uncertainty in c is compensated for by the fact that the value of c has a small effect for large arrays since it is divided by the square root of the number of units. Thomas stated the method was applicable for arrays of 64 units or larger so at the very least c is divided by 8 in practical application.

Table I: 9975 Dimensions for SCALE Model

Component	Parameter	Specification (cm)
Primary Containment Vessel (Stainless Steel)	Inner Diameter	12.8194
	Outer Diameter	14.1300
	Inner Radius	6.4097
	Outer Radius	7.0650
	Inner Height	45.0850
	Outer Height	46.0248
	Bottom Thickness	0.6553
	Wall Thickness	0.6553
	Lid Thickness	3.5052
Secondary Containment Vessel (Stainless Steel)	Inner Diameter	15.4051
	Outer Diameter	16.8275
	Inner Radius	7.7026
	Outer Radius	8.4138
	Inner Height	58.0136
	Outer Height with air gap	59.6900
	Bottom Thickness	0.7112
	Wall Thickness	0.7112
	Lid Thickness	3.5052
Lead Shield	Inner Diameter	18.5979
	Outer Diameter	21.2014
	Inner Radius	9.2989
	Outer Radius	10.6007
	Wall Thickness (average)	1.2103
Stainless Steel Jacket	Thickness	0.0914
Aluminum Bearing Plates	Diameter	28.4480
	Radius	14.2240
	Thickness	1.2700
9975 Outer Drum (Stainless Steel)	Inner Diameter	46.3550
	Outer Diameter	46.5988
	Inner Radius	23.1775
	Outer Radius	23.2994
	Inner Height	88.2650
	Outer Height	88.5088
	Thickness	0.1219

Table II: SCALE Calculated Fissile Mass (g) per Package for a Cubic Critical Array

	Center-to-Center Spacing ($2*a_n$)						
Number of Units per Side, n	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
4	7798 g	7923 g	7975 g	8028 g	8058 g	8167 g	8231 g
5	7749 g	7871 g	7930 g	7975 g	8009 g	8134 g	8198 g
6	7725 g	7834 g	7880 g	7925 g	7969 g	8090 g	8171 g
7	7698 g	7804 g	7856 g	7896 g	7929 g	8061 g	8144 g
8	7691 g	7787 g	7829 g	7875 g	7913 g	8039 g	8126 g
9	7666 g	7763 g	7814 g	7853 g	7886 g	8014 g	8094 g
10	7668 g	7760 g	7802 g	7837 g	7865 g	7984 g	8081 g

Table III: L-LSD Method Prediction Error (%) for Cubic Array Fissile Mass per Container

	Center-to-Center Spacing ($2*a_n$)						
Number of Units per Side, n	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
4	4.00%	3.71%	3.58%	3.26%	3.12%	2.14%	1.53%
5	3.66%	3.78%	3.72%	3.60%	3.47%	2.41%	1.85%
6	3.02%	3.67%	3.94%	3.91%	3.72%	2.81%	2.09%
7	2.42%	3.48%	3.82%	3.96%	3.98%	3.03%	2.33%
8	1.59%	3.12%	3.74%	3.89%	3.92%	3.16%	2.46%
9	1.01%	2.88%	3.51%	3.85%	4.01%	3.34%	2.77%
10	0.09%	2.34%	3.24%	3.73%	4.03%	3.58%	2.84%

Table IV: N-LSD Method Prediction Error (%) for Cubic Array Fissile Mass per Container

	Center-to-Center Spacing ($2*a_n$)						
Number of Units per Side, n	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
4	0.44%	0.04%	0.1%	0.06%	0.23%	0.20%	0.42%
5	0.46%	0.09%	0.07%	0.13%	0.24%	0.02%	0.25%
6	0.29%	0.09%	0.23%	0.28%	0.27%	0.09%	0.12%
7	0.23%	0.07%	0.15%	0.26%	0.39%	0.08%	0.07%
8	-0.01%	-0.05%	0.15%	0.19%	0.26%	0.02%	-0.03%
9	0.01%	-0.03%	0.05%	0.18%	0.31%	0.05%	0.08%
10	-0.28%	-0.25%	-0.06%	0.12%	0.32%	0.17%	-0.01%

Table V: S-LSD Estimation Error (%) for Cubic Array Fissile Mass per Container

	Center-to-Center Spacing ($2*a_n$)						
Number of Units per Side, n	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
Sensitivity Predictor Evaluated at $2*a_n$ =46.6 cm							
4	0.00%	0.36%	1.13%	1.89%	2.94%	5.76%	9.10%
5	0.00%	0.92%	1.99%	3.24%	4.61%	8.36%	12.81%
6	0.00%	1.58%	3.20%	4.81%	6.41%	11.28%	16.58%
7	0.00%	2.11%	4.01%	6.04%	8.14%	13.90%	20.17%
8	0.00%	2.70%	5.08%	7.36%	9.73%	16.55%	23.74%
9	0.00%	3.15%	5.73%	8.44%	11.20%	18.96%	27.21%
10	0.00%	3.63%	6.64%	9.73%	12.88%	21.69%	30.58%
Sensitivity Predictor Evaluated at $2*a_n$ =90 cm							
4	2.41%	1.07%	0.61%	0.16%	0.00%	-0.73%	-0.89%
5	2.16%	0.94%	0.46%	0.16%	0.00%	-0.74%	-0.73%
6	1.71%	0.73%	0.48%	0.23%	0.00%	-0.53%	-0.55%
7	1.27%	0.42%	0.16%	0.04%	0.00%	-0.49%	-0.38%
8	0.91%	0.26%	0.18%	0.03%	0.00%	-0.26%	-0.02%
9	0.63%	0.06%	-0.09%	-0.08%	0.00%	-0.11%	0.37%
10	0.08%	-0.34%	-0.32%	-0.20%	0.00%	0.17%	0.59%
Sensitivity Predictor Evaluated at $2*a_n$ =150 cm							
4	1.77%	0.65%	0.34%	0.04%	0.03%	-0.26%	0.00%
5	0.90%	-0.04%	-0.32%	-0.42%	-0.39%	-0.56%	0.00%
6	-0.18%	-0.82%	-0.82%	-0.83%	-0.83%	-0.66%	0.00%
7	-1.22%	-1.66%	-1.64%	-1.48%	-1.24%	-0.91%	0.00%
8	-2.37%	-2.55%	-2.31%	-2.13%	-1.84%	-1.15%	0.00%
9	-3.48%	-3.52%	-3.29%	-2.92%	-2.48%	-1.51%	0.00%
10	-4.65%	-4.49%	-4.06%	-3.54%	-2.93%	-1.58%	0.00%

Table VI: SCALE Calculated Fissile Mass (g) per Package for a Non-Cubic Critical Array

	Center-to-Center Spacing ($2*a_n$)						
Dimensions (width, depth, height)	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
2x20x1	7876 g	8028 g	8093 g	8137 g	8174 g	8245 g	8304 g
2x30x1	7869 g	8020 g	8088 g	8145 g	8178 g	8250 g	8302 g
2x20x2	7847 g	7982 g	8045 g	8086 g	8123 g	8217 g	8259 g
2x20x3	7843 g	7961 g	8027 g	8066 g	8093 g	8200 g	8255 g
4x20x3	7737 g	7862 g	7922 g	7967 g	8009 g	8128 g	8198 g
5x5x3	7761 g	7892 g	7958 g	7999 g	8041 g	8154 g	8223 g

Table VII: Uncorrected L-LSD Method Prediction Error (%) for Non-Cubic Array Fissile Mass per Container

	Center-to-Center Spacing ($2*a_n$)						
Dimensions (width, depth, height)	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
2x20x1	5.59%	3.93%	3.23%	2.76%	2.36%	1.57%	0.90%
2x30x1	5.66%	4.02%	3.28%	2.65%	2.30%	1.51%	0.91%
2x20x2	5.05%	3.97%	3.43%	3.09%	2.76%	1.79%	1.35%
2x20x3	4.18%	3.68%	3.26%	3.03%	2.88%	1.85%	1.32%
4x20x3	5.53%	4.95%	4.60%	4.29%	3.94%	2.74%	2.02%
5x5x3	5.33%	4.62%	4.18%	3.92%	3.56%	2.44%	1.72%

Table VIII: Uncorrected N-LSD Method Prediction Error (%) for Non-Cubic Array Fissile Mass per Container

	Center-to-Center Spacing ($2*a_n$)						
Dimensions (width, depth, height)	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
2x20x1	-0.12%	-0.84%	-0.93%	-0.86%	0.77%	0.33%	-0.04%
2x30x1	-0.41%	-1.12%	-1.24%	-1.33%	-1.18%	-0.75%	-0.38%
2x20x2	-0.39%	-0.91%	-0.98%	-0.87%	-0.77%	-0.60%	-0.12%
2x20x3	-0.70%	-1.01%	-1.11%	-0.97%	-0.76%	0.75%	-0.41%
4x20x3	0.04%	-0.36%	-0.39%	-0.33%	-0.32%	0.46%	-0.29%
5x5x3	0.77%	0.28%	0.17%	0.28%	0.29%	0.22%	0.39%

Table IX: Shaping Factor Corrected L-LSD Method Prediction Error (%) for Non-Cubic Array Fissile Mass per Container

	Center-to-Center Spacing ($2*a_n$)						
Dimensions (width, depth, height)	46.6 cm	60 cm	70 cm	80 cm	90 cm	120 cm	150 cm
2x20x1	4.81%	3.51%	2.95%	2.58%	2.24%	1.56%	0.93%
2x30x1	4.83%	3.57%	2.98%	2.45%	2.17%	1.49%	0.94%
2x20x2	4.29%	3.55%	3.16%	2.91%	2.64%	1.77%	1.39%
2x20x3	3.80%	3.50%	3.16%	2.98%	2.86%	1.90%	1.39%
4x20x3	3.91%	4.01%	3.94%	3.81%	3.59%	2.60%	1.97%
5x5x3	4.49%	4.16%	3.87%	3.71%	3.42%	2.42%	1.75%

Table X: Multiplication and Reactivity for Changing Unit Mass in a 10x14x3 Array of 9975 Shipping Packages

Unit Mass (kg)	k_{eff}	Δk/k	SCALE k_{eff}
3.4	0.761	-0.082	0.768
3.9	0.797	-0.039	0.804
4.4 (base case)	0.830	--	0.836
4.9	0.860	0.037	0.866
5.4	0.888	0.071	0.894
7.703	1.000	N/A[1]	1.002

[1]This is the calculated critical state and 7.703 kg serves as basis for the other reactivity perturbation values, hence Δk/k is not applicable here. See Equation 26 and Section IV.

Figure 1: Design and KENO Model Renderings of the 9975 Shipping Package

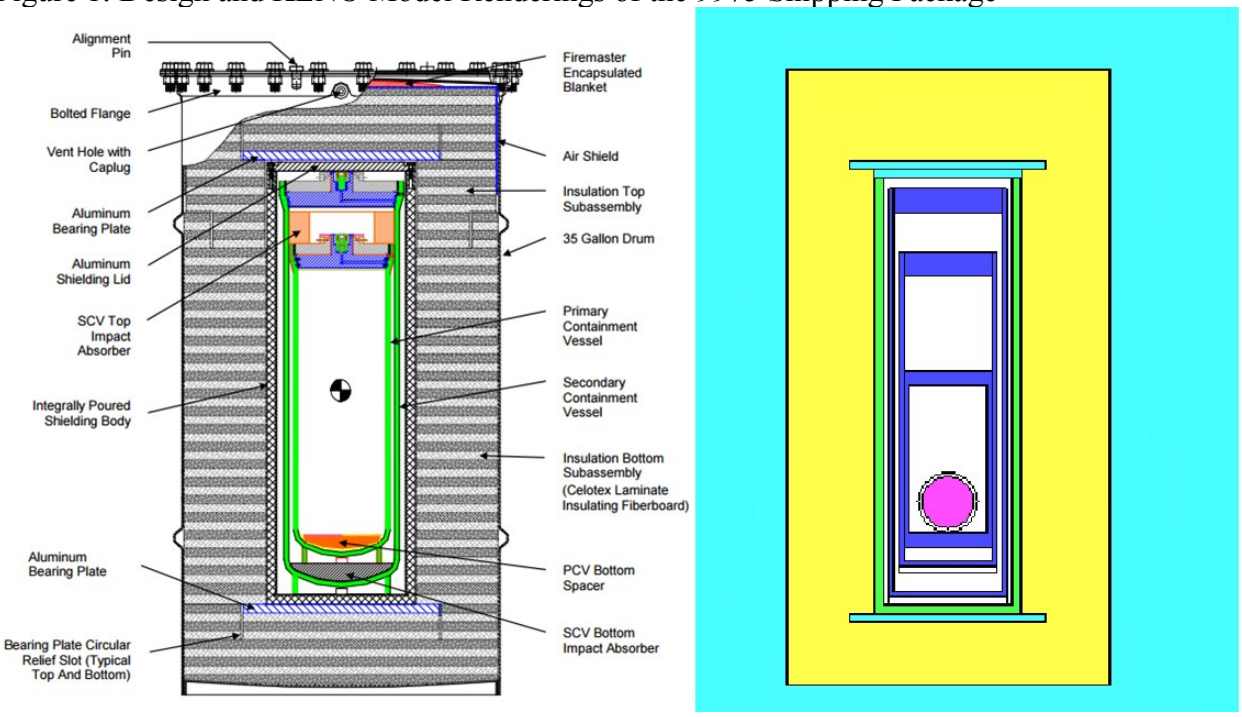

Figure 2: Plot of Surface Density Functions for an Example Array

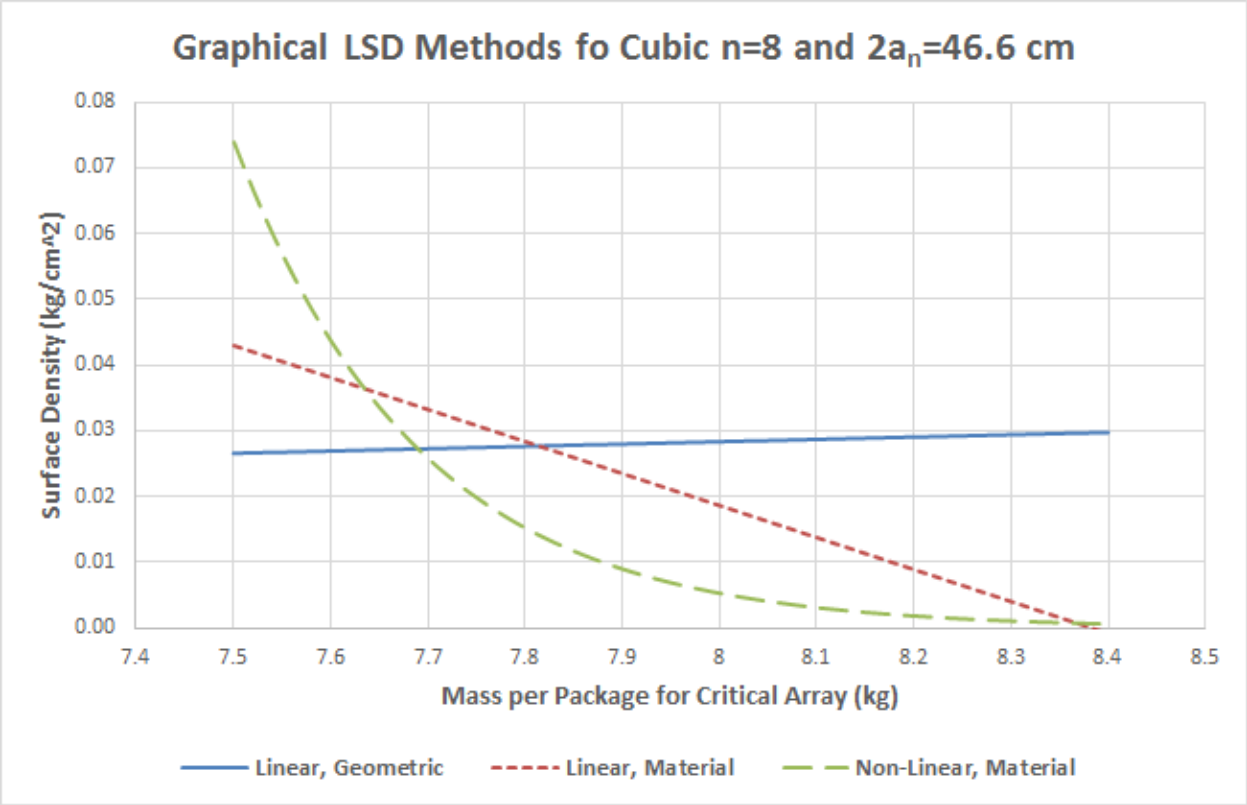

Figure 3: Surface Density versus Package Fissile Mass Resulting in a Critical Array

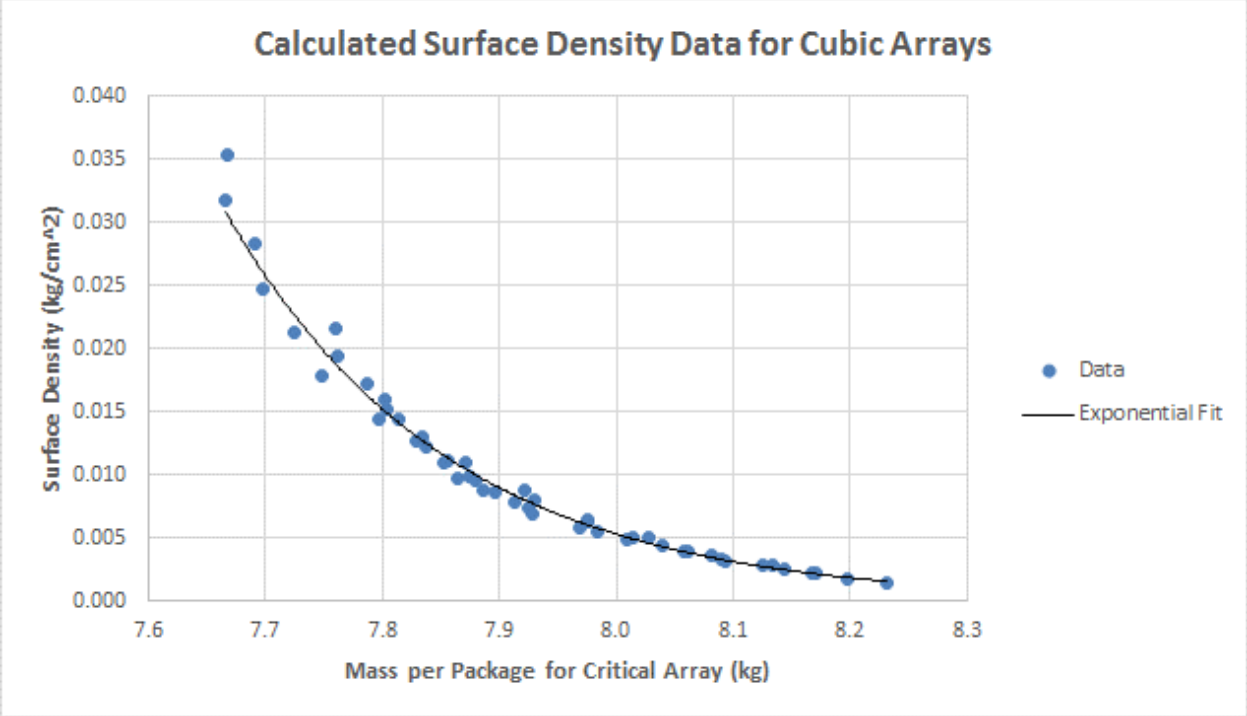

Figure 4: Scatter Plot of $NB_N^2\ {\lambda_{array}}^2$ Data