# Application of the Limiting Surface Density Method to Arrays of 9975 Shipping Packages with Plutonium Oxide 

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## Introduction

- Reducing our computational burden by extending the Limiting Surface Density (LSD) Method to apply to arrays of 9975 shipping packages with Pu Oxide

- LA-14244-M (Hand Calculation Primer) has an overview and several example applications for the original method by Joe Thomas.


## Background

- Previous work for Pu Metal contents is given in:
- 2017 NCSD Topical Meeting, Verification Suite for the Application of the Limiting Surface Density Method to Arrays of 9975 Shipping Packages, J. Baker, T. Stover, M. Ratliff and G. Mitschelen.
- Nuclear Science and Engineering, Volume 190, Issue 2, pp 176-194, Limiting Surface Density Method Adapted to Large Arrays of Heterogeneous Shipping Packages with Nonlinear Responses, T. Stover, J. Baker, M. Ratliff and G. Mitschelen, May 2018.


## Full Derivation of LSD Relationships

- Start with basic reactor physics relationships:

$$
B_{g}^{2}=\frac{\pi^{2}}{\left(d_{x}+2 \lambda_{x}\right)^{2}}+\frac{\pi^{2}}{\left(d_{y}+2 \lambda_{y}\right)^{2}}+\frac{\pi^{2}}{\left(d_{z}+2 \lambda_{z}\right)^{2}}
$$

- After 7 pages of algebra you have:

$$
\frac{\mathrm{m}_{\mathrm{c}} \mathrm{n}}{\left(2 \mathrm{a}_{\mathrm{n}}\right)^{2}}\left(1-\frac{\mathrm{c}}{\sqrt{\mathrm{~N}}}\right)^{2}=\mathrm{c}_{2}\left(\mathrm{~m}_{\mathrm{c}}-\mathrm{m}_{\mathrm{o}}\right)
$$

- See derivation in excruciating detail in our Journal paper


## Deriving New Constants

- From Thomas' classic (original) method derivation:

$$
\frac{\mathrm{m}_{\mathrm{c}} \mathrm{n}}{\left(2 \mathrm{a}_{\mathrm{n}}\right)^{2}}\left(1-\frac{\mathrm{c}}{\sqrt{\mathrm{~N}}}\right)^{2}=\mathrm{c}_{2}\left(\mathrm{~m}_{\mathrm{c}}-\mathrm{m}_{\mathrm{o}}\right)
$$

- where:

$$
c=\sqrt{\frac{4 \lambda_{\text {array }^{2} N B_{N}^{2}}^{3 \pi^{2}}}{} \text {. }}
$$

$-c$ and $c_{2}$ are empirically determined constants

- How to derive c??
- Clues given in Thomas' paper Y-CDC-10, Appendix B


## Deriving the Constants (cont'd)

- KENO-VI calculations for critical mass of arrays across the parameter ranges of interest: array size \& spacing ( $2 a_{n}$ )
- Cubic arrays with number per side, n , from 4 to 10
$-N=n_{x}{ }^{*} n_{y}{ }^{*} n_{z} \quad 64 \leq N \leq 1000$
- Unit Spacing: $46.6 \mathrm{~cm} \leq 2 \mathrm{a}_{\mathrm{n}} \leq 150 \mathrm{~cm}$
- Reflected by 30 cm thick concrete on all 6 sides
- Critical mass found for each combination of array size and spacing (49 different arrays)
- Pu oxide assumed to be theoretical density with $0.5 \mathrm{wt} \%$ moisture


## Simplified 9975 KENO-VI Model



## Vertical Slice of $4 \times 4 \times 4$ Cubic Close-Packed Array



## Horizontal Slice of Array Model



## Critical Array Fissile Mass (kg) per Package



## Non-Linear Response for Surface Density

 $\left[=c_{2}\left(\mathrm{~m}_{\mathrm{c}}-\mathrm{m}_{0}\right)\right]$

## Computing the Constants

- From the derivation of array buckling (leakage):

$$
\begin{aligned}
& N B_{N}^{2}=\frac{3 \pi^{2}}{m_{c}} c_{3} e^{c_{4} m_{c}} \\
& \text { where: } c_{3}=2.63031 \mathrm{E}+4, \text { and } c_{4}=-0.694645
\end{aligned}
$$

- Extrapolation distance is calculated from:

$$
\lambda_{\text {array }}{ }^{2}=\frac{N 3 \pi^{2}}{4 N B_{N}^{2}}\left(1-\sqrt{\frac{4 a_{n}^{2} N B_{N}^{2}}{n 3 \pi^{2}}}\right)^{2}
$$

## Computing the Geometric Constant, c

- Average value of $N B_{N}^{2} \lambda_{\text {array }}{ }^{2}=3.23$,
- Returning to the definition of c :

$$
c=\sqrt{\frac{4 \lambda_{\text {array }}{ }^{2} N B_{N}^{2}}{3 \pi^{2}}}
$$

- Yields c = 0.66
- Similar to Thomas' value of $0.55+/-0.18$


## Checking the Method-Using Cubic Arrays

- The relationship to estimate critical mass is:

$$
m_{c}=\frac{\left(2 a_{n}\right)^{2} c_{3} e^{c_{4} m_{c}}}{n\left(1-\frac{c}{\sqrt{N}}\right)^{2}}
$$

- Using this to calculate $m_{c}$ for the 49 cubic arrays
$-4 \leq n \leq 10,46.6 \mathrm{~cm} \leq$ Pitch $\leq 150 \mathrm{~cm}$
- Comparing the LSD and KENO-VI critical mass values:
- Average $\Delta \%=0.62$
- Maximum $\Delta \%=1.7$


## LSD vs. KENO-VI Critical Unit Mass

## for Realistic Arrays with Pu Oxide

- 42 non-cubic arrays were chosen: $2 \times 20 \times 1,2 \times 30 \times 1,2 \times 20 \times 2,2 \times 20 \times 3$, $4 \times 20 \times 3,5 \times 5 \times 3$. Also varying pitch: $46.6 \mathrm{~cm} \leq 2 a_{n} \leq 150 \mathrm{~cm}$
- Comparing the LSD and KENO-VI critical mass values:
- Average $\Delta \%=2.5$
- Maximum $\Delta \%=5.2$
- LSD values generally under-predict the KENO-VI value
- Agreement not as good as for same arrays with Pu metal contents. For those:
- Average $\Delta \%=0.6$
- Maximum $\Delta \%=1.3$


## Empirical Adjustment to Critical Mass Based on Array Shape and Pitch

$$
m_{c, a d j}=m_{c} \frac{\left(1+R^{2.5}\right)}{100} *\left(1.01-\left(14.3 P^{-1.58}\right)\right)
$$

where: $\quad R=$ Shape Factor, given by:

$$
R=\frac{\sqrt[3]{N}}{3}\left(\frac{1}{n_{x}}+\frac{1}{n_{y}}+\frac{1}{n_{z}}\right)
$$

$\mathrm{P}=$ Horizontal Pitch (unit cell dimension) in cm

With this adjustment, overall results improved:

- Average $\Delta \%=0.8$
- Maximum $\Delta \%=2.2$


## Application Considerations

- There is much more safety margin for Pu oxide contents that with Pu metal
- For quick reactivity effect estimates, great precision is not needed
- Empirical adjustment might not be needed
- Does not improve results significantly for minimum pitch (no spacing), where the $\Delta$ is less than $+/-2.5 \%$.


## Sample Application

- Program relationships into a spreadsheet:

$$
m_{c}=\frac{\left(2 a_{n}\right)^{2} c_{3} e^{c_{4} m_{c}}}{n\left(1-\frac{c}{\sqrt{N}}\right)^{2}} \quad k_{e f f}=\left(\frac{m}{m_{c}}\right)^{1 / 3}
$$

- Examples for $10 \times 14 \times 3$ array, with $5 \mathrm{~kg} \mathrm{PuO}_{2}$ in each package
- What is safety margin for normal conditions?
- What is the effect of:
- Excess stacking (4 high)?
- Double batching ( 10 kg )?
- Changing the array pitch?


## Example 1: $10 \times 14 \times 3$ Array of $9975 \mathrm{~s}, 5 \mathrm{~kg} \mathrm{PuO} 2$ Each, Units Touching

- What is the critical mass per unit?
- What is $\mathrm{k}_{\mathrm{eff}}$ ?

| 4 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 5 |  |  |  | $\mathrm{c}=$ | 0.6602 |  |  |  |  |  |  |  |  |
| 6 |  |  |  | c3 $=$ | 26303 |  |  |  |  |  |  |  |  |
| 7 |  |  |  | c4 $=$ | -0.6946 |  |  |  |  |  |  |  |  |
| 8 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 9 |  |  |  |  |  |  | Array |  |  |  |  |  |  |
| 10 |  |  |  |  |  | Shape | Pitch | $\mathrm{a}_{\mathrm{n}}$ | Constants | Solver | LSD | Loading | k-eff |
| 11 | $\mathrm{n}_{\mathrm{x}}$ | $\mathrm{n}_{\mathrm{y}}$ | $\mathrm{n}_{2}$ | N | $\mathrm{N}^{1 / 3}$ | Factor | (cm) | (cm) | Multiplier | Equation | $\mathrm{m}_{\mathrm{c}}$ | (kg) |  |
| 12 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 46.6 | 23.3 | 8143340 | -7.1E-13 | 18.7 | 5.000 | 0.644 |
| 13 |  |  |  |  |  |  |  |  |  |  |  |  |  |

## Example 2: Excess Stacking 4 High

- What is the critical mass per unit?
- What is $\mathrm{k}_{\mathrm{eff}}$ ?

| 8 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 9 |  |  |  |  |  |  | Array |  |  |  |  |  |  |
| 10 |  |  |  |  |  | Shape | Pitch | $\mathrm{a}_{\mathrm{n}}$ | Constants | Solver | LSD | Loading | k-eff |
| 11 | $\mathrm{n}_{\mathrm{x}}$ | $\mathrm{n}_{\mathrm{y}}$ | $\mathrm{n}_{2}$ | N | $\mathrm{N}^{1 / 3}$ | Factor | (cm) | (cm) | Multiplier | Equation | $\mathrm{m}_{\mathrm{c}}$ | (kg) |  |
| 12 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 46.6 | 23.3 | 8143340 | -7.1E-13 | 18.692 | 5.000 | 0.644 |
| 13 | 10 | 14 | 4 | 560 | 8.243 | 1.158 | 46.6 | 23.3 | 7333166 | -2.9E-07 | 18.552 | 5.000 | 0.646 |
| 14 |  |  |  |  |  |  |  |  |  |  |  |  |  |

## Example 3: Excess Mass, 10 kg PuO , Each

- What is $\Delta k_{\text {eff }}$ ?

| 8 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 9 |  |  |  |  |  |  | Array |  |  |  |  |  |  |
| 10 |  |  |  |  |  | Shape | Pitch | $\mathrm{a}_{\mathrm{n}}$ | Constants | Solver | LSD | Loading | $\mathbf{k}$-eff |
| 11 | $\mathrm{n}_{\mathrm{x}}$ | $\mathrm{n}_{\mathrm{r}}$ | $\mathrm{n}_{\mathbf{z}}$ | N | $\mathbf{N}^{1 / 3}$ | Factor | $\mathbf{( c m})$ | $\mathbf{( c m})$ | Multiplier | Equation | $\mathrm{m}_{\boldsymbol{c}}$ | $\mathbf{( k g})$ |  |
| 12 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 46.6 | 23.3 | 8143340 | $-7.1 \mathrm{E}-13$ | 18.692 | 5.0 | 0.644 |
| 13 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 46.6 | 23.3 | 8143340 | $-7.1 \mathrm{E}-13$ | 18.692 | $\mathbf{1 0 . 0}$ | $\mathbf{0 . 8 1 2}$ |
| 14 |  |  |  |  |  |  |  |  |  |  |  |  |  |

## Example 4: Changing Spacing

- Assume decrease of 5 cm , or an increase of 10 cm
- What is new critical mass?
- What is $\Delta \mathrm{k}_{\text {eff }}$ ?

| 8 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 9 |  |  |  |  |  |  | Array |  |  |  |  |  |  |  |
| 10 |  |  |  |  |  | Shape | Pitch | $\mathrm{a}_{\mathrm{n}}$ | Constants | Solver | LSD | Loading | k-eff | $\Delta k$-eff |
| 11 | $\mathrm{n}_{\mathrm{x}}$ | $\mathrm{n}_{\mathrm{y}}$ | $\mathrm{n}_{2}$ | $N$ | $\mathrm{N}^{1 / 3}$ | Factor | (cm) | (cm) | Multiplier | Equation | $\mathrm{m}_{\mathrm{c}}$ | (kg) |  |  |
| 12 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 46.6 | 23.3 | 8143340 | -7.1E-13 | 18.692 | 5.0 | 0.644 |  |
| 13 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 41.6 | 20.8 | 6489592 | -3.2E-06 | 18.389 | 5.0 | 0.648 | 0.004 |
| 14 | 10 | 14 | 3 | 420 | 7.489 | 1.260 | 56.6 | 28.3 | 12013335 | -8.8E-07 | 19.213 | 5.0 | 0.638 | -0.006 |
| 15 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

## Conclusions

- LSD Method provides good agreement with KENO-VI for arrays of 9975 shipping packages with Pu Oxide.
- Allows rapid estimates for safety margin for varying mass, spacing, and array sizes.
- Can be used to evaluate variety of normal and credible abnormal conditions.
- Helps develop understanding of the physics.


## Questions?



## Supplemental Discussion: Basic Concept

- Buckling relationships can be used to relate one critical array to another, using empirically derived constants.
- First, assume that one has a critical array of identical fissile items, specified by its isotopics, mass/unit, spacing, array shape, etc.
- Changes in one parameter (e.g., mass or spacing) may be compensated by changes in another parameter so that the resulting array is also critical.


## Can LSD work for shipping package arrays?

- Thomas' LSD method is very good for air-spaced arrays of solid items (see Hand Calculation Primer Sec. 7)
- Caveat 1: Derivation uses cubic arrays of cubic units
- Caveat 2: Each unit may be surrounded by $\leq 1 / 2$ inch of steel
- Problems and Challenges:
- 9975s are not cubic; nor are the arrays
- 9975s have several nested layers of packaging material (steel, lead, Celotex ${ }^{\top M}$ )
- Some packaging varies among 9975s
- Unclear how to derive the necessary constants

