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ENSURING THE VALIDITY OF CALCULATED SUBCRITICAL LIMITS

by

H. K. Clark

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Savannah River Laboratory
E. I. du Pont de Nemours and Company
Aiken, S.C. 29801

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DISCLAIMER

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ABSTRACT

The care taken at the Savannah River Laboratory and Plant to ensure the validity of calculated subcritical limits is described. Close attention is given to ANSI N16.1-1975, *"Validation of Calculational Methods for Nuclear Criticality Safety."* The computer codes used for criticality safety computations, which are listed and are briefly described, have been placed in the SRL JOSHUA system to facilitate calculation and to reduce input errors. A driver module, KOKO, simplifies and standardizes input and links the codes together in various ways. For any criticality safety evaluation, correlations of the calculational methods are made with experiment to establish bias. Occasionally subcritical experiments are performed expressly to provide benchmarks. Calculated subcritical limits contain an adequate but not excessive margin to allow for uncertainty in the bias. The final step in any criticality safety evaluation is the writing of a report describing the calculations and justifying the margin.

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INTRODUCTION

Great care is taken at the Savannah River Laboratory and Plant to ensure the validity of calculated subcritical limits. Careful attention is given to ANSI N16.9-1975, *"Validation of Calculational Methods for Nuclear Criticality Safety."* With any method, there are two principal areas of concern. The first is that the method be used in the intended manner, free of input error and of an improper selection of options. The second is that the method be correlated with pertinent experimental data to establish bias and that allowance for uncertainty in the bias be adequate to ensure subcriticality.

COMPUTER CODES

The principal computer codes used at SRL for criticality safety analyses are listed in Slide 1. MGBS is a simple 12-group B_o calculation that computes buckling, migration area, and two-group diffusion theory parameters from cross sections incorporated in the code.[1] It performs lattice calculations for cylindrical cells by a P_3 treatment in the thermal group and by the use of Hellstrand resonance integrals.[2] TGAN is a one-dimensional, analytical two group diffusion theory code for slab, cylinder, and sphere. HRXN processes Hansen-Roach cross sections[3] into macroscopic cross sections and contains a B_1 calculation to determine critical buckling and migration area, and if desired, to collapse cross sections. GLASS[4], the successor to HAMMER[5], performs integral transport theory cylindrical cell calculations with 84-group cross sections drawn from the HAMMER library or

processed from ENDF/B-IV. It also contains a B_1 calculation to determine critical buckling and to collapse cross sections into fewer groups. ANISN[6] performs one-dimensional Sn calculations for slab, cylinder, and sphere and TWOTRAN-II performs two dimensional Sn calculations.[7] Monte carlo calculations are performed by KENO-IV[8] and KENO-IV/CG[9]. Cross sections for Sn and Monte Carlo are commonly Hansen-Roach but may be derived from GLASS.

The codes MGBS and TGAN are quite old, having originally been written in machine language for the IBM-650. They have been successively rewritten in FORTRAN II for the IBM-704 and in FORTRAN IV for the present SRL-SRP computer, the IBM-360 Model 195. Despite the approximations in MGBS and those involved in assuming separable one-dimensional solutions in applying TGAN to three-dimensional shapes, the combination MGBS-TGAN is still widely used because of its great speed of execution and because of extensive correlation with experiment to determine bias. The combination MGBS-TGAN was used to generate the limits for slightly enriched uranium appearing in ANSI-N16-1-1975 "Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors". The reference for these limits[10] is a good example of the care taken at SRL to determine the bias of a method and to establish valid limits. Input to MGBS and TGAN is quite simple, and there are few options. However, because of approximations and cross section limitations the combination of codes is not generally used beyond the area covered by experimental data except to

delineate areas to be investigated by other methods or as a rough check on more accurate calculations.

JOSHUA SYSTEM

All the codes used for criticality safety evaluations are modules in the SRL JOSHUA system[4]. This system permits codes to be executed in specified sequences (e.g. MGBS-TGAN) by a driver module, and one has been written (KOKO). Besides executing the modules KOKO prepares specialized input for standard types of problems, often operating on the output from one module to prepare input for the next. Input data and intermediate data passed from one module to another are handled in named data records. Records that may be required for executing KENO, for example, are listed in Slide 2. The records are named with a tree structure. The variables ?NAME and ?M are, respectively, a name assigned to a study and a problem number. The variables ?N are assigned to the macroscopic cross section records, odd numbers for P_0, even for P_1. The variables ?L and ?K identify the albedo and adjoint biased weight records, which are stored in a standard data set.

Input records are prepared by the user at a cathode ray tube terminal through a template and reside in the user's data set A template is simply a means of displaying the data with identifying labels. Such labels help the user avoid errors in supplying input. Slide 3 shows the first page of the INPUT. KENO. GNRL. ?NAME. ?M record as filled in for a particular problem. A tab key positions the cursor on the terminal screen at the colon.

Failure to enter an item on a blank page which appears when the data are first entered, causes the item to be zero. The zeros for "No. of groups" and "No. of energy transfers" default to 16 and 6 in KENO. Records may rapidly be copied or renamed. Thus, to set up a batch of similar KENO problems, the user creates the data records required for one problem, copies them into records for the remaining problems, and then modifies them as required. The JOSHUA system facilitates the accurate entry of data, minimizes data manipulation by the user in proceeding from one module to another, and permits standardization of methods while preserving flexibility.

MACROSCOPIC CROSS SECTIONS

With the modular capability of JOSHUA available, it was considered desirable to generate macroscopic Hansen-Roach cross sections, which are used in both Sn and Monte Carlo calculations, in a separate module, HRXN. Atom densities are calculated by the module from a wide variety of forms of input data. Regardless of the form, mixture densities and compositions by concentration and weight fraction of components are printed so that errors may readily be detected. The macroscopic potential scattering cross section is computed from data contained in a standard cross section record and resonance cross sections are interpolated from standard Hansen-Roach cross section records as a function of potential scattering per atom of absorber. A B_1 calculation is provided to determine buckling and migration area and to collapse cross sections, if desired. Collapsing is performed so as to maintain the buckling and the migration area.

To provide a standard method for computing the densities of aqueous solutions of U and Pu, apparent specific volumes of UO_2F_2 in water solutions and of UO_3 and PuO_2 in nitric acid solutions are incorporated in HRXN so that only U, Pu, and NO_3 concentrations need be specified. The specific volume of UO_2F_2 is given for natural uranium by the formula developed by Johnson and Kraus[11] as shown in Slide 4. In HRXN the parameters are extrapolated to 20°C and allowance is made for isotopic composition. A study of available solution composition data made about 4½ years ago revealed large scatter in the apparent specific volume of PuO_2 in nitric acid solutions, with nitric acid density read from the International Critical Tables. Less scatter was shown in the apparent specific volume of UO_3. Despite the scatter, specific volumes as a function of solution concentration were estimated as given in Slide 5. The scatter was too great to detect conceivable dependence on nitrate concentration. Use of these specific volumes provides a standard method for proceeding from experimental data to establish bias and then proceeding to establish limits for aqueous solutions.

STANDARDIZATION OF METHODS

Although it is desirable to preserve the flexibility provided by the options in GLASS, ANISN, and KENO, it is important to provide standardized methods since bias established with one set of options may differ significantly from that with another selection. This standardization is provided by subroutines in KOKO which write input records for other modules in a standard

manner. For example, for the usual type of ANISN problem, one need fill out only two pages of input. The first page is shown in Slide 6. Unless groups are to be collapsed by ANISN and cross sections other than Hansen-Roach or GLASS are to be used, the five items following "No. of Zones" may be skipped since they will default to the proper values. Only 4, 8, or 16 may be selected for quadrature and particular sets will be read. The last two items refer to flux weighting and may be skipped except where weighting is desired as in a cell calculation or group collapsing. On the next page (Slide 7) omission of the "mesh factor" causes zones to be divided into subzones and the mesh to be selected by a scheme which assigns more points in regions of rapidly varying flux. A standard selection is made by KOKO of the various integer and floating-point parameters required by ANISN, and a GNRL (15$ and 16* arrays) record and a FIDO (remainder of data) record are written which are read by ANISN. These records may be prepared directly by the user, but their preparation in a standard form through KOKO is preferable and is far simpler and less prone to error.

BIAS

Once an appropriate method has been selected for an evaluation, bias is established for the "Area of Applicability". Validation is required for any method, however sophisticated. Since many calculations are required to establish bias and since many more are usually required to establish subcritical limits, it is generally inadvisable to use a highly sophisticated method if,

as is usually the case, sophistication increases computing time.

A search is made for pertinent data. Reference is generally made to the original source of the data. The data are carefully examined for consistency. All available data are included in the correlation. Including all the data tends to provide an estimate of the uncertainty in the bias beyond that estimated by the experimenter for individual data points since calculations (other than Monte Carlo) should exhibit smooth trends; abrupt changes are presumably due to experimental errors. Even where KENO is to be used, correlations with one-dimensional systems are generally made with ANISN extrapolated to S_∞, of course with the same cross sections, since the two should be equivalent. Due to lack of data, effects sometimes have to be considered separately as for example when experimental data for a particular reflector exist only with a core differing from that being evaluated. In some cases, notably for handling U-Al alloy driver assemblies for SRP reactors, and the forms from which they are extruded, in H_2O, exponential and other subcritical experiments are performed to provide a basis for establishing bias (e.g. Reference 12).

The bias established by the correlation is carefully examined for trends, particularly where the conditions being evaluated are outside the range of experimental data. Reasons are sought for the trends. Where an extension of the area of applicability is

required, the method being validated is supplemented by other methods. Finally, an adequate margin of subcriticality is selected. The margin may be greater where the uncertainty in the bias is greater. The margin is of course arbitrary and is chosen to be ample but not excessive. The smaller the margin the greater the effort required to justify its adequacy. However, the increase in limits associated with increasing the limiting value of k_{eff} by, say, 0.01-0.02 is generally not worth the effort required to justify the increase. Much greater increases in limits are likely to result from restricting an additional parameter such as concentration in addition to mass.

DOCUMENTATION

The final part of any criticality safety evaluation is the writing of a report describing the calculations and giving the results of the evaluation. This is a valuable exercise. Often additional calculations will be shown to be necessary as the writing proceeds. The author feels the need to be clear, convincing, and complete. This need is apt to become especially apparent when he has occasion to review a previous evaluation; hence it is advisable to set the draft aside for a while before finally reviewing and issuing it. The report need not be overly long. The methods of calculation may have been well described in internal and external reports, and bias established and reported for several areas of applicability; hence reference to appropriate reports may often be sufficient for describing the method and giving the bias.

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PRINCIPAL COMPUTER CODES

MGBS

TGAN

HRXN

GLASS

ANISN

TWOTRAN-II

KENO-IV

KENO-IV/CG

SLIDE 1

KENO RECORDS

INPUT.KENO.?JOB

INPUT.KENO.GNRL.?NAME.?M

INPUT.KENO.GEOM.?NAME.?M

INPUT.KENO.BXLN.?NAME.?M

INPUT.KENO.GNGM.?NAME.?M

INPUT.KENO.CMGM.?NAME.?M

INPUT.KENO.PCTR.?NAME.?M

OUTPUT.XSEC.?NAME.?N

KOKO.KENO.ALBD.?L.16.4

KOKO.KENO.WGHT.?K.16

SLIDE 2

```
:     1149.INPUT.KENO.GNRL.HXRY.1

  | TITLE FOR |  :7 CYLINDERS OF ORALLOY EMBEDDED IN ALUMI |
  | PROBLEM   |  :NUM CUBOID. MIXED BOX + AUTO REFL.       |
:  1.5  MAXIMUM TIME                :103  NO. OF BATCHES
  :300  NO./BATCH                   : 3  NO. OF BATCHES TO SKIP
   : 0  NO. OF GROUPS               : 0  NO. OF ENERGY TRANSFERS
          :000000000000 RANDOM NUMBER SEED
   : 0  NOT USED                    :  3  NO. UNITS IN X DIRECTION
  :  4  NO. UNITS IN Y DIRECTION    :  1  NO. UNITS IN Z DIRECTION
 :   0  PRINT OPTIONS                : 0  BATCHES BEFORE RESTART
    :0  DUMMY RNDM NO. CALLS         :1  >0 PICT, >1 GEOMCHK ONLY
```

SLIDE 3

UO_2F_2 SOLUTIONS

$$1/d = 1/d_0 + aF_2 + bF_2^2$$

d_0 = density of H_2O $\qquad$ F_2 = weight fraction of UO_2F_2

T, °C	a	b
25	-0.9120	0.0567
30	-0.9126	0.0569

$$v = 1/d_0 + \frac{ac - \sqrt{(1-ac)^2 + 4bc^2/d_0}}{2c}$$

v = apparent specific volume of UO_2F_2 (cm^3/g)

c = concentration, g UO_2F_2/cm^3

SLIDE 4

$UO_2(NO_3)_2$ AND $Pu(NO_3)_4$ SOLUTIONS

	Specific Volume, cm^3/g	
Molarity	UO_3	PuO_2
0	0.038	-0.038
0.5	0.092	0.010
0.1	0.120	0.027
1.5	0.135	0.035
≥ 2.0	0.142	0.038

SLIDE 5

```
:      TEMPLATE.INPUT.KOKO.ANSN.?.?

    TITLE   :AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA |
:III NO. OF ZONES                   :II NO. OF FEW GRPS (O = SAME)
:III NO. OF GROUPS                  :II NO. DOWN + SELF SCATTERS
 :II NO. UPSCATTERS (- = RMVL)       :I ORDER OF SCATTER
 :II QUADRATURE (- = ADJOINT)        :I 1/2/3=PLANE/CYLINDER/SPHERE
  :I L 0-3=BARE/REFL/PER/WHITE       :I R 0-3=BARE/REFL/PER/WHITE
  :I 0-6=Q/K/ALPHA/C/Z/R/B**2     :III ZONE FOR DIMENSION SEARCH
:F.FFFF KEFF FOR DIM. SRCH.          :I >0 TO PRINT FLUX & BALANCE
:E.EEEEEEEEE TRANSVERSE BCKLNG    :E.EEEEEEEEE ALBEDO
  :I 0/1/2/3=NO/CELL/D.F./BOTH       :I >0 FOR CURRENT & FLUX WTS.
```

SLIDE 6

```
:      TEMPLATE.INPUT.KOKO.ANSN.?.?

ZONE MATL  THICKNESS   MSH FTR    ZONE MATL  THICKNESS   MSH FTR
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
:111:IIII :E.EEEEEEEEE :F.FF      :111:IIII :E.EEEEEEEEE :F.FF
```

SLIDE 7