INTERIM REPORT

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Program for Standardized Analysis of Fuel Shipping Containers

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UNION CARBIDE CORPORATION, NUCLEAR DIVISION
operating the
Oak Ridge Gaseous Diffusion Plant . Oak Ridge National Laboratory
Oak Ridge Y-12 Plant . Paducah Gaseous Diffusion Plant
for the
DEPARTMENT OF ENERGY

INTERIM REPORT

PROGRAM FOR THE STANDARDIZED ANALYSIS

OF FUEL SHIPPING CONTAINERS

Quarterly Summary

January 1, 1980 to March 31, 1980

Personnel Time -- 2804 man hours

(a) This Quarter . . . . $ 89,850*

(b) Fiscal Year-to-Date 198,472

(c) Projected to End of Fiscal Year 267,282**

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*Excludes $32,000 of BNL computer charges outstanding and under consideration by NRC for transfer.

**Includes additional $65,000 authorized under SOEW #60-80-112 dated 3/10/80.

QUARTERLY REPORT ON PROGRAM FOR THE STANDARDIZED

ANALYSIS OF FUEL SHIPPING CONTAINERS

SCALE System Development

During this quarter, activity centered on documenting the operational portions of the SCALE system, implementing and testing the system on the Brookhaven National Laboratory CDC-7600 computer for NRC personnel and assisting the Radiation Shielding Information Center (RSIC) in packaging SCALE for distribution. The progress is briefly summarized by category.

1. Functional Modules

Work proceeded on the documentation of the KENO-V module. An input data guide as well as sections describing the analytical model and the error messages have been prepared. A new angular selection scheme for treating P_1 scattering was implemented into KENO-V.

Recommendations were developed for applying MORSE-SGC/S in calculating radiation dose levels exterior to spent fuel shipping casks. A more extensive effort involving a study of various biasing techniques for this problem has been proposed for FY1981. Documentation of MORSE-SGC/S including the MARS geometry package is in preparation.

The SCALE system documentation of the ORIGEN-S program is being typed.

Documentation of the NITAWL-S program is proceding. Minor programming errors detected during the validation of the analytical model have been corrected.

2. Data Base

Preparations were made to analyze three of the storage pool critical experiments[1] performed by the Babcock and Wilcox Company (B&W). The initial B&W analyses with the 123 group library showed a negative analytical bias for those experiments with a wide spacing between fuel assemblies. The immediate interest is to study this effect with the SCALE system version of the 123 group library. The B&W staff has provided KENO-IV input specifications for twenty-one critical experiments. These input specifications will be included in the CESAR (Critical Experiment Storage And Retreival) Library being released to the public with the SCALE system.

The SCALE system standard Compositions Library was updated with the inclusion of an additional standard concrete, REG-CONCRETE, with specifications taken from ARH-600.[2]

Revised versions of the four neutron cross section libraries to be used with the criticality safety analytical sequences were transmitted to RSIC for packaging.

3. Control Modules

The SCALE manual sections on CSAS1 and CSAS2 have been typed and matted. A proofread and corrected copy will go to RSIC for inclusion in their package documentation. Fifty copies of the document will be distributed internally at Oak Ridge. Then mats and binders will be shipped to the NRC for distribution under RC-14 and under a special external distribution.

Portions of the documentation on the control modules CSAS4, SAS2 and SAS3 have been prepared. Work is proceding on this documentation.

Under the support of another project, the SAS2 analytical sequence was applied in a study of the importance of the presence of fission products on the neutron-spectrum-weighted ORIGEN-S data. In this study, the ENDF/B-IV Data Base was applied for 13 isotopes of the heavy elements and 177 isotopes of the fission products. The results are summarized in four tables. Table 1 contains the benchmark problem specifications. Table 2 lists the model assumptions, libraries, and parameter options applied in computing the problem. The computed values of k_∞, accumulated fissions and atom concentrations as a function of fuel burnup are given in Table 3. Table 4 lists the relative importance of the fission products in terms of neutron absorption. The total absorption due to fission products is 10.83%.

4. BNL-CDC-7600 Implementation

The CRT-terminal interactive-input processors for CSAS1, CSAS2 and SAS3 are now operational on the BNL-CDC-7600 computer.

An effort to package CDC-7600 versions of these control modules has been initiated.

The charges for computing on the BNL system have been much larger than anticipated. In order to avoid a severe impact on SCALE system development funds, arrangements are being made to have these charges transferred to the appropriate NRC account.

Table 1. Unit Cell Benchmark Problem #1

This problem is intended to be a fictitious calculation of an infinite array of identical unit cells. No leakage (e.g., B^2) should be taken into account. The spectra and depletions should be calculated for the non-critical keff = k∞ (i.e., modification of fission source) conditions with no criticality search.

Engineering Specifications

Fuel Temperature = 1200°F (utilize also for Doppler calculation)

Clad Temperature = 620°F

Moderator Temperature = 572°F

Pressure = 2250 psia

Power = 190 Watts/cm of core height

Weight Fraction U-235 = .03 in U

Fuel Density = 91% theoretical density
or 91% of 10.96

Clad Material = Zr-4

Grid Material = Inconel (used only for calculation of pitch expansion, material not to be included in problem)

Cold Dimensions (to be expanded to hot dimensions at referenced temperatures)

Pellet OR	0.18 in
Clad IR	0.19 in
Clad OR	0.21 in
Square Pitch	0.56 in

Equivalent Hot 3 Region Cylindrical Physics Representation

Fuel OR	.45956 cm
Clad OR	.53436 cm
Cell OR	.80573 cm

Fuel Nuclide Densities x 10^{24}, atoms/cm^3

O-16	$.438101 \times 10^{-1}$
U-235	$.665303 \times 10^{-3}$
U-238	$.212398 \times 10^{-1}$

Clad Nuclide Densities x 10^{-24}, atoms/cm^3

Zr	$.300279 \times 10^{-1}$
Sn	$.320332 \times 10^{-3}$
Fe	$.102119 \times 10^{-3}$
Cr	$.052228 \times 10^{-3}$
Ni	$.001850 \times 10^{-3}$

Table 1. (cont.)

Moderator Nuclide Densities x 10^{-24}, atoms/cm^3

H-1	.486262 x 10^{-1}
O-16	.243131 x 10^{-1}

Calculate

At 0.0 (no Xe) - 100(equil. Xe) - 10,000-20,000-30,000 MWD/TONNE

TONNE to correspond to metric tons of metal at BOL
Cell k∞, accumulated fissions, and fuel region nuclide densities of U-235, U-238, Pu-239, Pu-240, Pu-241, Pu-242 and Xe-135

Report: whether used Engineering or Physics representation; code, data libraries and options utilized (reference if possible); deviations from specifications or assumptions required

Table 2. Problem Description and Chief Assumptions of Model

1. Name:

   Unit Cell Benchmark - Problem #1.

2. Choice between two representatives:

   Equivalent Hot Cylindrical Physics.

3. Deviations from specifications or assumptions:

   None.

4. Code applied:

   Shielding Analysis Sequence #2, or SAS2 Model of SCALE[1] System.

   Specifically invoked execution of the following:

   a. NITAWL[1,2] Code (for Nordheim Integral treatment)

   b. XSDRNPM[1,2] Code (for obtaining time-dependent cross sections from transport flux calculation)

   c. COUPLE[1] Code (for revising ORIGEN Libraries with XSDRNPM results)

   d. ORIGEN[1,3] Code (for generating final and intermediate nuclide densities at appropriate time periods)

5. Data Libraries:

   a. Used standard LWR Nuclear Data Library[3] as "initial" ORIGEN-S Binary Library.

   b. Used 27-Group Master Library of SCALE System plus the fission product library produced by M. A. Bjerke for making improved ORIGEN libraries. These were produced by applying standard methods of the AMPX[2] System using the ENDF/B-IV Data Base. Isotopes for which cross sections were updated or added in the ORIGEN-S Library were: ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{244}Cm and 177 fission products.

6. Options utilized (othèr than those fixed by SCALE):

   a. Applied 27-Group Master AMPX Library.

   b. Number of libraries (time-dependent) = 2, 4, and 6 for the 10, 20, and 30 GWD/MTU cases, respectively.

   c. Power = 30 MW/MTU.

   d. Burn time = 333 1/3, 666 2/3 and 1000 days for the three cases.

   e. SZF = 0.5, which produced 48 spacial mesh intervals for the unit cell.

   f. Convergence epsilon = 4×10^{-5}.

   g. Angular quadrature order = S_8.

7. Assumptions or options fixed by model:

   a. One-dimensional discrete ordinate transport calculation for deriving flux weighted cross sections.

   b. Order of scattering = P_3.

   c. One-region in burnup calculation.

Table 2. (continued)

d. Resolved resonance cross sections determined by Nordheim Integral Method; slowing-down fluxes calculated with scattering from ^{16}O and ^{238}U and an external 1/E source.

e. Use of the last "time-dependent library" to generate densities at mid-time of the next library for the input densities used in determining the library cross sections. This type of extrapolation error is reduced by increasing number of libraries.

f. All of the cross sections in ORIGIN-S library other than those updated from the XSDRNPM weighted library (e.g., for nuclides listed in 5.b.) are obtained by weighting their two-group values in the master ORIGEN-S library with the corresponding two-group flux computed by XSDRNPM. The thermal weight factor is directly obtained by adding a small quantity of "1/v Absorber" to the fuel.

g. The generation and depletion of nuclide densities is determined chiefly through the matrix exponential expansion method. Where matrix elements are ill-behaved, Bateman Equations or secular equilibrium is applied.

h. The ORIGEN-S Code converts burnup to flux applying ENDF/B data for removable energy per fission reaction of the various fissile isotopes plus the energy released from the corresponding the (n,γ) reactions of the computed actinide, fission product, clad and moderator nuclides.

Table 3. Densities* and k_∞ Computed by SCALE (SAS2-ORIGENS-ENDF/B IV) SYSTEM.

MWD/TONNE	10,000	20,000	30,000
k_∞**	1.1459	1.0533	0.9789
k_∞***	1.1445	1.0514	0.9769
^{135}Xe	7.83-9	7.53-9	7.11-9
^{235}U	4.45-4	2.93-4	1.86-4
^{238}U	2.11-2	2.09-2	2.07-2
^{239}Pu	8.05-5	1.12-4	1.25-4
^{240}Pu	1.28-5	3.02-5	4.51-5
^{241}Pu	5.69-6	1.79-5	2.86-5
^{242}Pu	4.54-7	3.26-6	8.60-6
Fissions	2.32-4	4.61-4	6.85-4
Other:			
^{239}Np	1.45-6	1.60-6	1.74-6
^{236}U	3.91-5	6.44-5	7.97-5
^{237}Np	1.93-6	5.27-6	9.06-6
^{238}Pu	1.76-7	9.84-7	2.65-6
^{241}Am	6.29-8	3.80-7	8.15-7
^{243}Am	2.56-8	4.14-7	1.70-6
^{242}Cm	7.10-9	8.07-8	2.44-7
^{244}Cm	1.55-9	5.74-8	3.94-7

*Atoms/barn-cm.

**Average of the lamdas computed by XSDRNPM at "burnup-2,500 MWD/TONNE" and "burnup + 2,500 MWD/TONNE."

***Corrected for the ^{148m}Pm absorption, which was computed by ORIGENS and not included in XSDRNPM.

Table 4. Fission Products Computed by SCALE (SAS2-ORIGENS-ENDF/B IV) System

MWD/TONNE	% of Total Absorption Rate 20,000	30,000	Accumulative 30,000	Densities (atoms/barn-cm) 10,000	20,000	30,0
^{135}Xe	1.95	1.815	1.815	7.83-9	7.53-9	7.11-9
^{103}Rh	7.42-1	1.045	2.860	6.66-6	1.43-5	2.08-5
^{143}Nd	6.95-1	9.06-1	3.766	1.15-5	2.08-5	2.75-5
^{149}Sm	7.07-1	7.03-1	4.469	8.13-8	9.04-8	9.12-8
^{133}Cs	4.56-1	6.40-1	5.109	1.50-5	2.89-5	4.12-5
^{131}Xe	4.33-1	5.82-1	5.691	6.12-6	1.15-5	1.60-5
^{99}Tc	3.66-1	5.15-1	6.206	1.38-5	2.66-5	3.80-5
^{147}Pm	4.64-1	5.06-1	6.712	3.63-6	5.33-6	5.91-6
^{152}Sm	3.04-1	4.20-1	7.132	1.41-6	2.82-6	4.00-6
^{151}Sm	3.52-1	4.12-1	7.544	3.14-7	4.11-7	4.88-7
^{153}Eu	1.83-1	3.09-1	7.853	7.09-7	1.91-6	3.27-6
^{145}Nd	1.92-1	2.65-1	8.118	8.54-6	1.60-5	2.25-5
^{148m}Pm*	1.82-1	2.01-1	8.319	2.50-8	3.80-8	4.27-8
^{150}Sm	1.29-1	1.95-1	8.514	2.85-6	6.21-6	9.59-6
^{95}Mo	1.27-1	1.95-1	8.709	8.30-6	2.12-5	3.30-5
^{154}Eu	8.59-2	1.87-1	8.896	1.14-7	5.07-7	1.13-6
^{155}Eu	9.23-2	1.84-1	9.080	8.01-8	2.15-7	4.36-7
^{109}Ag	9.29-2	1.60-1	9.240	5.84-7	1.67-6	2.94-6
^{129}I	9.19-2	1.56-1	9.396	1.79-6	3.81-6	5.62-6
^{101}Ru	1.02-1	1.50-1	9.546	1.21-5	2.43-5	3.63-5
^{147}Sm	6.75-2	1.09-1	9.655	4.28-7	1.29-6	2.12-6
^{105}Pd	5.37-2	9.05-2	9.745	4.24-6	1.05-5	1.79-5
^{134}Cs	4.09-2	8.29-2	9.828	5.26-7	1.97-6	4.06-6
^{93}Zr	5.05-2	7.08-2	9.899	1.35-5	2.55-5	3.62-5
^{105}Rh	6.06-2	6.90-2	9.968	3.56-8	4.60-8	5.35-8
^{141}Pr	4.54-2	6.72-2	10.035	1.14-5	2.41-5	3.63-5
^{83}Kr	4.62-2	5.94-2	10.095	1.04-6	1.82-6	2.38-6
^{108}Pd	3.18-2	5.84-2	10.153	1.06-6	3.47-6	7.89-6
^{148}Pm	4.71-2	5.42-2	10.207	1.68-8	2.68-8	3.19-8
^{139}La	3.66-2	5.27-2	10.260	1.46-5	2.85-5	4.18-5
^{135}Cs	3.05-2	4.48-2	10.305	4.70-6	9.37-6	1.39-5

Table 4. (continued)

	% of Total Absorption Rate			% of F.P. Abs. Rate
MWD/TONNE	20,000	30,000	Accumulative 30,000	Accumulative 30,000
^{97}Mo	2.55-2	3.73-2	10.342	95.5
^{107}Pd	1.89-2	3.44-2	10.377	
^{157}Gd	2.26-2	3.28-2	10.409	
^{106}Pd	8.12-3	2.12-2	10.431	
^{113}Cd	1.72-2	1.86-2	10.449	96.5
^{144}Nd	9.52-3	1.77-2	10.467	
^{148}Nd	9.53-3	1.39-2	10.481	
^{98}Mo	9.20-3	1.36-2	10.494	
^{102}Ru	8.04-3	1.24-2	10.507	97.1
^{127}I	7.01-3	1.17-2	10.518	
^{91}Zr	7.46-3	1.07-2	10.529	
^{133}Xe	1.04-2	1.01-2	10.539	
^{155}Gd	5.05-3	1.00-2	10.549	
^{96}Zr	6.94-3	1.00-2	10.559	97.5
^{143}Pr	1.04-2	9.78-3	10.569	
^{100}Mo	6.35-3	9.40-3	10.578	
^{104}Ru	5.48-3	8.97-3	10.587	
^{115}In*	6.99-3	8.71-3	10.596	
^{104}Pd	3.70-3	8.65-3	10.605	
^{156}Gd	3.37-3	8.55-3	10.613	98.0
^{103}Ru	7.[illegible]-3	7.90-3	10.621	
^{156}Eu	4.03-3	7.85-3	10.629	
^{146}Nd	4.61-3	6.94-3	10.636	
^{151}Pm	5.68-3	6.94-3	10.643	
^{149}Pm	6.20-3	6.63-3	10.649	
^{147}Nd	6.76-3	6.53-3	10.656	
^{141}Ce	6.40-3	6.12-3	10.662	98.5
^{148}Sm	2.95-3	6.08-3	10.668	
^{132}Xe	3.29-3	5.17-3	10.673	
^{150}Nd	3.21-3	4.90-3	10.678	
^{142}Ce	3.38-3	4.87-3	10.683	
^{100}Ru	2.03-3	4.62-3	10.688	98.7
Total (All F.P.)			10.826	100.0

*Only nuclide for which ORIGEN weighted cross section was applied in place of ENDF B-IV data.

References

1. G. S. Hoovler, et al., "Critical Experiments Supporting Close-Packed Water Storage of Power Reactor Fuel," Trans. Am. Nucl. Soc. 33, 374 (1979).

2. R. D. Carter, et al., "Criticality Handbook," Atlantic Richfield Hanford Co., ARH-600 (1968).

ATTACHMENT

Standardized Analysis of Fuel Shipping Containers

Thermal Analysis Support

C. A. Sady
W. D. Turner

The task of incorporating additional features into HEATING6 to render the code more versatile as a tool in the thermal studies associated with the design and safety analysis of spent fuel shipping containers was continued during the past quarter.

1. Implementation of HEATING6 into SCALE

A series of cases were designed to test error handling features involving the input data. A number of coding errors that were deleted in executing these test cases on HEATING6 were corrected.

2. Implementation of HEATING6 on the CDC-7600

The task of implementing HEATING6 on the CDC-7600 computing system at Brookhaven National Laboratory (BNL) was initiated during the past quarter. It was decided to complete a portion of this implementation on the Oak Ridge computing systems prior to sending the code to BNL. This preliminary work included the following coding changes. Most of the multiple entries and the argument lists in many subroutines were restructured to meet requirements of CDC FORTRAN. This required subdividing a number of large subroutines into several smaller ones. The multiple return feature present in a number of subroutines was restructured. The coding to call local IBM systems routines was redesigned to reference CDC systems routines at BNL. Arrays were selected for large core memory (LCM), and the initial coding was added to place those arrays in LCM.

3. Documentation of HEATING6

A draft of most of the body of the report documenting HEATING6 has been prepared and is being typed. This includes chapters on numerical techniques, input data description, and a discussion of output generated by the code. A major portion of the chapters concerning the logical flow of the code and modeling concepts has been written.

4. REGPLOT Conversion

Debugging on the HEATING6 version of REGPLOT continued during the quarter. A draft of a document describing the use of the code has been completed.