INTERIM REPORT

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Program for Standardized Analysis of Fuel Shipping Containers

Subject of this Document: Technical Progress

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Office of Nuclear Regulatory Research

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UNION CARBIDE CORPORATION, NUCLEAR DIVISION
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for the
DEPARTMENT OF ENERGY

INTERIM REPORT

OAK RIDGE NATIONAL LABORATORY
OPERATED BY
UNION CARBIDE CORPORATION
NUCLEAR DIVISION
POST OFFICE BOX X
OAK RIDGE, TENNESSEE 37830

ORNL/CSD/INF-80/4

DATE: July 29, 1980

SUBJECT: Quarterly Report on Program for the Standardized Analysis of Fuel Shipping Containers

TO: U. S. Nuclear Regulatory Commission

FROM: G. E. Whitesides

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PROGRAM FOR THE STANDARDIZED ANALYSIS OF FUEL SHIPPING CONTAINERS

Quarterly Summary

April 1, 1980, to June 30, 1980

Personnel Time -- 2804 man-hours

(a)	This Quarter	$ 70,829*
(b)	Fiscal Year-to-Date	269,301
(c)	Projected to End of Fiscal Year	(2,019)**

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

**Present deficit.

QUARTERLY REPORT ON PROGRAM FOR THE STANDARDIZED ANALYSIS OF FUEL SHIPPING CONTAINERS

SCALE System Development

During this quarter, activity was oriented towards documenting the operational portions of the SCALE system, converting HEATING6 for operation on the Brookhaven National Laboratory CDC-7600 computer and assisting the Radiation Shielding Information Center (RSIC) in packaging SCALE for distribution. A major objective was reached in the completion of the initial version of the SCALE manual leading to the release of the SCALE system by RSIC. The progress is briefly summarized by category.

1. Functional Modules

Work proceeded on the documentation of the KENO-V module, the HEATING6 module, the ORIGEN-S module, the MORSE-SGC/S module and the NITAWL-S module. The estimated level of completion of this documentation is given in Table 1. Copies of the work in progress have been forwarded to the NRC project manager.

2. Data Base

Input specifications for 21 critical experiments performed by the Babcock and Wilcox Company to simulate fuel storage pool situations have been incorporated into the CESAR (Critical Experiment Storage And Retrieval) library being released to the public with the SCALE system. Analyses of three of these experiments with the 123 group GAM-THERMOS library is being reported under NMSS Project No. B0009-7.

Under a special arrangement with the University of Tennessee, one of their visiting scientists has performed a study of critical experiments designed to simulate hypothetical accident situations occurring during fuel fabrication and storage. The study was performed with the CSAS2 analytical sequence and with three cross-section libraries in the SCALE system. The study was performed on a no-personnel-time cost basis. A paper presenting the results of this study is attached as Appendix A. The calculated multiplication factors range from critical to approximately 3% Δk supercritical for systems with hydrogenous materials between the fuel assemblies. Although these results are conservative from the criticality safety point of view, they also indicate that the procedure for resonance processing in CSAS2 could be expanded to yield more accurate results. That is, a separate treatment for these pins next to the hydrogenous material would yield lower values of the multiplication factor.

Table 1. SCALE System Tasks Nearing Completion

Task	Individual Responsible	Part Completed	Estimate Man-Months to Completion
MORSE-SGC/S IBM Conversion and Checkout	Jim West	0	3-4
JUNEBUG Graphics IBM Conversion	Jim West	0	½-1
MORSE-SGC/S Documentation* (CDC)	Jim West	0.5	2-3
JUNEBUG Documentation* (CDC)	Jim West	0.9	¼-½
SAS3* (CDC) Documentation and Benchmarking	Jim West	0.5	1-2
HEATING6 CDC Conversion (CDC)	Doyle Turner	0.6	1
HEATING6 Documentation (CDC)	Doyle Turner	0.8	½
SAS2 Checkout and Documentation	Bill Hermann	0.2	2-3
COUPLE Documentation	Bill Hermann	0.4	1
CSAS4 Checkout and Documentation	Nancy Landers	0.2	2-3
ORIGEN-S Documentation (CDC)	Bill Hermann	0.95	¼-½
KENO-V Documentation	Nancy Landers	0.5	1-2
NITAWL-S Documentation	Mike Westfall	0.7	½-1
ORIGEN-S CDC Conversion (CDC)	Bill Hermann Jim West	0.9	½-1
XSDRN-2 Documentation	Lester Petrie	0.1	2-3
Interactive Input Processor Documentation	John Knight	0.3	¼-½
Cross Section Libraries Documentation	Mike Westfall	0.1	½-1

3. Control Modules

The SCALE manual sections on CSAS1 an CSAS2 have been completed. Binders, binder inserts, index tabs and a set of camera-ready plates of the manuscript have been forwarded to the NRC for publication and distribution.

4. BNL-CDC-7600 Implementation

A major portion of the effort to convert HEATING6 for operation on the BNL computer was performed. Progress made at the time the work was suspended for lack of funds is described in Appendix B.

The effort to package the CDC version of the operational portions of the SCALE system was completed. Correspondence pertinent to this task is attached as Appendix C.

APPENDIX A

SCALE SYSTEM CROSS-SECTION VALIDATION FOR CRITICALITY SAFETY ANALYSIS

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The purpose of this study is to test selected data from three cross-section libraries for use in the criticality safety analysis of UO_2 fuel rod lattices. The libraries, which are distributed with the SCALE system,[1] are used to analyze potential criticality problems which could arise in the industrial fuel cycle for PWR and BWR reactors. Fuel lattice criticality problems could occur in pool storage, dry storage with accidental moderation, shearing and dissolution of irradiated elements, and in fuel transport and storage due to inadequate packing and shipping cask design. The data were tested by using the SCALE system to analyze 25 recently performed critical experiments.

The SCALE system consists of a driver module, control modules, functional modules and a data base. One of the control modules is CSAS2 which stands for Criticality Safety Analytical Sequence No. 2. The CSAS2 control module reads a single unified set of input. After "messaging" the input and performing several auxiliary calculations, (e.g., Dancoff factor determination) problem-dependent cross-section processing and a subsequent calculation of the system multiplication factor are performed. The execution path includes the functional

modules BONAMI and NITAWL for problem-dependent cross-section processing, and the KENO-IV module for a Monte-Carlo determination of the system multiplication factor.

The three cross-section libraries utilized in the analysis presented here are the 27-group CSRL library,[2] the 123-group GAM-THERMOS library[3] and the 16-group Hansen-Roach library.[4] The 27-group library was collapsed from the 218-group CSRL library,[5] which was derived from ENDF/B-IV data.[6] Each of these libraries is available in the SCALE system data base.

Two series of experiments[7] involving 4.75 wt % enriched UO_2 rods were analyzed. The rods had a fuel diameter of 0.79 cm, an active fuel length of 90 cm, and an AG5 aluminum clad of 0.06 cm.

The first series of experiments utilized a square pitch lattice immersed in a sodium nitrate solution ($NaNO_3 + H_2O$). The parametric variations in this series were lattice pitch, $NaNO_3$ concentration, and the total number of rods in nearly square arrays. Criticality was determined by varying the height of the sodium nitrate solution.

The second series utilized four assemblies of rods in an 18x18 square pitch lattice. Cross-shaped, water-tight containers with various gap thicknesses (2.5, 5, and 10 cm) were positioned between the four assemblies. The containers were filled with either water, air, expanded polystyrene $(C_8H_8)_n$, polyethylene powder, or polyethylene balls, thus providing different concentrations of hydrogenous material.

The parameters of interest in this series were the composition and density of the hydrogenous materials and the separation distance (i.e., gap thickness) between the assemblies. Criticality was determined by varying the lattice water height.

The results obtained with the SCALE system for the first series of experiments are presented in Table 1. Using the 27-group ENDF/B-IV library, the average k_{eff} is 0.998 ± 0.004; using the 123-group GAM-THERMOS library, k_{eff} is 1.003 ± 0.004; and using the 16-group Hansen-Roach library, k_{eff} is 1.007 ± 0.004. Of the three libraries, the 27- and the 123-group results are more accurate than the 16-group results. When both data accuracy and computing efficiency are considered, the 27-group ENDF/B-IV library is preferred because it has substantially smaller computer storage requirements than the 123-group library.

In Table 2, results are presented for the second series of experiments. For assemblies with water only as the interstitial material, the 27-group library gives better agreement with experiment (i.e., measured k_{eff} = unity) than the other two libraries. For assemblies separated by the aluminum container filled with different materials, the calculated $k_{eff's}$ using all three libraries are, for the most part, equal to or slightly greater than unity. Also, considering statistical uncertainties, k_{eff} increases slightly with increasing hydrogen concentration for gap thicknesses of 2.5 and 5.0 cm - but not for the 10.0 cm gap. Finally, for this series of experiments,

the three libraries give essentially the same values for k_{eff}. Therefore, for assemblies separated by the hydrogenous materials used in this work, either the 16-group Hansen-Roach or the 27-group ENDF/B-IV library would be preferred over the 123-group library because of their much smaller (approximate factor of five) computer storage requirements.

References

1. R. M. Westfall et al., SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation, NUREG CR-0200 (1980). Distributed by the Radiation Shielding Information Center, P. O. Box X, Oak Ridge, Tennessee 37830.

2. R. M. Westfall et al., "Procedure for Determining Broad-Group Energy Structure or Criticality Safety Calculations," Trans. Am. Nucl. Soc., 22, 291 (1975).

3. Undocumented ORNL Library of ancient vintage.

4. G. E. Hansen et al., Six and Sixteen Group Cross Sections for Fast and Intermediate Critical Assemblies, LAMS-2543 (1961).

5. W. E. Ford et al., A 218-Group Neutron Cross-Section Library in the AMPX Master Interface Format for Criticality Safety Studies, ORNL/CSD/TM-4 (1976).

6. M. K. Drake, Ed., Data Formats and Procedures for the ENDF Neutron Cross-Section Library, BNL-50274 (ENDF 102 Vol. 1) (1970).

7. J. G. Manaranche et al., Dissolution and Storage Experimental Program with 4.75 wt % ^{235}U Enriched UO_2 Rods, Trans. Am. Nucl. Soc. (1980).

Table 1. CSAS2 Analysis of 4.75% UO_2 Rods in Sodium Nitrate Solution

Lattice		Solution			Calculted k-eff ± 1 σ		
Lattice Pitch cm	Array Size	Density g/cm^3	NaNO Conc. g/cm^3	Critical Height cm	27-Group ENDF/B-IV	123-Group GAM-THERMOS	16-Group Hansen-Roach
1.26	24x25	1.1521	0.247	80.9	0.99598 ± 0.00464	1.00401 ± 0.00477	0.98823 ± 0.00478
1.6	18x18	1.1503	0.243	76.1	0.98728 ± 0.00478	1.00216 ± 0.00455	0.99259 ± 0.00484
2.1	17x17	1.1523	0.246	76.2	0.99817 ± 0.00402	1.00846 ± 0.00379	1.01476 ± 0.00441
2.1	16x16	1.1094	0.178	89.5	1.00157 ± 0.00442	0.99509 ± 0.00430	1.01586 ± 0.00421
2.1	15x16	1.0565	0.090	84.8	1.00586 ± 0.00416	1.00658 ± 0.00389	1.0128 ± 0.00477
2.52	20x21	1.1523	0.246	85.9	0.99812 ± 0.00385	1.00239 ± 0.00418	1.01895 ± 0.00363

Table 2. CSAS2 Analysis of Four Assemblies of 18x18 U(4.75%)O_2 Rods at 1.35 cm Lattice Pitch, Separated by Various Hydrogenous Materials

Assembly Configuration					Calculated k_{eff} ± 1 σ		
		Compounds		Water Critical			
Δ cm*	Interstitial Material	Density gm/cm³	Conc.H gm/cm³	Height cm	27-Group ENDF/B-IV	123 Group GAM-THERMOS	16-Group Hansen-Roach
0	Water	1.0	0.1119	23.8	1.00806 ± 0.00507	1.02868 ± 0.00545	1.01481 ± 0.00514
	Box + Air	0	0	29.03	1.01663 ± 0.00488	1.01591 ± 0.00476	1.00460 ± 0.00504
	Box + $(C_8H_8)_n$	0.0323	0.0025	28.61	1.00506 ± 0.00499	1.01608 ± 0.00491	0.99856 ± 0.00517
2.5	Box + Powder $(CH_2)_n$	0.2879	0.0414	26.98	1.02348 ± 0.00472	1.02786 ± 0.00455	1.00797 ± 0.00471
	Box + Ball $(CH_2)_n$	0.5540	0.0800	25.54	1.03263 ± 0.00504	1.03542 ± 0.00457	1.02599 ± 0.00461
	Box + Water	1.0	0.1119	25.66	1.02827 ± 0.00454	1.03379 ± 0.00474	1.02991 ± 0.00485
	Water		0.1119	24.48	1.00391 ± 0.00399	1.02718 ± 0.00481	1.00673 ± 0.00376
	Box + Air	0	0	34.48	0.99886 ± 0.00462	1.01276 ± 0.00495	1.00366 ± 0.00451
	Box + $(C_8H_8)_n$	0.0262	0.002	34.39	1.00614 ± 0.00537	1.01100 ± 0.00477	1.00696 ± 0.00432
5	Box + Powder $(CH_2)_n$	0.3335	0.0480	30.16	1.02215 ± 0.00527	1.03381 ± 0.00412	1.0290 ± 0.00464
	Box + Balls $(CH_2)_n$	0.5796	0.0833	30.73	1.02913 ± 0.00446	1.02881 ± 0.00494	1.03299 ± 0.00519
	Box + Water	1.0	0.1119	32.78	1.02257 ± 0.00415	1.03349 ± 0.00463	1.02909 ± 0.00478
	Water	1.0	0.1119	31.47	0.99973 ± 0.00451	1.01139 ± 0.00473	1.01094 ± 0.00424
	Box + Air	0	0	46.08	0.99138 ± 0.00441	1.01345 ± 0.00498	0.99519 ± 0.00537
	Box + $(C_8H_8)_n$	0.0288	0.0022	45.62	1.01184 ± 0.00488	1.01393 ± 0.00526	0.98867 ± 0.00579
10	Box + Powder $(CH_2)_n$	0.3216	0.0464	42.05	1.01247 ± 0.00424	1.03046 ± 0.00454	1.02375 ± 0.00444
	Box + Balls $(CH_2)_n$	0.5680	0.0816	49.94	1.01674 ± 0.00450	1.00612 ± 0.00514	1.00898 ± 0.00499
	Box + Water	1.0	0.1119	64.12	0.99758 ± 0.00453	0.99949 ± 0.005	1.00396 ± 0.00512
	Water	1.0	0.1119	64.34	0.99352 ± 0.00446	0.98991 ± 0.00499	0.99659 ± 0.00521

*Δ is the value of the gap width between the assemblies, including 0.6 cm which is twice the wall thickness of the aluminum container box.

APPENDIX B

Changes to HEATING6 for Conversion to CDC

The following modifications were necessary for the conversion of HEATING6 from IBM FORTRAN to CDC FORTRAN.

1. All variables and constants were changed from double precision to single precision because CDC single precision uses a 60 bit word which is sufficient for the desired accuracy. All calls to double precision intrinsic functions and subroutines were changed to call the single precision versions.
2. Multiple returns from subroutines are set up differently in CDC FORTRAN. A RETURNS list has to be included with both the subroutine call and the SUBROUTINE statement. All the statements indicating multiple returns had to be modified.
3. The END=nnnn in a READ statement is not valid in CDC FORTRAN. There is a variable EOF which is set not equal to 0 when the end-of-file is detected. All the READ statements using END=nnnn were changed and a check on EOF was made to determine if the end-of-file was reached.
4. Calls to ERRSET in MAIN and MAINQ were commented out.
5. All entry points in subroutines must have the same argument list as the main entry point. Changes due to this restriction are enumerated later.
6. The number of arguments in a subroutine call is limited to 63 including the multiple return points. Many subroutines had to use SCM arrays CORE, ICORE, and LCORE and LCM arrays COREL,

ICOREL, and LCOREL to pass values between routines. The pointer commons had to be included in these routines to give access to the variably dimensioned arrays stored in these larger arrays. To eliminate duplication of a variable name already used in the subroutine, names of a few pointers had to be changed in some routines. Changes necessitated by the limit to the number of arguments are listed later.

7. All variable dimensions of arrays in a subroutine must be passed as arguments to that subroutine. They cannot be in COMMON. Many argument lists needed to be changed to include the variable dimensions in the subroutine.

8. CDC versions of some Oak Ridge systems routines had to be written. These subprograms are ICOMPA, ICLOCK, IDAY, INTBCD, JOBNUM, and MODEL.

9. All CALL CORE statements were changed to use ENCODE and DECODE, CDC FORTRAN statements which reformat data as it is transferred from one area of memory to another.

10. An ALOCAT subroutine which uses arrays in SCM and LCM was written. Any array whose dimension is based on MAXPTS is in LCM. The large arrays of LCM are COREL (real), ICOREL (integer), and LCOREL (logical). ALOCAT uses MEMORY to obtain the amount of SCM and LCM available.

11. LEVEL 2 statements were added to all subroutines that have variably dimensioned arrays in LCM.

12. When the program is compiled, I/O unit numbers must be included on the PROGRAM statement in the form of TAPEnn where nn is the

unit number. Therefore, the I/O unit numbers cannot be changed without recompiling the main program. I/O unit numbers for all the possible I/O files have been set in the BLOCK DATA subprogram and the I/O unit number variables have been taken out of the NAMELIST statement in MAIN.

Most of the above changes have very little effect on the logic or the structure of the routines. The limit to the number of arguments and the restriction to the arguments at entry points caused the major changes. Any routine which was restructured is listed below. Changes due to the limitation on the number of arguments and the restriction to the arguments at entry points will be denoted as L and E, respectively. With any division of a program, an attempt was made to maintain the linear and logical structure of the original program in the smaller routines. The major changes were made in the following routines:

ANALFN was divided into ANALFN and TABLFN (E).

DCHAR was divided into DCHAR, CVERTI, and CNVERT (E).

ERRCK was eliminated as a separate routine (L). Calls to subroutines ERRBND, ERRHGN, ERRINT, ERRMAT, and ERRREG are included in INPUT.

HGENS is divided into HGENS and ITEMPS (E).

INPUT entry points INPCM1 and INPCM2 were eliminated and the argument list was changed (E). CORE, ICORE, and LCORE are used in the argument list (L). The call to PREANA to initialize variables was eliminated (E). The arguments in the call to READER were changed, the call to WRITER was changed to call WRITE1, WRITE2, and WRITE3, and the call to ERRCK was

changed to call ERRBND, ERRHGN, ERRINT, ERRMAT, and ERRREG (L).

PREANA entry point was eliminated and the argument list was changed (E). Since the entry point was eliminated, PREANA is no longer called from INPUT to initialize variables. The name of the subroutine was changed from PREANA to ANALYT.

PRETAB was divided into PRETAB and TABLE (E).

PRTOUT was divided into PRTOUT, NODEMN, SPCPRT, and SPECPL (E).

READER uses CORE, ICORE, LCORE, COREL, ICOREL, and LCOREL in the argument list (L).

REORDR was divided into REORDR, REORMT,REORPC, REORHG, REORIT, REORBC, REORAF, and REORTF (E).

TEMPR was divided into TEMPR, SSPARM, TRANS, and TRANS2 (E).

WRITER was divided into WRITE1, WRITE2, and WRITE3 (L).

BDCOND entry point BDCOCM was eliminated and the argument list was changed (E).

FINEV1 entry point was eliminated (E). The name of the subroutine was changed from FINEV1 to FINEVL.

FUNCTN entry point FUNCTM was eliminated and the argument list was changed (E). FUNCTN is called with a call to FUNCT2 in all routines.

POINTS no longer calls THRMPR (L). The call to THRMPR is in HEATN6 immediately after the return from POINTS.

SURBC entry point SURBCM was eliminated and the argument list was changed (E).

THRMPR entry point THRCOM was eliminated and the argument list was changed (E). THRMPR was divided into THRMPR, THRINI, THRM1, THRMX, THRMY, THRMZ, and THRMWU (L).

PLOTIN entry point PLOTOU was eliminated and the argument list was changed (E).

PREP entry point PREPCM was eliminated and the argument list was changed (E).

TMPOUT entry point TMPCM was eliminated and the argument list was changed (E).

TMSTEP's argument list was changed so that TMSTEP and entry point UDTS have same arguments (E).

TRANO's argument list was changed so that TRANC and entry point TRANIM have same arguments (E).

UMONTR's entry point USRMON was changed to use same arguments as UMONTR (E).

CALQLT's argument list was changed (L).

DIRECT's argument list was changed (L).

INFACE's argument list was changed (L).

HEATN6. Pointers of arrays whose dimensions depend on MAXPTS were changed so these arrays start at the first word in LCM. Multipliers for indexing variable dimensioned arrays were changed from PDP10 and IBM to CDC factors. Number of words and amount of core used were changed to use CDC word lengths and units. Calls to MEMORY to release unused SCM or LCM or to acquire additional SCM or LCM were added. All calls which initialized variables in subroutines, i.e., INPCM1, INPCM2, THRCOM, BDCOCM, SURBCM, FINEV1, FUNCTM, and PREPCM, were eliminated (E). Argument lists in calls to INPUT, POINTS, and CALQLT were changed (E and L). A call to THRMPR was added after the call to POINTS (L) (moved from POINTS subroutine).

APPENDIX C

NUCLEAR DIVISION

July 11, 1980

TO: Betty F. Maskewitz

FROM: J. T. West

SUBJECT: CDC SCALE

The CDC SCALE system is operational on the CDC-7600 at Brookhaven National Laboratory. Frozen versions of criticality sequences CSAS1 and CSAS2, along with shielding sequences SAS3 and SAS3X, have been delivered to TDMC for processing. The delivery package includes: BONAMI, NITAWL, XSDRN-PM, ICE-2, MORSE-SGC/S, JUNEBUG, KENO-IV, COMPOZ, and AIM.

The above package includes the only CDC version of super-group MORSE, and the only nested array lattice modeling capability, the MARS system with combinatorial geometry, in the public domain which has no proprietary restrictions. The JUNEBUG graphics allow 3-d isometric drawings of the MARS lattice geometries.

Requests for the above CDC code systems have been received from Adolph Garcia of Argonne-West, Ivan Fergus of Exxon Nuclear, Mike Strayer of CDC, Wolfgang Thomas of the Technical University of Munich, Federal Republic of Germany. Interest has been expressed by others.

Release of the above CDC SCALE system is held up pending completion of documentation.

JTW/mwl

cc: Marie Anthony
Betty McGill
R. M. Westfall
G. E. Whitesides

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 on the CDC-7600

The CDC version of HEATING6 was loaded on the 7600 CDC computer at Brookhaven National Laboratory. The program was compiled but no test case was successfully executed before work on the project was suspended. A memorandum was issued documenting the status of the conversion at the termination of the project.

2. Documentation of HEATING6

A draft of the report documenting HEATING6 has been completed and the typing has been essentially completed. A number of figures is still at Graphic Arts. The draft of the document should be ready for peer review in late June 1980. Additions that should be added to the documentation when funding is available are: a section on control cards; an expanded section on the logical structure of the code to include more information on the interaction between subroutines, a description of various warning and error messages, and descriptions of the variables and commons; additional sample problems designed to address new features of the code; acknowledgements; and a distribution list. Several errors in the HEATING6 code were detected in preparing the documentation. In addition to routine maintenance, the reprogramming necessary to correct these errors should be completed when funding is available. A series of test problems with analytical solutions should be developed, executed on HEATING6 and documented.

3. REGPLOT Conversion

The documentation describing the HEATING6 version of REGPLOT was issued.