Conf-780506--23

STANDARDIZED SAFETY ANALYSIS OF NUCLEAR FUEL SHIPPING CONTAINERS*

R. M. Westfall and L. M. Petrie

Computer Sciences Division
at Oak Ridge National Laboratory
Union Carbide Corporation, Nuclear Division

*Research sponsored by the Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission under Interagency Agreement DOE 40-550-75 with the U.S. Department of Energy under contract W-7405-eng-26 with the Union Carbide Corporation.

STANDARDIZED SAFETY ANALYSIS OF NUCLEAR FUEL SHIPPING CONTAINERS

Robert M. Westfall and Lester M. Petrie
Computer Sciences Division at Oak Ridge National Laboratory
Union Carbide Nuclear Division, Oak Ridge, TN 37830

INTRODUCTION

This paper describes a US Nuclear Regulatory Commission-supported effort to develop standardized methods for performing safety analyses of nuclear fuel shipping containers. The objective of this effort is a modular system of computer programs called SCALE. (SCALE is an acronym for Standardized Computer-Analysis for Licensing Evaluation.) The anticipated NRC applications and design criteria for the SCALE system are described in a companion paper by R. H. Odegaarden. The purpose of the present paper is to describe the components and capabilities of the initial version of the SCALE system, with emphasis being placed on those aspects of the system that lead to analytical standardization.

The SCALE system draws heavily from basic neutron-transport, data-processing, and heat-transfer methods technology developed at Oak Ridge over the past several years. The data-processing is a direct outgrowth of that employed in AMPX,[1] a modular code system for processing coupled neutron-photon cross sections from ENDF/B. Modified versions of the AMPX problem-dependent data-processing modules NITAWL and XSDRNPM are incorporated into SCALE. However, even though some of the functions performed in AMPX and SCALE are the same, the overall purpose and organizational structure of SCALE is substantially different from that of AMPX.

The overall purpose of SCALE is systems analysis with associated data-processing. For example, the objective of systems analysis may be to establish the criticality safety of the configuration under study. Then the associated data processing would involve the preparation of neutron cross sections representative of the system being analyzed. Systems analysis in the initial version of SCALE is comprised of criticality safety and radiation shielding determinations. Advanced versions of SCALE will perform heat transfer and, possibly, structural integrity analyses. Thus, one major difference between SCALE and AMPX is that data processing in SCALE is restricted to the problem dependent phase and, rather than being the primary objective, it is incidental to the systems analysis.

The second major difference between SCALE and AMPX is the manner in which the two systems are organized. In AMPX, the user selects a sequence of modules to be executed and prepares a set of input data for each module. In the SCALE system the user selects an analytical sequence characterized by the type of analysis to be performed and geometric complexity of the system being analyzed. The user then prepares

a single set of input for the control module corresponding to this analytical sequence. The control module input is in terms of easily-visualized engineering parameters specified in a simplified, free-form format. The control modules use this information to derive additional parameters and prepare the input for each of the functional modules in the analytical sequence.

The components of the initial version of the SCALE system are shown in Figure 1. The SCALE system consists of a driver module, control modules, functional modules and a data base.

SCALE SYSTEM DRIVER

The driver module resides in-core at all times and, upon various types of commands, loads and unloads the control and functional modules from the central processor unit. Thus the core storage requirement for a sequence involving the execution of several modules corresponds roughly to the largest needs of any single module in the sequence. The intermodular execution paths are normally determined by the control modules. The control modules communicate with the system driver through a small common block of special parameters. Ordinarilly, the user specifies the control module to be executed on a data card read by the driver. For example, to execute Criticality Safety Analytical Sequence 1, CSAS1, the user submits =CSAS1 to the driver, which in turn, loads CSAS1 into the central processor unit. However, provvision has been made to allow the user to execute the functional modules on a standalone basis, e.g., =KENO. Thus the user has the option of determining his own (or nonstandard) execution path.

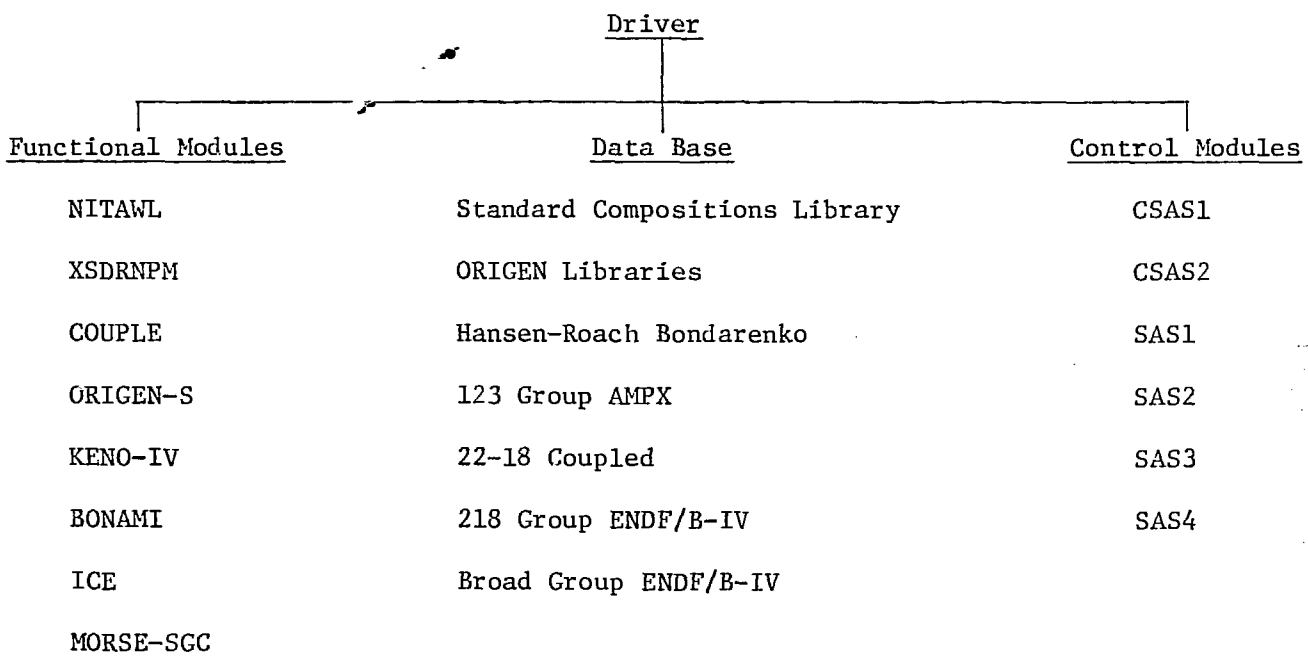

Figure 1. SCALE SYSTEM COMPONENTS

SCALE SYSTEM CONTROL MODULES

Six control modules have been developed for the initial version of SCALE.

1. CSAS1 performs data processing and criticality safety analysis on systems which can be adequately modeled in one-dimensional geometries. The execution path includes the functional modules NITAWL and XSDRNPM.

2. CSAS2 performs data processing and criticality safety analysis on systems which must be modeled in three-dimensional geometry. The execution path includes NITAWL, XSDRNPM (if lattice-cell cross section processing is specified), and KENO-IV.

3. SAS1 performs data processing and radiation shielding analysis on systems for which the user specifies the radiation source distribution and which can be adequately modeled in one-dimensional geometries. The execution path includes NITAWL, XSDRNPM for data processing, and a final pass through XSDRNPM for the shielding analysis.

4. SAS2 performs data processing, radiation source determination and radiation shielding analysis on systems which can be adequately modeled in one-dimensional geometries. The execution path includes NITAWL, XSDRNPM, COUPLE and ORIGEN-S for data processing, fuel burnup and radiation source determination and a final pass through XSDRNPM for the shielding analysis. The data processing can be updated for fuel compositions determined by the burnup analysis.

5. SAS3 performs data processing and radiation shielding analysis on systems for which the user specifies the radiation source distribution and which must be modeled in three-dimensional geometry. The execution path includes NITAWL, XSDRNPM (if lattice-cell cross section processing is specified), ICE and MORSE-SGC.

6. SAS4 combines the more sophisticated capabilities of SAS2 and SAS3 to include data processing, radiation source distribution determination, and three-dimensional geometry modeling. The execution path includes NITAWL, XSDRNPM, COUPLE, ORIGENS, ICE and MORSE-SGC.

An example of the simplified input for the control modules is given in Figure 2. The first card contains user-specified title information. The second card contains a general specification of problem parameters. These include the name of the cross section library, the geometry type, and the number of material mixtures, standard compositions, material zones and fuel solution compositions in the problem. The first standard composition is a uranyl nitrate solution specified in terms of the heavy metal density, the excess acid molarity, the temperature, and the uranium isotopic distribution in weight percent. The standard compositions are followed by a specification of geometry parameters including boundary conditions, dimensions and the material mixture numbers by zone. The last set of data contains special parameters with which the user can override default values set in the XSDRNPM input.

This example includes all the information required by CSAS1 to execute NITAWL and XSDRNPM. A package of routines called the materials information processor is incorporated into all of the control modules. This processor reads the materials-related information, accesses the SCALE system standard compositions library, and calculates isotopic atom densities. It also prepares the physics parameters required by the resolved resonance analysis in the NITAWL module. For example, the materials information processor includes a calculation of the Dancoff factor for problems in which the LATTICE CELL geometry option has been specified.

Upon processing the user-specified input, the SCALE system control modules immediately print an input check list in which the user (or reviewer) can easily

```
=CSAS1
34.6 CM RADIUS UO2(NO3)2 CRITICAL SPHERE.
25GROUPAMPX  2 2 2 MULTIREGION  1 1
SOLNUO2(NO3)   1 20.123 0.14 1 298 92234 1.04 92235 93.18
  92236 0.27 92238 5.51      END
AL    2 1.0  END
SPHERICAL  VACUUM  REFLECTED  0
1 34.6 NOEXTERMOD  2 34.92 NOEXTERMOD      END
SZF=2  ICM=180  PTC=1-5  EPS=1-5  IUS=0   END
END
```

Figure 2. CARD IMAGES OF CSAS1 INPUT

establish that the input describes the system to be analyzed. The input check list given in Figure 3 summarizes the user-specified input given in Figure 2. The SCALE system control module input format has been designed to minimize input errors and therefore lead to analytical standardization. Where appropriate, parameters are entered in an alphameric form. Also, associated parameters, whether alphameric, integer or floating, are entered in their relative logical order within a single group. For example, all the input variables required to use a standard composition are entered together.

SCALE SYSTEM FUNCTIONAL MODULES

The functional modules included in the initial version of the SCALE system are shown in Figure 1. The modules perform data processing, radiation source determination, criticality safety analysis and radiation shielding analysis. The list includes NITAWL, XSDRNPM, COUPLE, ORIGEN-S, KENO-IV, BONAMI, ICE, and MORSE-SGC. Advanced versions of SCALE will perform heat transfer analysis using the three-dimensional finite-difference program HEATING5[2] and a new Monte Carlo heat transfer program that is presently under development at Oak Ridge. Here we present a brief summary of the capabilities of the functional modules in the initial version of the SCALE system.

1. NITAWL - The Nordheim Integral Technique[3] is applied in NITAWL to perform neutron cross section processing in the resonance energy range. This technique involves a fine energy group calculation of the slowing-down flux across each resonance with subsequent flux-weighting of the resonance cross sections. This is the major function of NITAWL in its conversion of cross section libraries from a problem-independent to a problem-dependent form. However, NITAWL also assembles group-to-group transfer arrays from the elastic and inelastic scattering components and performs other tasks in producing the problem-dependent library.

2. XSDRNPM - This is a substantially modified version of the one-dimensional, discrete-ordinates transport program XSDRN.[4] The transport analysis is essentially the same as that performed in ANISN, a well-established program used in both criticality safety and shielding analyses. XSDRNPM performs both data-processing and systems analysis in the SCALE system. Probably its most important role is in providing lattice-cell-averaged cross sections. Other functions include one-dimensional criticality safety and radiation shielding analyses. Also, the neutron spectrum as calculated by XSDRNPM is used to develop the spectral parameters applied in the ORIGEN-S module.

3. COUPLE - This is a relatively new module whose function is to update ORIGEN-S libraries with flux-weighted cross sections provided by XSDRNPM. COUPLE uses the multigroup fluxes from XSDRNPM to calculate THERM, RES, and FAST, the spectral parameters used in ORIGEN-S. This is done in a manner that is

```
34.6 CM RADIUS UO2(NO3)2 CRITICAL SPHERE.

**** PROBLEM PARAMETERS ****

LIB 25GROUPANPX  LIBRARY
MXX            2 MIXTURES
MSC            2 COMPOSITIONS SPECIFICATIONS
IZM            2 MATERIAL ZONES
GE  MULTIREGION  GEOMETRY
MORE           1 0/1 DO NOT READ/READ SPECIAL PARAMETERS
MSLN           1 FUEL SOLUTIONS

**** PROBLEM COMPOSITION DESCRIPTION****

SC  SOLNUO2(NO3) STANDARD COMPOSITION
MX             1 MIXTURE NO.
FD       20.1230 SOLUTION FUEL DENSITY
AML       0.1411 ACID MOLARITY
VF        1.0000 VOLUME FRACTION
TEMP       298.0 DEG KELVIN
           92234  1.04%
           92235 93.18%
           92236  0.27%
           92238  5.51%
END

SC  AL           STANDARD COMPOSITION
MX             2 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
END

****PROBLEM GEOMETRY****

CS  SPHERICAL    COORDINATE SYSTEM
BR  VACUUM       RIGHT BOUNDARY
BL  REFLECTED    LEFT BOUNDARY LOCATION
ORGN        0.0  CM LEFT BOUNDARY LOCATION
DY          0.0  CM BUCKLING HEIGHT
DZ          0.0  CM BUCKLING DEPTH

ZONE NUMBER    1
MZX            1 MIXTURE NO.
RZ         34.60 CM RIGHT BOUNDARY LOCATION
XMOD NOEXTERMOD  EXTERNAL MODERATOR INDEX

ZONE NUMBER    2
MZX            2 MIXTURE NO.
RZ         34.92 CM RIGHT BOUNDARY LOCATION
XMOD NOEXTERMOD  EXTERNAL MODERATOR INDEX

**** SPECIAL PARAMETERS ****

ISN            8 ORDER OF ANGULAR QUADRITURE
IIM           20 INNER ITERATION MAXIMUM
ICM          180 OUTER ITERATION MAXIMUM
SZF  2.00000E 00 SIZE FACTOR FOR SPATIAL MESH
EPS  1.00000E-05 OVERALL PROBLEM CONVERGENCE
PTC  1.00000E-05 SCALAR FLUX CONVERGENCE
BLK  1.42089E 00 BUCKLING FACTOR
IUS            0 THERMAL UPSCATTER SCALING
```

Figure 3. CSAS1 INPUT CHECKLIST

consistent with the use of the data in the ORIGEN library for those nuclides which are not being updated with XSDRNPM cross sections.

4. ORIGEN-S - This is a version of the ORIGEN[5] program which had been modernized with flexible dimensioning and free-form input processing before being implemented into SCALE. ORIGEN-S performs a fuel depletion, actinide transmutation and fission product buildup analysis yielding isotopic compositions and radiation source terms. In the SCALE system analytical sequences, the user specifies the physical description of the fuel bundle and its radiation history in terms of the various cycles of burntime at a given power level followed by downtime. Also the user can specify the number of times during each cycle that new isotopic compositions calculated by ORIGEN-S are fed back into NITAWL, XSDRNPM, and COUPLE to produce updated cross section libraries.

5. KENO-IV[6] - This is the latest version of the KENO Monte Carlo criticality programs in general use. The criticality safety sequence employing KENO-IV provides for automated cross section processing and simplified materials input specifications. However, all of the features of the three-dimensional geometry specifications have been reserved as options for the user. A combinatorial geometry version of KENO, KENO-IV/CG, and a supergroup version, KENO-V, will be incorporated into new analytical sequences of the advanced versions of SCALE.

6. BONAMI - This is a new program which performs resonance cross section processing by the shielding factor method most frequently associated with Bondarenko.[7] The initial application of BONAMI in SCALE is in the automation of the use of the Hansen-Roach[8] 16 group library in the criticality safety analytical sequences. Eventually, BONAMI will be used to perform problem-dependent unresolved resonance processing with the cross section libraries based upon ENDF/B.

7. ICE[9] - This module prepares supergrouped macroscopic cross sections from multigroup microscopic cross sections. Supergrouping reduces the core storage required by Monte Carlo analysis with fine multigroup libraries. The storage required to mix macroscopic constants is eliminated altogether from the Monte Carlo program CPU needs. Thus the Monte Carlo programs will execute on computers with relatively modest CPU capabilities. Initially, MORSE-SGC will be the only SCALE module to use ICE prepared constants. Eventually KENO-V will use ICE data.

8. MORSE-SGC[10] - This is a supergrouped version of the MORSE[11] Monte Carlo radiation shielding analysis programs. The capabilities of MORSE to analyze radiation transport in complex three-dimensional geometries is well established. The analytical sequences employing MORSE have simplified input specifications for the flux-at-a-point estimators used in determining the radiation dose levels at locations of interest.

The functional modules in the SCALE system have been selected on the basis of both their sophisticated, state-of-the-art, analytical capabilities and their proven records of reliable performance. An ongoing effort is being directed towards minimizing computer storage requirements, automating data processing, and simplifying input requirements.

SCALE SYSTEM DATA BASE

The SCALE system data base contains a standard compositions library, various neutron and coupled neutron-photon libraries, and the ORIGEN-S libraries. The standard compositions library is used by the materials input processor in developing nuclide atom densities. Also the library contains data on each nuclide which is used in developing the input for the resonance processors and for the mesh-spacing algorithms used with the deterministic codes. The library consists of a

standard compositions directory, a standard compositions table, an isotope distribution directory, an isotope distribution table, and a nuclide information table. The library is configured as a permanent direct access data set. Presently, it contains 109 standard compositions, 78 nuclides, 3 elements with variable isotopic distributions and data for the specification of three aqueous fuel solutions. The physical data contained in the library is taken from standard references.[12,13]

A single nuclide identification scheme is common to both the standard compositions library and all of the cross section libraries. The cross section libraries were selected on the basis of their completeness and the wide experience that has been built up in their use. The ORIGEN libraries include the small and large (800 element) fission product and light element libraries, the LWR libraries and the LMFBR library. The Hansen-Roach-Bondarenko library includes all of the original Hansen-Roach 16 group data supplemented by ENDF/B-IV data for nuclides not present in the original library. The 123 group AMPX library contains data originally compiled for the GAM-II[14] and THERMOS[15] programs. Although this data is old, the library is known to be quite effective in the analysis of systems containing light water reactor fuel. The 22-18 coupled neutron-photon library was developed for shipping cask analysis[16] and it has also been widely used. The 218 group ENDF/B-IV library[17] was developed as a reference-source for the broad group ENDF/B-IV library. The broad group library is currently being validated[18] through the calculation of critical experiments containing the fuel, structural materials, and neutron absorbers commonly found in shipping cask designs.

SCALE SYSTEM FEATURES LEADING TO ANALYTICAL STANDARDIZATION

The initial version of the SCALE system is being documented[19] in a modular format under which new sections can be added to the report as new modules are added to the system. Separate sections describe the SCALE system driver, the data base, and each of the standard analytical sequences. The functional modules are being documented as appendices in the report. The documentation complies with the ANSIN413-1974 standard for the documentation of computer programs. The objective of this effort is to provide the SCALE system user the capability of performing analysis in an easily-referenced, well-documented manner.

In addition to thorough documentation, the SCALE system features which lead to analytical standardization are:

1. the coupling of data processing and systems analysis into standard analytical sequences,

2. simplified, easily-verified input based upon selections from a standard compositions library,

3. the application of well-established functional modules with proven records of reliable performance,

4. the use of cross section and other data libraries which have demonstrated ranges of applicability.

The development of the SCALE system has involved a cooperative effort from many members of the Computer Sciences Division at Oak Ridge. Particular recognition should be given to the work of J. A. Bucholz, O. W. Hermann, J. R. Knight and J. T. West. R. H. Odegaarden and W. R. Lahs of the Nuclear Regulatory Commission have participated in this project since its inception and have contributed many worthwhile ideas.

REFERENCES

1. N. M. Greene et. al., "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL-TM-3706 (March 1976).

2. W. D. Turner et al., "HEATING5-An IBM-360 Heat Conduction Program," ORNL/CSD/TM-15, (March 1977).

3. L. W. Nordheim, "The Theory of Resonance Absorption," *Proc. Symp. In Apl. Math, XI*, 58, American Mathematical Society, Providence (1961).

4. N. M. Greene et al., "XSDRN: A discrete Ordinates Spectral Averaging Program," ORNL-TM-2500 (July 1969).

5. M. J. Bell, "ORIGEN-The ORNL Isotope Generation and Depletion Code," ORNL-4628 (May 1973).

6. L. M. Petrie et al., "KENO-IV, An Improved Monte Carlo Criticality Program," ORNL-4938 (November 1975).

7. I. I. Bonarenko et al., "Group Constants for Nuclear Reactor Calculations," Consultants Bureau, New York (1964).

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

9. S. K. Fraley, "Users Guide to ICE," ORNL/CSD/TM-9 (July 1976).

10. S. K. Fraley, "Users Guide to MORSE-SGC," ORNL/CSD/TM-7 (1976).

11. E. A. Straker et al., "The MORSE Code-A Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code," ORNL-4585 (1970).

12. Handbook of Chemistry and Physics, 51st Edition, Chemical Rubber Company, Cleveland (1971).

13. Chart of the Nuclides, Eleventh Edition, Nuclear Energy Division, General Electric Co., San Jose (April 1972).

14. G. D. Joanou et al., "GAM-II-A B_3 Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants," GA-4265 (September 1963).

15. H. C. Honeck, "THERMOS, A Thermalization Transport Theory Code for Reactor Lattice Calculations," BNL-5826 (September 1961).

16. G. W. Morrison, "CASK, 40 Group Coupled Neutron and Gamma-Ray Cross Section Data," Radiation Shielding Information Center DLC-23.

17. W. E. Ford et al., "A 218-Neutron-Group Master Cross Section Library for Criticality Safety Studies," ORNL/CSD/TM-4 (July 1976).

18. N. F. Cross et al., "Validation of Criticality Safety Broad-Group Library Using Uranium Systems," *Trans. Am. Nuc. Soc.*, 27,406 (November 1977). (March 1975).

19. R. M. Westfall et al., "SCALE: A Modular Code System for Performing Standardized Computer-Analysis for Licensing Evaluation," to be published as ORNL/NUREG/CSD-2 and NUREG-0358.