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STANDARDIZED ANALYSES OF NUCLEAR SHIPPING CONTAINERS*

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INTRODUCTION

This paper describes improved capabilities for analyses of nuclear fuel shipping containers within SCALE - a modular code system for Standardized Computer Analyses for Licensing Evaluation (1). The SCALE system was conceived and funded by the U. S. Nuclear Regulatory Commission (via the Transportation Branch of the Office of Nuclear Material Safety and Safeguards) to satisfy a strong need for standardized methods of analysis for the evaluation of nuclear facility and package designs. Earlier papers have described the initial components and overall capabilities of the SCALE system, the SCALE features that lead to analytical standardization, and an NRC perspective on its use in design reviews (2,3). Therefore, this paper will provide only a brief description and history of the SCALE system prior to presenting the improved SCALE capabilities for criticality, shielding, and thermal analyses.

OVERVIEW OF SCALE

The overall goal of the SCALE project has been to develop easy-to-use analytical sequences which are automated to perform the necessary data processing (e.g., cross-section preparation) and manipulation of well-established computer codes (functional modules) required by the sequence. Thus, the user is able to select an analytical sequence characterized by the type of analysis (criticality, shielding, or heat transfer) to be performed and the 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 existing components of the SCALE system are shown in Fig. 1.

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. Ordinarily, the user specifies the control module to be executed on a data card read by the driver. For example, to execute Criticality Safety Analysis Sequence No. 1 (CSAS1) the user submits =CSAS1 to the driver, which in turn loads CSAS1 into the central processor unit. However, provision has been made to allow the user to execute the functional modules on a stand-alone basis, e.g., =KENO5. Thus the user has the option of determining his own (or nonstandard) execution path.

A limited version of SCALE (SCALE-0) was made available to the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory in July 1980. A more

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extensive version of SCALE (SCALE-1) (complete with functional module documentation) was made available to RSIC in January 1982. Recently (May 1983), several new or revised SCALE components were made available to RSIC. Two of these new components (SAS2 and HTAS1) are discussed in this paper along with the components currently being tested for public release in early 1984.

IMPROVEMENTS IN CRITICALITY ANALYSIS

The KENO V.a Functional Module

The earliest version of SCALE used the existing KENO IV Monte Carlo program as the functional module for criticality safety analysis of multidimensional systems. Subsequently KENO V was developed as a functional module within the SCALE system. KENO V features not previously available in KENO IV include simplified data input, supergrouping of energy-dependent data, a P_n scattering treatment, extended use of differential albedo reflection and an improved restart capability. Recently KENO V has been further improved (KENO V.a) by inclusion of an advanced geometry capability that provides 1) construction of arrays from previously described arrays (arrays of arrays), 2) placement of a unit or array at any desired location (or hole) within a geometry region, and 3) generation of printed geometry "pictures" that aid in verifying the problem description when arrays of arrays or holes are used.

The arrays of arrays option greatly simplifies the setup of arrays involving different units at different spacings. The depth of nesting is limited only by computer space restrictions. At all levels of nesting, the constraint on array construction is that adjacent faces of adjacent units in an array must match exactly in size and shape. The unit or array located with the hole option cannot intersect any geometry region boundary and thus must be wholly contained within a particular region. As many holes as will snugly fit without intersecting can be placed in a region. Any number of holes can be described in a problem and holes can be nested to any depth. The new picture capability can be optionally used to check the model by printing the material (mixture number) by location or the unit number by location. Any number of pictures can be specified. Timing studies indicate that the cost of the additional geometry capability is small in terms of extra execution time.

These new features in KENO V allow the modeling of complex geometry configurations not possible with KENO IV. As an example, consider the typical shipping cask model illustrated by Fig 2. Note that a very detailed model of the shipping cask can be obtained. The shipping cask contains seven 17x17 PWR Fuel assemblies with each pin in each assembly modeled. The rods placed between the fuel assemblies are B_4C rods with stainless steel cladding. The geometry input consisted of only 53 statements. The stand-alone KENO V.a calculation took 8 min. of cpu time (IBM 3033) for 30,000 histories and yielded a k-effective of 0.954 ± 0.004.

Fig. 2. Cross-section of a typical PWR shipping cask model for KENO V.a.

The CSAS4 Control Module

The Criticality Safety Analysis Sequence No. 4 was developed within SCALE to 1) incorporate the use of KENO V in a control module and 2) provide an option for an optimum pitch search that determines the spacing between units (e.g., fuel pins or assemblies) corresponding to the maximum value of k-effective for the global array. Like all criticality and shielding control modules in SCALE, a standardized procedure is applied to calculate number densities for the nuclides specified in the input data and to generate appropriate cross sections for use in the calculation. In order to minimize human error, this is automated as much as possible. The sequence utilizes (1) a Material Information Processor to generate number densities and related information, as well as geometry data for XSDRNPM-S (a one-dimensional discrete ordinates code) and resonance data for NITAWL-S (for resonance self-shielding using the Nordheim Treatment); (2) a Data Preprocessor to prepare data input for the cross section processing codes; (3) a KENO V Data Processor to read and check the KENO V data; and (4) a Search Data Processor to read and check the search data. The Material Information Processor is responsible for reading the standard composition data and other engineering-type specifications including volume fraction or percent theoretical density, temperature, and isotopic distribution. It checks the data for obvious errors and generates information used in processing the cross sections.

After the data is read and checked, BONAMI-S (for resonance self-shielding with Bondarenko data), NITAWL-S, XSDRNPM-S (for cell-weighted calculations only), and ICE-S (for cross-section mixing) are executed sequentially to prepare cross sections for use in KENO V. For an optimum pitch search, the module MODIFY repeatedly alters the pitch and executes KENO V until the optimum pitch is determined or the calculation is terminated. The search module initially obtains k-effectives for the specified problem, the minimum constraint (units touching), the maximum constraint (presently arbitrary), and a fourth case with a spacing chosen to fall between the specified design spacing and the more distant of the bounding constraints. Utilizing a weighted least squares fit to a cubic polynomial on the data points, MODIFY investigates the local behavior of the cubic equation. A cubic with no local extrema indicates an optimum pitch on one of the boundaries, whereas a cubic with two local extrema requires iteration to determine the optimum pitch.

The data input required to obtain the optimum pitch for an array of fuel bundles in a square aluminum cask is shown in Fig. 3. The input utilizes a cell-weighted mixture (500) to represent a BWR-like fuel bundle. The cask contains a 2x2x1 array of fuel bundles. Each fuel bundle consists of a 17x17x1 array of zirconium clad, 2.35% enriched UO_2 fuel pins arranged in a square pitch. The pin diameter is 0.823 cm, and its length is 366 cm. The clad is 0.1393 cm thick, and the pitch is 1.275 cm. Each fuel bundle is contained in a 0.6615-cm-thick boral sheath. The bundles are separated by 1 cm of water, representing a flooded cask. The square aluminum cask is 10 cm thick on all faces and is reflected by 15 cm of water. The input consists of a sequence keyword, title, cross-section library specification (HANSEN-ROACH), type of calculation keyword (LATTICECELL), standard composition input, fuel pin cell specification, KENO V data, and search data. The output from the above sample problem indicated a maximum k-effective value of 0.754 ± 0.048 when the fuel bundles were touching (i.e., at the minimum constraint).

With the completion of CSAS4 in 1982, the SCALE-1 package currently has five available sequences involving multidimensional criticality calculations. The initial sequence (CSAS2) performs cross-section processing followed by a KENO IV calculation for k-effective. With the development of CSAS4, one is now able to run a sequence (CSAS25) essentially identical to CSAS2 except KENO V is used in place of KENO IV. Cell-weighting is also automatically available as variations on CSAS25 and CSAS4 by specifying CSAS2X or CSAS4X, respectively. Current development is underway to upgrade the sequences presently using KENO V to use KENO V.a. The search data input to CSAS4 and CSAS4X is also being altered to allow user specification of the boundary constraints.

IMPROVEMENTS IN SHIELDING ANALYSIS

The SAS2 Control Module

The Shielding Analysis Sequence No. 2 (SAS2) processes fuel assembly cross sections, computes photon and neutron source spectra and evaluates dose rates from shipping casks by a one-dimensional transport shielding analysis. The execution includes: repeated passes through BONAMI-S, NITAWLS, XSDRNPM-S, COUPLE and ORIGEN-S for cross-section processing and fuel burnup; radiation source computations; the radial shipping cask shielding analysis applying the calculated spent-fuel composition and sources; and the final determination of dose rates by XSDOSE from the angular flux leakage. See Fig. 4 for a flow diagram of this sequence. The SAS2 sequence is a very versatile tool particularly in light of the HALT and RESTART features discussed below.

Fuel assembly cross-section processing is done using the same procedures and input requirements described for CSAS4. Other input requirements include parameters for the depletion segment (specific power, burn time, and down time per cycle), and the shielding analysis (shielding cross-section library and geometry specification). An automatic mesh generator provides a conservative mesh for use in XSDRNPM; however, the mesh size can be easily scaled up or down using an input factor. Detector locations may be input, however, the standard but default locations are 0, 3, and 10 feet from the cask surface.

A radial shielding analysis was performed on the typical PWR shipping cask of Fig. 5. The four cases of Table 1 were analyzed via the following steps

1) 3.2% enriched fuel was depleted through three cycles, each with 80% full power irradiation at 37.5 MW/MTU and 20% downtime. The final spent fuel burnup was 33 GWD/MTU. Use of the HALT03 feature stopped the computation after the third cycle which corresponds to 180 days of cool time. Step 1 generates a library of burnup dependent cross sections which can be used in subsequent stand-alone ORIGEN-S calculations where a slightly different irradiation history or specific power is used. Necessary restart files were saved.
2) The RESTART feature allowed the analysis of case 1 to be completed.
3) Case 2 was run by using a short HALTXX job to change the cask water content and then restarting the SAS2 calculation.
4) Case 3 required an intermediate ORIGEN-S calculation to decay the fuel from 180 days to 3 years followed by a SAS2 RESTART.
5) Case 4 again required a HALTXX job followed by a RESTART.

Cases 1 and 4 correspond to normal conditions of transport for wet and dry shipments, respectively. Cases 2 and 3 correspond to accident conditions. The results could be obtained by running four complete SAS2 cases. However, following the above procedure saved about 40% on the required cpu time.

Table 1. Results of SAS2 shielding analysis.

Fig. 4. Basic flow invoked by SAS2.

Fig. 5. Typical shipping cask calculational model.

The SAS5 Control Module

The latest feature in SCALE provides the option to automatically incorporate adjoint fluxes from a one-dimensional (1-D) discrete ordinates calculation (functional module XSDRNPM-S) to generate biasing parameters for the Monte Carlo calculation of radiation levels exterior to a shipping cask. The feature is available within the Shielding Analysis Sequence No. 5 (SAS5) which prepares the cross section data, generates biasing parameters, and performs a multidimensional shielding analysis using the MORSE-SGC/S functional module. Proper biasing of the Monte Carlo histories substantially reduces the high cost of the deep-penetration calculations needed for axial dose rates in shipping casks.

In generating the biasing parameters, a one-to-one correspondence is made between the zones, IZ, of XSDRNPM-S and the importance regions, IR, in MORSE-SGC/S. The energy-dependent and zone-averaged adjoint flux, $\phi^*(IG,IZ)$, is then used directly as the importance function for selection of emergent particle energy and source energy biasing. The Russian roulette survival weights are set equal to $\lambda/\phi^*(IG,IZ)$ where λ is the effect of interest (dose rate) approximated with the 1-D adjoint calculation. Similarly, the weight above which splitting occurs and the weight below which Russian roulette is played is determined respectively by the lowest and highest adjoint flux in IZ. The path length biasing parameter is determined by minimizing the least square error between 1) the adjoint-based approximation to the optimal probability density function (pdf), and 2) the pdf used in MORSE-SGC for choosing the next collision site for particles directed at the detector. Estimation probabilities are also generated to alleviate the necessity of obtaining response contributions from each collision site. Reference 4 provides a detailed discussion of the automatic biasing techniques and their implementation.

The biasing techniques were initially tested using a dry shipping cask model and five detectors. Excellent agreement was obtained between the biased MORSE-SGC calculation and a DOT-IV (5) calculation of neutron dose (4). The test problem comparison also indicated a considerable savings in cpu time on the IBM 3033 between the biased MORSE-SGC calculation (10.8 min.) and the DOT-IV calculation (97.2 min.). Final development and testing of the SAS5 control module will continue until mid-1984 when a version will be released to RSIC.

The SAS5 control module will contain a simple geometry input that allows calculational models such as that of Fig. 5 to be easily described using keyword identifiers. [Optionally, a SCALE combinatorial geometry package (MARS) containing the arrays of arrays feature can be used where detailed models of the fuel assemblies are desired.] The pre-release version of SAS5 was used to obtain the dose rates shown in Table 1 for the shipping cask of Fig. 5. Note that separate calculations are required for the gamma and neutron doses since the generated biasing parameters are highly dependent on the type of radiation.

IMPROVEMENTS IN THERMAL ANALYSIS

The thermal analysis capability within SCALE is centered around the HEATING6 functional module which was made available with the SCALE-1 release. HEATING6 is a general use code for solving multidimensional, steady-state and/or transient heat conduction problems using finite-difference techniques. The code allows a great deal of flexibility in specifying material and thermal properties, heat generation rates, boundary conditions, and finned surfaces. In addition, one may specify radiative heat transfer across gaps or regions embedded in the model. Several numerical schemes are available for both steady-state and transient problems. Selected materials may undergo a change of phase for transient calculations involving one of the explicit numerical schemes.

HEATING6 is a complex code requiring a large amount of input and careful consideration of the time and/or space mesh. Thus, the Heat Transfer Analysis Sequence No. 1 (HTAS1) was developed within SCALE to generate the necessary HEATING6 input and automatically manipulate the module to perform a two-dimensional (R-Z) thermal analysis for a specific class of shipping containers during normal, fire, and post-fire conditions. Keywords, free format, and extensive use of default parameters and options simplifies the HTAS1 input to the point that a novice user can easily obtain a shipping cask thermal analysis. Each shipping cask component (e.g., inner shell, neutron shield, etc.) is identified by a keyword and appropriate axial and radial thicknesses. A standard material properties library in HTAS1 makes identification of thermal properties a simple matter of designating the correct identifier for each component material of the cask. Default materials are available for each shipping cask component.

The HTAS1 sequence begins by establishing the steady-state pre-fire conditions based on an input fuel heat generation, a default solar heat load, and default radiative and natural convective boundary per requirements of Appendix A, 10CFR71. From the input heat generation, (available from the thermal decay heat calculated by SAS2), HTAS1 establishes the heat flux impinging on the axial and radial wall of the inner shell. Following the steady-state analysis, the sequence proceeds through a 30-minute fire and post-fire transient lasting three hours. The default fire conditions are established to meet the requirements of Appendix B, 10CFR71. Following the transient analysis, a post-fire steady-state analysis is performed. The entire analytical sequence, or an optional segment of the sequence, is run with a single HTAS1 calculation using repeated calls to HEATING6.

The specific class of shipping containers that can be analyzed using HTAS1 are shipping casks which can be modeled as concentric cylinders that may be axially asymmetric. Typical components include an inner and outer shell, water jacket, neutron and gamma shields, and impact limiters. Allowance is made for optional removal of the water jacket and impact limiters and/or loss of the neutron shield after any of the analyses noted above. HTAS1 has been developed to allow the user to input fin data, emissivity data (to alter the default), and change of phase data in a particular component. Each of the analyses noted above is specified by a keyword. Following each keyword the user may alter the default values for the ambient temperature and the coefficients and exponents used in the heat transfer correlation for natural convection from radial and axial surfaces. The default numerical technique may also be overridden for each phase of the sequence.

The shipping cask of Fig. 5 was analyzed using HTAS1 with slight changes in the model due to the HTAS1 requirement for having concentric cylinders (i.e., the axial and radial gamma shields were connected). The simple input for this analysis is shown in Fig. 6. Note that the input is in mixed English units (inches, Btu/hr, minutes, and °F). The integer values following the axial and radial thicknesses of each cask component are the number of mesh intevals for that thickness. The last entry on the cavity (210000) card is the heat generation rate. Note that material 12 (uranium metal) was used for the gamma shield, thus overriding the default material (lead). Also, fins were added to the axial and radial outer shell surfaces and the neutron shield was deleted (water removed and replaced with air) following the PREFIRE steady-state analysis. Fig. 7 provides transient temperature profiles for three axial mid-points within the cask.

SUMMARY

This paper has presented several of the improvements recently completed or currently being developed for the SCALE system. Criticality analysis improvements include the new KENO V.a code which contains an enhanced geometry package and a new control module CSAS4 which uses KENO V and allows a criticality search on optimum pitch (maximum k-effective) to be performed. The SAS2 sequence is a new shielding analysis module which couples fuel burnup, source term generation, and radial cask shielding. The SAS5 shielding sequence allows a multidimensional Monte Carlo analysis of a shipping cask with code generated biasing of the particle histories. The thermal analysis sequence (HTAS1) provides an easy-to-use tool for evaluating a shipping cask response to the accident scenario prescribed by 10CFR71. These tools should hopefully improve the capability of the SCALE system to provide the cask designer or evaluator with a computational system that provides the automated procedures and easy-to-understand input that leads to standardization.

REFERENCES

1. SCALE: A Modular Code System For Performing Standardized Computer Analyses For Licensing Evaluation, Vols. 1-3, NUREG/CR-0200 (January, 1982). Available from GPO Sales Program, Division of Technical Information and Document Control, USNRC, Washington, DC.

2. R. M. Westfall and L. M. Petrie, "Standardized Safety Analysis of Nuclear Fuel Shipping Containers," pp. 842-849 in Proceedings of the Fifth International Symposium on Transportation of Radioactive Materials, Las Vegas, NV, May 7-12, 1978.

3. R. H. Odegaarden, "Application of SCALE System to Nuclear and Thermal Review of Radioactive Material Package Designs," pp. 837-841 in Proceedings of the Fifth International Symposium on Transportation of Radioactive Materials, Las Vegas, NV, May 7-12, 1978.

4. T. J. Hoffman and J. S. Tang, "XSDRNPM-S Biasing of MORSE-SGC/S Shipping Cask Calculations," NUREG/CR-2342 (ORNL/CSD/TM-175), Computer Sciences at Oak Ridge National Laboratory, Oak Ridge, TN (October 1982).

5. W. A. Rhoades et. al., The Dot-IV Two-Dimensional Discrete Ordinates Transport Code with Space-Dependent Mesh and Quadrature, ORNL/TM-6529, Oak Ridge National Laboratory, Oak Ridge, TN (1979).

```
=CSAS4X
SAMPLE FUEL CASK
HANSEN-ROACH LATTICECELL
U02  1 .84 293. 92235  2.35 92238 97.65 END
ZR  2 1 END
H20  3 1 END
B4C  4 0.367 END
AL  4 0.636 END
H20  5 1 END
AL  6 1 END
END COMP
SQUAREPITCH  1.2751 .823 1 3 .9627 2 END
SAMPLE SQUARE FUEL CASK
READ PARAM  TME=5.0  NUB=YES FAR=YES GEN=53
END PARAM
READ ARRAY NUX=2  NUY=2  NUZ=1 END ARRAY
READ GEOM
CUBOID 500 1 10.8385 -10.8385 10.8385 -10.8385 183.1 -183.1
CUBOID 4 1 11.5 -11.5 11.5 -11.5 183.1 -183.1
CUBOID 5 1 12.0 -12.0 12.0 -12.0 184.0 -184.0
CORE     0 1 3*0
REFLECTOR 6 1 6*10.0 1
REFLECTOR 5 2 6*3 5
END GEOM
READ BIAS ID=500 2 6 END BIAS
END DATA
READ SEARCH  OPTIMUM  PITCH  END SEARCH
END
```

Fig 3. CSAS4 Input for square aluminum fuel cask.

```
=HTAS1
TYPICAL PWR SHIPPING CASK
CAVITY  18.75 5 84.75 5 210000
INNER SHELL  0.5 1 1.0 1 1.25 1
SHIELDING  4.0 5 3.0 4 3.75 4
MATERIAL  12
OUTER SHELL  1.5 2 2.0 2 1.5 2
FINS  1 1
7.0 0.75 0.75 2.5 0.0 1.0
7.0 0.75 0.75 2.5 0.0 1.0
NEUTRON SHIELD  4.5 4 63.75 80.25
DELETE  PREFIRE  0 0.6 0.6
WATER JACKET  .125 1
PREFIRE  100 .3827
FIRE
POSTFIRE  180 100 .3827
FINAL  100 .3827
%
END
```

Fig. 6. Typical shipping cask input for HTAS1.

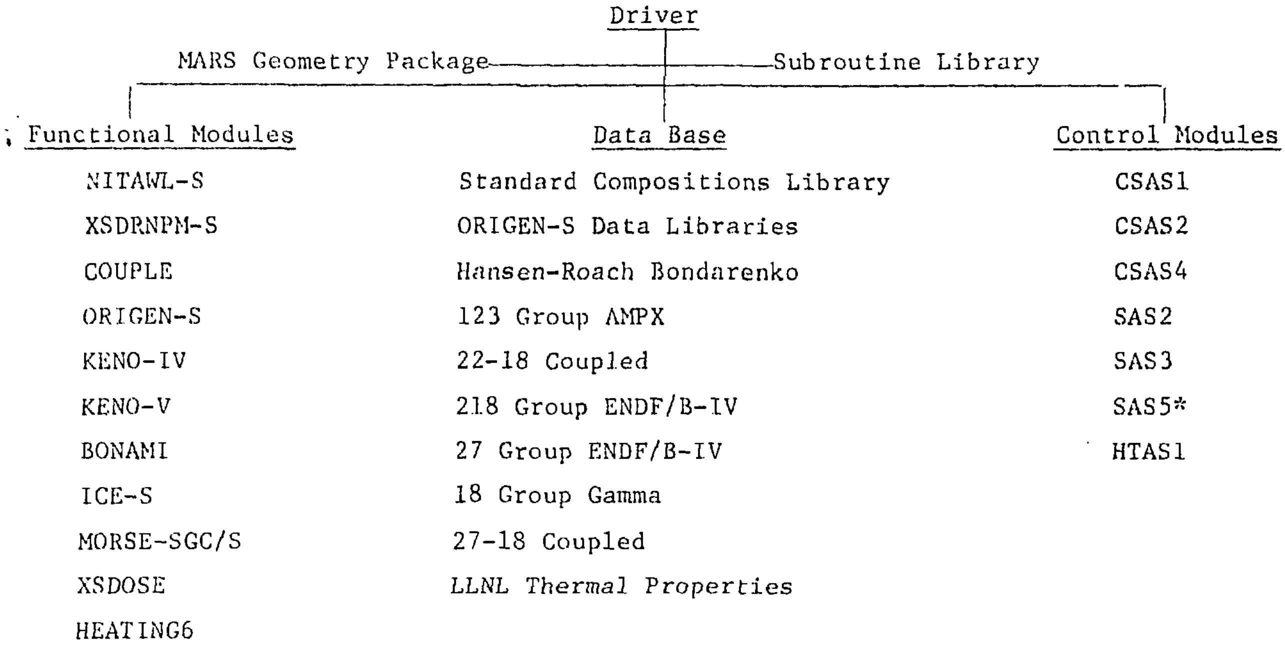


Figure 1. Scale system components

*Public release in 1984.

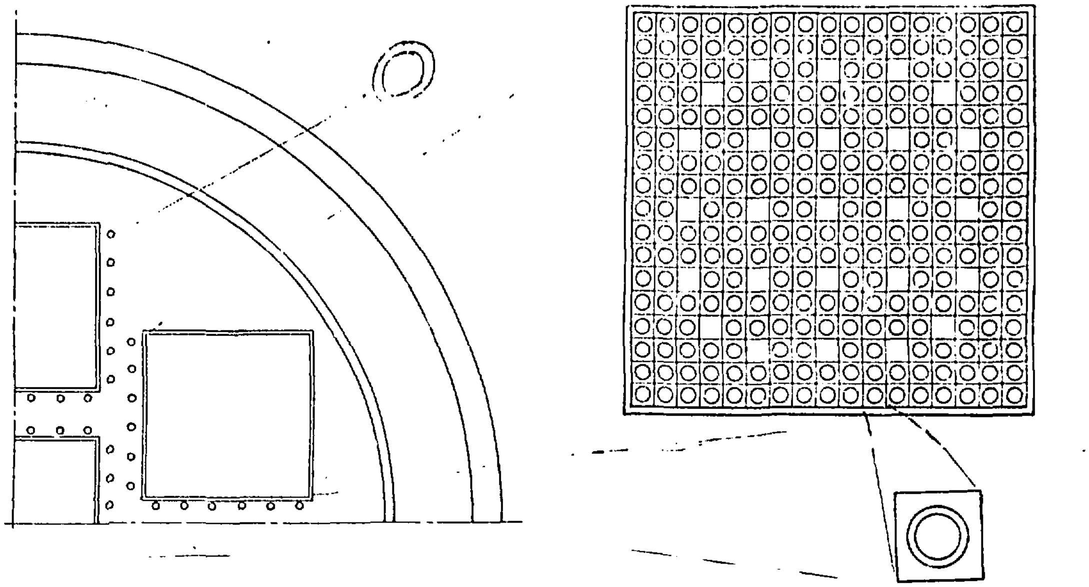
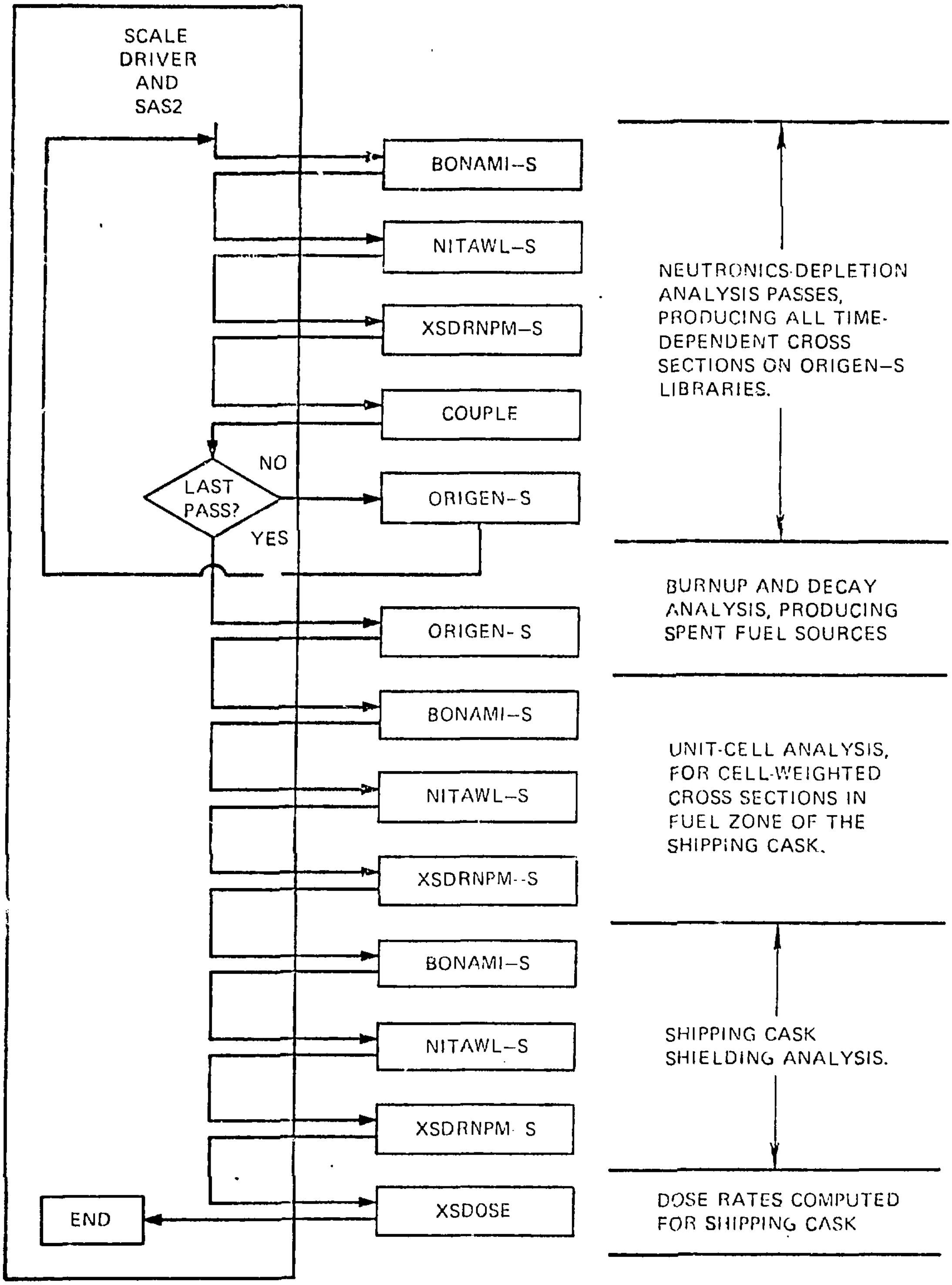


Fig. 2

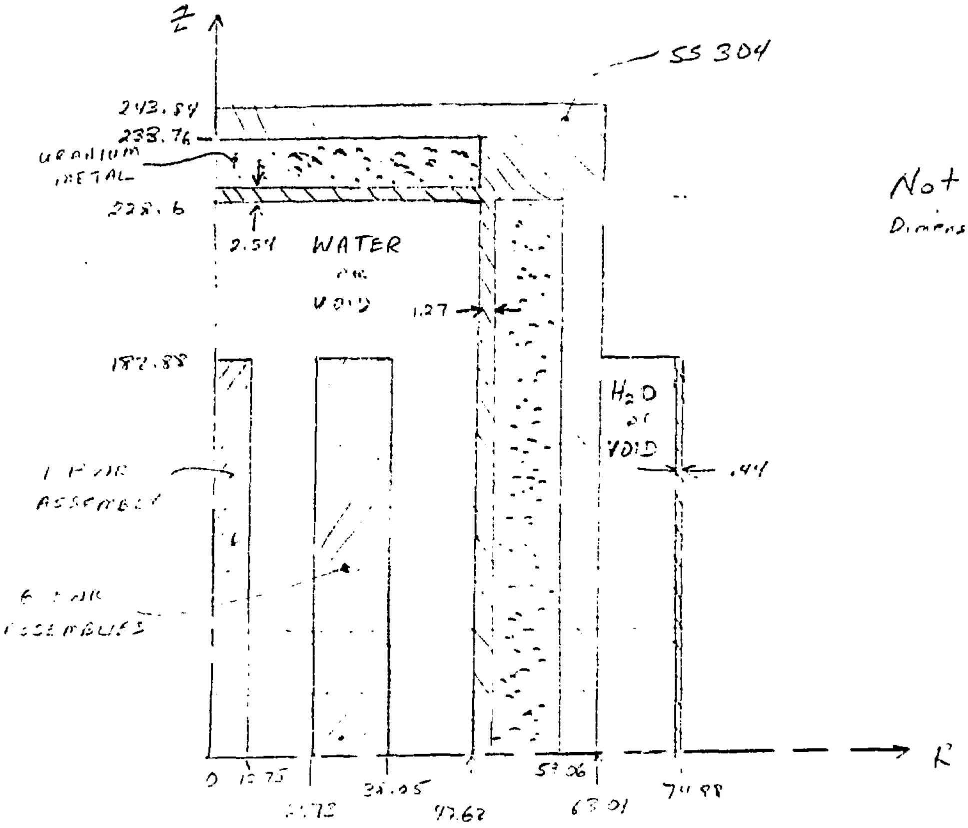
ORNL-DWG 82-20409



~~Fig. 32.2.1~~. Basic flow invoked by SAS2.

Fig. 4

83-12795



Not to scale.
Dimensions in cm.

Fig. 5. Typical shipping cask calculational model.

1 slide (color ~~if possible~~)

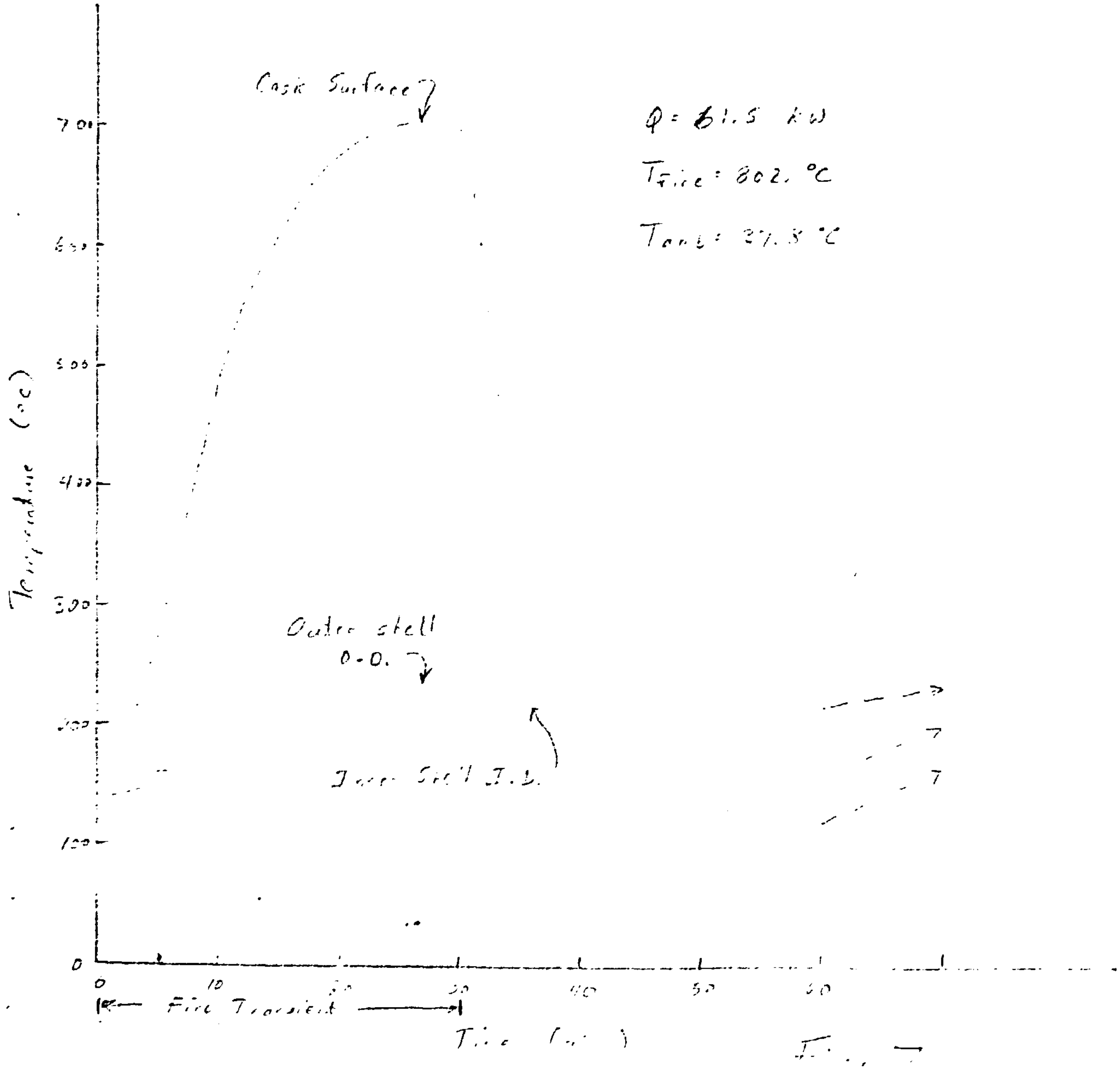

Temperature (°C)
0
100
200
300
400
500
600
700
Cask Surface
Outer shell O.D.
Inner Shell I.D.
$Q = 61.5$ kW
$T_{Fire} = 802.$ °C
$T_{amb} = 37.8$ °C
0
10
20
30
40
50
60
Fire Transient
Time (min)

TABLE 1: Dose rates at axial midplane for typical shipping cask.

Case	Cool Time	Internal Cavity	Neutron Shield	SAS2 Total Dose Rates (mR/hr)			SAS5 Total Dose Rates (mR/hr)	
				Surface	3 ft.	10 ft.	3 ft.	10 ft
1	180 d.	Wet	Wet	38.64	14.83	4.89	*	-
2	150 d.	Dry	Dry	582.8	199.6	55.6	*	*
3	5 yr.	Dry	Dry	293.5	95.2	[illegible]	*	-
4	5 yr.	Dry	Wet	93.7	39.2	12.7	*	*

* SAS5 dose rates presently being calculated.

DISCLAIMER