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ABSTRACT

The SCALE (Standardized Computer Analyses for Licensing Evaluation) code system is used extensively to perform away-from-reactor safety analysis (particularly criticality safety, shielding, heat transfer analyses) for spent light water reactor (LWR) fuel. Spent fuel characteristics such as radiation sources, heat generation sources, and isotopic concentrations can be computed within SCALE using the SAS2 control module. A significantly enhanced version of the SAS2 control module, which is denoted as SAS2H, has been made available with the release of SCALE-4. For each time-dependent fuel composition, SAS2H performs one-dimensional (1-D) neutron transport analyses (via XSDRNPM-S) of the reactor fuel assembly using a two-part procedure with two separate unit-cell-lattice models. The cross sections derived from a transport analysis at each time step are used in a point-depletion computation (via ORIGEN-S) that produces the burnup-dependent fuel composition to be used in the next spectral calculation. A final ORIGEN-S case is used to perform the complete depletion/decay analysis using the burnup-dependent cross sections. The techniques used by SAS2H and two recent applications of the code are reviewed in this paper.

INTRODUCTION

In the late 1970s, Nuclear Regulatory Commission (NRC) and Oak Ridge National Laboratory (ORNL) staff formulated the framework for the SCALE[1,2] modular code system. The system development criteria included (1) the use of well-established computer codes and data libraries, (2) an input format designed for the occasional user and/or novice, (3) the automation of analyses requiring multiple computer codes or calculations into standard analytic sequences, and (4) complete documentation and public availability. Since the initial release of SCALE in 1980, the code system has been heavily used by the NRC, Department of Energy (DOE) contractors, and industry to perform criticality, shielding, and thermal analyses for the storage and transport of depleted light water reactor (LWR) fuel.

The SAS2 control module was originally developed for SCALE to provide a sequence that generated radiation source terms for spent fuel and subsequently utilized these sources within a 1-D shielding analysis of a shipping cask. Although the shielding portion of the sequence can still be accessed, the principal use of SAS2 over its history has been fuel depletion analyses to obtain radiation sources, decay heat, and spent fuel isotopics. Earlier SAS2 versions used an infinite lattice pin-cell model for the neutronics analysis and so only variations in lattice design and composition could be considered. This simple procedure has been shown to produce conservative actinide inventories for PWR spent fuel and does not provide the versatility required for depletion of BWR fuel.[3] Thus, the original SAS2 sequence has been considerably enhanced to produce the

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SCALE-4 version which will be denoted SAS2H.[4] With the SAS2H model, the presence of water holes, control rods, burnable poison rods, orifice tubes, and other assembly design features can be considered in an approximate fashion. This new capability allows a more accurate evaluation of isotopic concentrations and source terms at long cooling times (>10 years) where actinide contributions are more important.

The purpose of this paper is to describe the SAS2H analysis sequence used to calculate the characteristics of spent LWR fuel. Recent applications that demonstrate the flexibility and usefulness of the sequence will also be discussed.

MODULES AND DATA

The SAS2H control module performs the depletion/decay analysis sequence using the well-established codes (or functional modules) and data libraries provided in the SCALE system.[1,2] The applicable modules and data libraries are briefly reviewed in this section.

Problem-dependent resonance processing of neutron cross sections is performed by SAS2H using the BONAMI-S and NITAWL-II modules. BONAMI-S applies the Bondarenko method of resonance self-shielding for nuclides which have Bondarenko data included with their cross sections. NITAWL-II is an updated version of the NITAWL code and performs resonance self-shielding corrections using the Nordheim Integral Treatment for nuclides that have resonance parameters included with their cross sections.

The XSDRNPM-S module, as applied by SAS2H, is used to produce weighted and collapsed cross sections for the fuel depletion calculations. XSDRNPM-S performs a 1-D discrete-ordinates transport calculation based on various specified geometries requested in the data supplied by SAS2H. Data from the weighted, cross-section library and spectra produced by XSDRNPM-S are used by the COUPLE module to update an ORIGEN-S nuclear data library and modify the ORIGEN-S spectral parameters (THERM, RES, and FAST).[5]

The last module used in the depletion/decay portion of SAS2H is the ORIGEN-S module. This module computes time-dependent concentrations and source terms of a large number of isotopes which are simultaneously generated or depleted through neutronic transmutation, fission, radioactive decay, input feed rates, and physical or chemical removal rates. The ORIGEN-S module uses a point-depletion model that has no spatial dependence. All data provided to ORIGEN-S (i.e., cross sections or spectral data) should be averaged over the spatial region of interest. The time dependence of the nuclide concentrations is solved by using the matrix expansion technique. A generalized form of the Bateman equations is used to solve for concentrations of short-lived nuclides removed from the transition matrix to ensure better accuracy.

Any master AMPX cross-section library[6] with SCALE nuclide identifiers can be used by the SAS2H module. Of the available SCALE libraries, the hybrid 27-group neutron cross-section library is typically applied. This library primarily has ENDF/B-IV data, but ENDF/B-V data have been added where needed for fission products and higher-order actinides. The ORIGEN-S data libraries[7] are accessed for the half-lives, decay constants, fission yields, and Q-values.

Input data for each SCALE module is prepared by SAS2H based on a single set of input consisting of basic engineering parameters (e.g., fuel pin-cell dimensions and compositions) and keywords cast in a simple, free-form format. The SAS2H program uses this basic information to derive additional parameters (e.g., number densities or associated physics data) and prepare the input for each of the functional modules in the sequence. Nuclide densities required by the codes are prepared by the SCALE Material Information Processor Library (MIPLIB) from both the user input (e.g., material densities or volume fractions) and the contents of the SCALE Standard Composition library. MIPLIB is also an essential tool in preparing applicable physics (e.g., Dancoff factors) for the neutronics modules.

METHOD AND TECHNIQUES

The method applied by SAS2H starts with data describing a fuel assembly as it is initially loaded into a particular reactor. The composition, temperatures, geometry, and time-dependent specific power of the fuel assembly are required. Fundamentally, the chief function of the SAS2H control module is to convert this user input data, plus data available within the SCALE system, into the input required by functional modules and output it onto the interface units read by the codes. A diagram of the basic flow path invoked by SAS2H and the SCALE driver is shown in Fig. 1. Appropriate parameters are returned to the SCALE driver to properly invoke the functional modules in the SAS2H method. The methods and techniques employed by SAS2H through the execution of the final ORIGEN-S case are discussed in the remainder of this section.

NEUTRONIC MODELS

The flow chart of Fig. 1 indicates two computational paths (path A and path B) for the neutronics portion of the depletion analysis. Although the neutronics modules used in these sequential flow paths are similar (both access BONAMI/NITAWL/XSDRNPM), the models analyzed are quite different. The model used in path A is similar to that used in earlier SAS2 versions, through SCALE-3, inclusively. The addition of flow path B and its model produces the new version of the SAS2 control module that is denoted SAS2H.

Basically, the model used in path A represents the fuel by an infinite lattice of fuel pins. Cross- section processing is followed by a discrete-ordinates 1-D transport computation of the neutron flux in a unit cell with white boundary conditions. The cell-weighted cross sections produced by this path A model are then applied to the fuel region of the path B model. The model used in path B is a larger unit cell model used to represent part or all of an assembly within an infinite lattice. The concept of using cell-weighted data in the 1-D XSDRNPM-S analysis of path B is an approximate method for evaluating two-dimensional (2-D) effects found in fuel-pin lattices containing different types of rods or water "holes." The path B model is used by SAS2H to calculate an "assembly-averaged" fuel region flux that considers the effects due to the path A model and channel moderation, if present.

Two examples of the larger unit cells are depicted in Fig. 2 where diagram (a) applies to a PWR control rod assembly and diagram (b) applies to a BWR burnable poison assembly. Variations to diagram (b) (e.g., omitting the casing and channel moderator) would apply to different types of BWR or PWR assemblies. The essential rule in deriving the zone radii is to maintain the relative volumes for all zones in the actual assembly. The control region of the larger cell can be modeled as an assembly guide tube, a burnable poison rod containing no fuel, an orifice rod, an axial peaking rod, a fuel rod containing a burnable poison, or almost any other pin-cell type rod. The moderator of the path A model is included with an outer radius equal to the unit cell radius. Then a fuel region surrounds the moderator with a radius which maintains volume conservation of fuel and moderator for the entire assembly. Also, the fuel assembly housing material, or casing, and channel moderator between assemblies may be added by conserving volumes. Assembly rod spacers and other hardware that may be present are usually ignored. However, if their effects are estimated to be significant, they may be input by using zone average or effective densities.

The models utilized by SAS2H, either in path A or path B, always assume a constant material composition and power in the axial direction of the fuel assembly. While some assembly designs may have axial variations in fuel and burnable poison compositions, there are axial changes in moderator densities and power in all assemblies. The approximation used to determine the average water density may have a significant effect upon the results.

A frequent and acceptable practice in using SAS2H for PWR assemblies is to derive the average density using the water pressure and the average core temperatures. However, there is a much greater axial change in the moderator density in fuel assemblies for the BWR than those for the PWR. An improved approximation of the effective water density in the BWR is an important requirement in achieving the same accuracy in isotopic results for the BWR as that obtained for the PWR. In general, the BWR assembly is contained within a

casing, which separates the water into the fuel zone moderator and the channel moderator. There are different methods of obtaining "effective" moderator densities. Acceptable values of effective moderator density may be known from previous analyses. If moderator density and relative power is known as a function of axial zone, a power-weighted density may be applied. When the data are available at various fuel burnups, the densities may be changed in SAS2H for each cycle used. Where only the moderator densities are given, BONAMI-S, NITAWL-II, and XSDRNPM-S may be applied to unit-pin-cell and slab models to estimate the axial power distribution.

BURNUP-DEPENDENT CROSS SECTIONS

Fuel cross sections vary with burnup because of the change in nuclide concentration and because of the resulting shift in the energy spectrum of the neutron flux. The neutronics-depletion procedure of Fig. 1 is applied repeatedly by SAS2H to produce cross-section libraries for the irradiation intervals requested in the input. The SAS2H sequence repeatedly "passes" through the neutronics-depletion procedure using a "bootstrapping" method. The major data differences for the sequential "passes" are in the nuclide densities and reactor history parameters.

The user input specifies the number of cycles (e.g., the number of years the assembly resides in the reactor), the number of libraries to make per cycle, the specific power in each cycle, and both the total operation time and downtime of each cycle. Thus, the irradiation-time interval associated with each library is derived from the input. With the exception of the initial fresh fuel library, each cross-section library is based on number densities obtained for the midpoint of the irradiation-time interval. The midpoint number densities for an irradiation interval are computed from an ORIGEN-S case that uses the library from the previous irradiation interval. Cross sections for all nuclides included in the XSDRNPM-S analysis are explicitly updated and included on each new ORIGEN-S working library. Trace amounts of the selected nuclides shown in Table 1 are automatically included by SAS2H in the XSDRNPM-S analysis to ensure appropriate cross sections are available for important nuclides which build up in the fuel during depletion. Additional trace nuclides can be input by the user.

The procedure is illustrated schematically in Fig. 3 for a two-cycle case where two libraries per cycle are requested. The first step is to produce the "PASS 0" library prepared using the fresh fuel isotopics. This initial library is used in the first ORIGEN-S case to generate number densities at the midpoint of the first irradiation interval. Next, the SAS2 module (1) computes density-dependent parameters for the resonance calculations, (2) increments the required data set unit numbers (3) adds "PASS 1" to the ORIGEN-S library title, (4) updates the ORIGEN-S input for the second case to save number densities for the starting point and the midpoint of the second irradiation interval, and (5) rewrites all code interfaces using the new data. Then, the "PASS 1" library is produced by invoking execution of the five codes in both path A and path B of Fig. 1 a second time with the new input interfaces. Each additional pass applies the same procedure as used for "PASS 1." The midpoint densities are applied to the neutronics analysis to produce a new library. The depletion computation applies this library and the densities calculated for the start of the pass. A decay computation with zero power is applied for reactor downtime, if specified for the end of a cycle, before deriving densities for the next pass. All ORIGEN-S libraries are saved, starting with the "PASS 1" library.

The time-dependent number densities applied in the neutronics analysis are obtained by different methods. Number densities for the heavy nuclides of the fuel, together with their activation products and fission products, are all computed by ORIGEN-S. In addition, ORIGEN-S calculates the depletion of the burnable poisons boron, gadolinium, and cadmium, and some of the specified structural materials or light elements (e.g., lithium). As noted above, the moderator (water) density does not change from the initial material specification unless requested by the user. The fraction of the first-cycle (initial material specification) density of the water or soluble boron may be specified by the user for each cycle.

FINAL DEPLETION AND DECAY ANALYSIS

Prior to the final pass, the purpose of the neutronics-depletion method was to produce a set of ORIGEN-S working libraries that apply to the specified fuel assembly at various points during its irradiation history. Now, these libraries and the initial nuclide densities form the input to the final ORIGEN-S depletion case. All of the nuclides in the large ORIGEN-S binary library[7] are available for the analysis. These presently include: 687 light elements, such as clad and structural materials; 101 actinides, including fuel nuclides and their decay and activation products; and 821 fission-product nuclides. All chains are automatically provided in the library processing by ORIGEN-S and COUPLE. Cross-section constants are either updated directly from XSDRNPM-S output, or, for those nuclides not included in the pin-cell analysis, from broad-group flux-weight factors.

First, in the procedure given here, the nuclide generation and depletion computation using the "PASS 1" library is performed. The first-cycle power and "PASS 1" time interval are applied. Four equal-size time steps are used during the irradiation time, followed by a single downtime interval. If no downtime is specified, a zero-time interval is applied. Next, a similar computation is performed using the compositions determined at the end of the "PASS 1" calculation and the cross-section data on the "PASS 2" library. The analysis proceeds with each succeeding library and corresponding assembly power and time interval. Ultimately, the nuclide inventory (actinides, fission products, and light elements) is computed at the burnup corresponding to the discharge of the assembly from the reactor. Finally, a decay-only subcase (six equal-size time steps) is computed for the requested spent fuel cooling time. These calculated compositions are applied in both the optional shielding analysis and the determination of radiation and heat generation.

The spent fuel gamma source is calculated for the photon energy group structure present on the cross-section library specified for use in the cask shielding analysis. The code first converts inventories of all nuclides of the cooled fuel assembly to disintegrations per second. Then, applying the ORNL Master Photon Data Base,[7] it sums individual nuclide photon spectra to determine the total gamma source spectrum. The procedures used maintain the conservation of energy, rather than photon intensity, which should give a more correct computation of dose rates in a shielding analysis. As a final correction, the ratio of total nuclide gamma energy (from data in the ORIGEN-S working library) to the gamma energy of only those nuclides having line data, is multiplied times the spectrum computed from the data base.

The isotopes ^{242}Cm and ^{244}Cm characteristically produce all except a few percent of the spontaneous fission and (α,n) neutron source in spent PWR fuel over a 10-year decay time. The next largest contribution is usually from the (α,n) reaction of alphas from ^{238}Pu, which is approximately 1 to 2% of the source. The energy distribution of the spontaneous fission neutron spectrum is computed based on measured spectral data for ^{242}Cm and ^{244}Cm and the calculated concentrations of those two isotopes. This spectrum is then renormalized to include the total neutron source from all spontaneously fissioning isotopes. A similar calculation, based on experimental data relevant to ^{244}Cm, ^{242}Cm, and ^{233}Pu is performed for the (α,n) neutron spectrum. The spectra are collapsed from the energy group structure of the data to that of the SCALE library requested for the cask computation. The procedure assumes uniform distribution within each group and simply sums the quantities based upon energy fractions common to both groups in the two group structures. The total neutron source spectrum is then computed as the sum of the spontaneous fission and (α,n) spectra. Neutrons produced by photofission and photoneutron reactions are not included in the source term computed by SAS2H.

APPLICATIONS

The SAS2H sequence was developed to provide an easy-to-use procedure that enables an accurate evaluation of a large number (several hundred) of isotopic concentrations that may be needed for spent fuel characterization and/or out-of-reactor safety analysis. In particular, decayed concentrations and concentrations for large numbers of individual fission products, light element impurities (e.g., ^{59}Co), and higher order actinides

(e.g., ^{242}Cm and ^{244}Cm) are not typically available from reactor analysis codes that perform fuel management or core-following. Codes like ORIGEN2[8] also generate the same type of data produced by the final ORIGEN-S case of SAS2H. The difference between the two methods is that ORIGEN2 can use only a limited set of burnup-dependent libraries that were developed for specific design and operating condition. SAS2H provides the user with some control of the neutronic analyses required to generate the burnup-dependent libraries.

Generation of radiation source terms for shielding analyses is still a primary function of the SAS2H module. In comparison to the earlier SAS2 version, the new SAS2H module yields lower neutron sources (because of lower actinide generation) and about the same gamma sources (dependent on total number of fissions) for PWR assemblies. Also, the new modeling capabilities now allow source terms for BWR assemblies to be obtained. This expanded capability to consider a large range of PWR and BWR assembly designs has significantly increased the types of problems for which the module can be applied. The value of the new capabilities is illustrated in the following discussion of two recent applications.

PROPOSED DECAY HEAT REGULATORY GUIDE

The NRC has provided technical guidance on decay heat with the issuance of Regulatory Guide 3.54, entitled "Spent Fuel Heat Generation in an Independent Spent Fuel Storage Installation." Work has recently been completed to produce a data base of decay heat rates for inclusion in a proposed revision to Regulatory Guide 3.54.[9] The SAS2H module of SCALE was selected to produce the data base because of its ability to obtain appropriate burnup-dependent cross-section data for PWR and BWR assembly models using a wide range of burnups, initial enrichments, and reactor power histories.

A preliminary SAS2H case was performed for each reactor type (i.e., BWR or PWR) to produce an ORIGEN-S library that was used as the starting library in all subsequent SAS2H cases. Both preliminary SAS2H cases provided cross sections for 181 fission products and all actinides at slightly burned fuel conditions (~5 MWd/kgU). The subsequent SAS2H cases used these base libraries and then updated cross sections as a function of burnup for 38 to 39 significant actinides and fission products (plus six gadolinium isotopes for the BWR cases).

The data base for the proposed guide revision was developed to cover the vast majority of spent fuel assemblies that have characteristics falling within the mainstream of normal reactor operations. The assembly design (Westinghouse 17 x 17 and General Electric 8 x 8) and operating characteristics applied in the SAS2H/ORIGEN-S cases represent generic, yet realistic, data and are presented in detail in reference 9. Each reactor type (BWR and PWR) was analyzed for six different burnups at three different specific powers. The burnup range (incremented by 5 MWd/kgU) was 20 to 45 MWd/kgU for the BWR cases and 25 to 50 MWd/kgU for the PWR cases. For each reactor type and burnup value, a typical initial ^{235}U enrichment was selected. The specific powers considered were 12, 20, and 30 kW/kgU for the BWR cases and 18, 28, and 40 kW/kgU for the PWR cases. Separate ORIGEN-S cases were used to compute final decay heat generation rates at 20 different cooling times in the range of 1 to 110 years.

Prior to development of the proposed guide revision, the reliability of the SAS2H/ORIGEN-S sequence was demonstrated by comparing calorimetric measurements of spent fuel assembly heat rates with computed values. In this study, results were compared for ten PWR and ten BWR spent fuel assemblies obtained from three reactors: Point Beach Unit 2 (PWR), Turkey Point Unit 3 (PWR), and Cooper Nuclear Station (BWR). The assemblies with the highest burnups and initial ^{235}U enrichments are from the Point Beach reactor. The measured decay heat values, along with the basic design and operating history data for each measured assembly, are provided in references 10-14. A more complete and compact description of this data is included in reference 9.

Measured and calculated decay heat rates of spent fuel assemblies from the three reactors in this study are compared in Tables 2-4. Percentage differences between measured and calculated values are reported for each measurement. The average percent difference for each assembly is reported in the last column of each table. The Point Beach PWR (Table 2) is the only reactor for which the assembly average difference exceeded its standard deviation (i.e., 3.0 ± 1.9%). The 3% difference for the C-64 assembly was the result of a comparison with a measurement by a static test, whereas the 16.2% resulted from a comparison with a measurement that was determined by a recirculation test. Had this assembly been excluded from consideration, the average percent difference of the other assemblies would have been 1.7 ± 0.9%.

The Turkey Point PWR results of Table 3 provide an update to a previous comparison[3] of SAS2 results using equal burnups and specific powers[12] for the three cycles of the D-assemblies. This estimate of operating history was replaced here with more complete data given by the utility. Three of the assembly average differences were within 2.3%. Assembly B-43 (which had a −4.5% difference) was the only one of the four that was in the reactor during the first cycle. Its lower calculated value could be due to exceptionally low operating powers during the first part of the first cycle. The average assembly percent difference, however, of −0.7 ± 1.7% indicates good overall agreement between measured and calculated values.

The percentage differences in the decay heat comparisons in Table 4 for the Cooper Nuclear Station BWR assemblies extended over a much wider range than those for the PWR reactors. However, the measurement values were in the range of 62.3 to 395.4 W, as opposed to 625 to 1550 W for the PWR reactors. Because measurement precision tends to be represented as a constant heat rate instead of a percentage of the total heat rate, larger percentage differences would result from the lower values being measured. The increase in the number of measurements and assemblies, however, has somewhat reduced the final standard deviation. The average assembly difference of -0.7 ± 2.6% indicates good overall agreement between calculated and measured values.

The comparison of measured and calculated decay heat rates shown in Tables 2-4 indicate the adequacy of SAS2H as a calculational tool to predict heat rates for PWR and BWR assemblies. The percentage difference between measured and calculated results was considered in the development of a safety factor to be included in the proposed revision to Regulatory Guide 3.54.

REACTIVITY CREDIT FOR SPENT FUEL ISOTOPICS

Criticality safety analysis for away-from-reactor storage and transport of spent fuel has typically assumed fresh fuel isotopics. In the past few years work has been done to investigate the possibility of using calculated spent fuel isotopics for the criticality analysis. The negative reactivity obtained from the net depletion of fissile isotopes and the buildup of actinide and fission-product absorbers are routinely referred to as burnup credit. The primary concern of spent fuel characterization for burnup credit analyses is the accuracy of calculated isotopic concentrations and the effect that varying design and neutronic conditions have on reactivity.

An initial validation of the SAS2H actinide inventory was performed by comparing computed results with measured data[15] for fuel rod sample DO1-G10-4 irradiated in the Turkey Point Unit 3 (PWR) reactor. An earlier comparison had already been performed using the older SAS2 code version that had only the infinite pin-cell lattice for the neutronics. The results of these two comparisons show that differences of calculated minus measured values before and after the new SAS2H version changed from 3% to −5% for $^{235}U/^{238}U$, from 19% to 3% for $^{239}Pu/^{238}U$, and 13% to −1% for total $Pu/^{238}U$. Preliminary (unreported) cases, using the new version and the same libraries for comparisons with other spent fuel measurements, indicate less ^{235}U differences and either the same or slightly higher ^{239}Pu differences. Also, there were indications that changing to ENDF/B-V cross sections tends to reduce the computed ^{239}Pu inventory (approximately 4%). A more extensive study to validate the SAS2H isotopic concentrations for PWR and BWR spent fuel is presently underway.

One of the more challenging applications of SAS2H to date was the task to investigate the feasibility of burnup credit for transport casks loaded with BWR fuel.[16] Earlier analyses with SAS2H had demonstrated that an average, single, axial-node BWR model yields good results for integral quantities such as radiation sources and decay heat rates. However, for criticality safety analyses, the axial variation of the spent fuel isotopics caused by moderator density changes would be important. The importance of using axial nodes and other BWR modeling effects were investigated for this task. This effort will be briefly discussed below.

The BWR assembly model used in this analysis corresponds to a typical 8 x 8 General Electric assembly. Five modeling effects were investigated: (1) water channel reactivity effects, (2) the appropriate assembly model with and without gadolinium (Gd) rods, (3) the Gd rod reactivity effects, (4) three-axial-node (one SAS2H case for each axial node) versus one-axial-node reactivities, and (5) use of average pin enrichments (3.4%) versus split pin enrichments. The specific models used in the SAS2H procedure varied depending on the presence of the Gd rods. Figure 4 shows the 1-D assembly representation for both cases. The initial fuel pin cell calculation (path A of Fig. 1) was identical for both cases. For the second-step calculation of the assembly without Gd rods, the full assembly was converted to an equivalent volume cylinder (Fig. 4a). The inclusion of the Gd rods presented modeling difficulties because of their irregular distribution within the assembly. Three different methods of treating these Gd rod effects were attempted. The first involved modeling the entire assembly with all six Gd rods placed in the center of the assembly. The reactivity for this case was nearly the same as the assembly without Gd rods. The second scenario was to smear the Gd rods uniformly over the entire assembly. This greatly enhanced the Gd effectiveness and resulted in a halving of the k_∞ value. The third method consisted of a 1/6 assembly model (Fig. 4b) and produced more consistent results in comparison to those from more exact neutronics models.

Table 5 gives the results of this initial model development and verification effort. These results are presented for three equally spaced axial nodes. Both the 1- and 2-D results treat each axial node as an independent calculation. The 3-D KENO V.a Monte Carlo[1] calculation treats all nodes simultaneously. For the non-Gd assembly cases, the water channel effects are significant in the top axial node. The k_∞ value increases from 1.05 (a pin-cell calculation as in Fig. 4, in which only the pin and surrounding low-density moderator are treated) to 1.33, with the inclusion of the high-density water channel (treated by the SAS2H full assembly model as in Fig. 4a). The effects are less striking for the bottom node, which contains very nearly the same water densities inside and outside of the fuel channel. The agreement between the 1-D SAS2H and the 2-D DORT[17] (modeled in x-y geometry with cell-weighted fuel cross sections) results using a 3.4% average enrichment is very good. Similarly, the KENO V.a result compares well with the three-node values.

The 1-D model used to approximate the assembly containing Gd rods (see Fig. 4b) represented a single Gd rod, surrounded by 1/6 of the assembly fuel, clad, and channel water (the assembly contains a total of six Gd rods). The 2-D DORT model for an assembly with Gd rods again uses x-y geometry but uses separate cell-weighted cross-section sets for standard fuel pins and Gd fuel pins. Based on the results in Table 5, the 1-D representation of a Gd assembly is not as accurate as that for the assembly without Gd rods. The 1-D results for the Gd assembly are higher by 4.5% Δk than the corresponding 2-D results. Apparently, this overprediction primarily stems from the inaccurate representation of the Gd rod position in the assembly. A separate calculation performed with the 1/6 model for the non-Gd assembly produced a 1% Δk difference with the multidimensional results. Thus, the remaining discrepancy should be caused by the approximate representation of the Gd rod locations. Again, the KENO V.a value agrees with the three-node 2-D values.

All cases thus far have assumed an average enrichment across the assembly. The final two results shown in Table 5 give k_∞ values, first for the actual pin-split enrichments, then assuming all pins contain the peak enrichment (4.15 wt %). The 2-D actual pin-split enrichment reactivity is only 2% Δk lower than the 2-D average enrichment case. The peak enrichment case produces a k_∞ value of 1.20 for the bottom node case, which is substantially higher than either the pin-split or average enrichment DORT results. Thus, the average enrichment assumption appears to be the best for this series of scoping calculations.

The 1-D model chosen for the scoping analyses consisted of an average enriched, 1/6 assembly, Gd-rod model that accounts for the water channel and Gd rod effects. The material density axial variations are accounted for by the use of three-axial-nodes.

All cases shown in Table 5 used fresh fuel in an effort to establish a valid 1-D model for the remaining analysis. In the case of the reactivity comparisons, it was possible to compare 1-D versus 2- and 3-D results to estimate the validity of the calculations. For the case of burned fuel, this direct comparison was not attempted. However, a comparison of the spectra and, in some cases, the fission fraction by neutron group (fission fractions) and the absorption fraction by neutron group (absorption fractions), was performed. The fission and absorption rates are directly the loss and/or generation rates for actinide materials. Thus, the fraction by group of these quantities constitutes an important measure for actinide production and loss.

The fission and absorption fractions from the two different DORT 2-D Gd assembly calculations based on explicit pin-split enrichments and the average pin enrichment were compared. Good agreement was seen in both cases (generally less than 1% difference for fissions and 2% for absorptions). A direct flux spectrum comparison was also made for the same 2-D cases. For all groups above 0.3 eV (group 22), the agreement was very good (generally 1% differences or less). For energies below 0.3 eV, the ^{155}Gd and ^{157}Gd cross sections rise rapidly, and the use of average enrichments in the Gd rods appears to cause a 6% underprediction of the flux.

A comparison of the flux spectra only was made for the same 2-D bottom node average enrichment case and a 1-D average enrichment case. The flux spectra generally agreed to within 3% for energies greater than 0.3 eV, with differences of nearly 20% seen for lower energies. However, because of cancellation effects, the fission and absorption rates are expected to agree better than those of the flux spectra. These spectra differences result from the geometric approximations necessary to model the Gd-pin assembly in one dimension. The same comparisons were also made for the top node. As expected, the agreement is not as good because the lower density/high density moderation changes across an assembly are more difficult to represent in one dimension than in two dimensions.

The flux spectrum differences and hence the fission and absorption rate differences that were observed are not a major cause for concern in the prediction of burnup and production results because the representation of the Gd appears to be the major cause of these differences. A 1-D to 2-D flux spectrum comparison for an assembly without Gd rods showed very good agreement. This type of agreement is expected to more closely represent the 1-D to 2-D comparisons over the lifetime of an assembly because the Gd rods typically lose their effect early in the depletion cycle.

In an operating BWR, the presence of a rapidly changing water density in the axial direction gives rise to axial power shapes that vary much more than corresponding PWR axial power shapes. This variation is commonly represented by a number of constant power "nodes." The SAS2H methods used here treat each of these nodes as independent points (i.e., no spatial variation of depletion within the node and no coupling between the nodes). Three equally spaced axial nodes used in this work represent the axial variation (only one radial point was used because the radial variation is less severe). The coupling between the nodes is accomplished by specifying the relative specific powers for each separate node from either the experimentally measured or calculated power distribution. These power distributions also vary with time because of the nonuniform burnup of the fuel.

Several differing assumptions were used in this work to ensure that the final results could be bounded with respect to the shape and time dependence of the relative power distribution. Perhaps the best and most realistic assumption was to set the specific powers equal for each node. This is an interesting case because in a sense it simulates the effect of control rods (not included previously), which tend to force equal specific powers axially. This simulation is only partial; the spectral effects of the control rods are not modeled, only the tendency of control rods to equalize the power axially by residing in the most reactive (bottom) portion of the core. Also, because a single-node analysis must also assume that the specific powers are equal, this case provides an excellent opportunity for multi- to single-node comparisons. Figure 4 shows the node k_∞ trend

curves for a constant specific power assumption together with the one-axial-node k_∞ values for comparison. This assumption was selected as the most realistic because (1) the end-of-life reactivities were very nearly the same for each node (fuel economy considerations); and (2) the reactivities for each axial node were similar over the last half of the assembly lifetime (reactor control considerations).

Using the various axial power distribution assumptions, predictions of the ending isotopic concentrations were produced for BWR fuel with an initial average ^{235}U enrichment of 3.4% undergoing a 40-GWd/MTU burnup. One question posed was how much variation in the isotopics would be produced by the various power distribution assumptions. Comparison of isotopics from a one-axial-node case and a three-axial-node case indicate that if the desired quantities are average concentrations over the entire assembly, the one-axial-node assumption should yield reasonable results. However, large differences are seen between fissile concentrations in the top node of the three-axial-node case and the one-axial-node values. The effect of inherent voiding in the upper levels of a BWR core offset the higher fissile concentrations and cause the fuel reactivity distribution during reactor operation to be only mildly sensitive to the large axial isotopic variations. In a shipping or storage cask filled with full-density water, quite a different situation exists. The higher fissile concentrations in the top node can cause the predicted reactivities to be dominated by the top effects.

The work described above for the BWR "burnup credit" model provides an indication of the effort used by the SAS2H developers to ensure an adequate method was used to generate adequate spent fuel isotopic concentrations for use in a BWR fuel cask.

SUMMARY

Away-from-reactor safety analyses routinely require spent fuel characterization of the radiation sources, decay heat rates, and isotopic concentrations. The SAS2 control module of the SCALE system is used to compute these spent fuel characteristics. The new version of SAS2, denoted SAS2H, provides an enhanced neutronic modeling procedure that enables burnup-dependent cross sections to be generated more accurately. Models for typical PWR and BWR have been developed and used successfully in recent applications. However, there are still definite geometric limitations in the SAS2H model capabilities, and its applicability to newer, more complex assembly designs will need to be addressed.

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Table 1. List of Fuel Nuclides Automatically Included by SAS2 for Inclusion in Neutronics Processing[a]

Xe-135	Pu-240
Cs-133	Pu-241
U-234	Pu-242
U-235	Am-241
U-236	Am-241m
U-238	Am-243
Np-237	Cm-242
Pu-238	Cm-243
Pu-239	Cm-244
	1/v-absorber[b]

[a]Unless overridden by user input, these nuclides are added to the initial fuel mixture with a number density of 10^{-20} atoms/barn-cm.

[b]Used to calculate the THERM parameters applied in ORIGEN-S (see Sect. F7.6.12).

Table 2. Point Beach PWR Measured[a] and Computed Decay Heat Rates

Assembly ID	Burnup, MWd/kgU	Initial ^{235}U wt %	Cooling time, d	Heat rate, watts		% difference $(\frac{\text{Calc.}}{\text{Meas.}} - 1)100\%$	% difference assembly average
				Meas.	Calc.		
C-52:	31.914	3.397	1635	724[b]	732.2	1.1	
			1635	723[c]	732.2	1.3	1.2
C-56	38.917	3.397	1634	921	943.3	2.4	2.4
C-64:	39.384	3.397	1633	931[b]	959.0	3.0	
			1633	825[c]	959.0	16.2	9.6
C-66	35.433	3.397	1630	846	852.2	0.7	0.7
C-67	38.946	3.397	1629	934	946.5	1.3	1.3
C-68	37.057	3.397	1630	874	898.0	2.7	2.7
Average						3.6	3.0
Std dev						±2.3	±1.9

[a]See Ref. 8.
[b]Static test.
[c]Recirculation test.

Table 3. Turkey Point PWR Measured[a] and Computed Decay Heat Rates

Assembly ID	Burnup, MWd/kgU	Initial ^{235}U wt %	Cooling time, d	Heat rate, watts		% difference $(\frac{\text{Calc.}}{\text{Meas}} - 1)100\%$	% difference assembly average
				Meas	Calc		
B-43	24.827	2.559	1782	637	608.1	−4.5	−1.5
D-15:	28.152	2.557	962	1423	1436.0	0.9	
			1144	1126	1172.0	4.1	
			2077	625	628.4	0.5	1.8
D-22	25.946	2.557	963	1284	1255.0	−2.3	−2.3
D-34	27.620	2.557	864	1550	1582.0	2.1	2.1
Average						0.1	−0.7
Std dev						±1.3	±1.7

[a] See Ref. 8.

Table 4. Cooper Nuclear Station BWR Measured[a] and Computed Decay Heat Rates

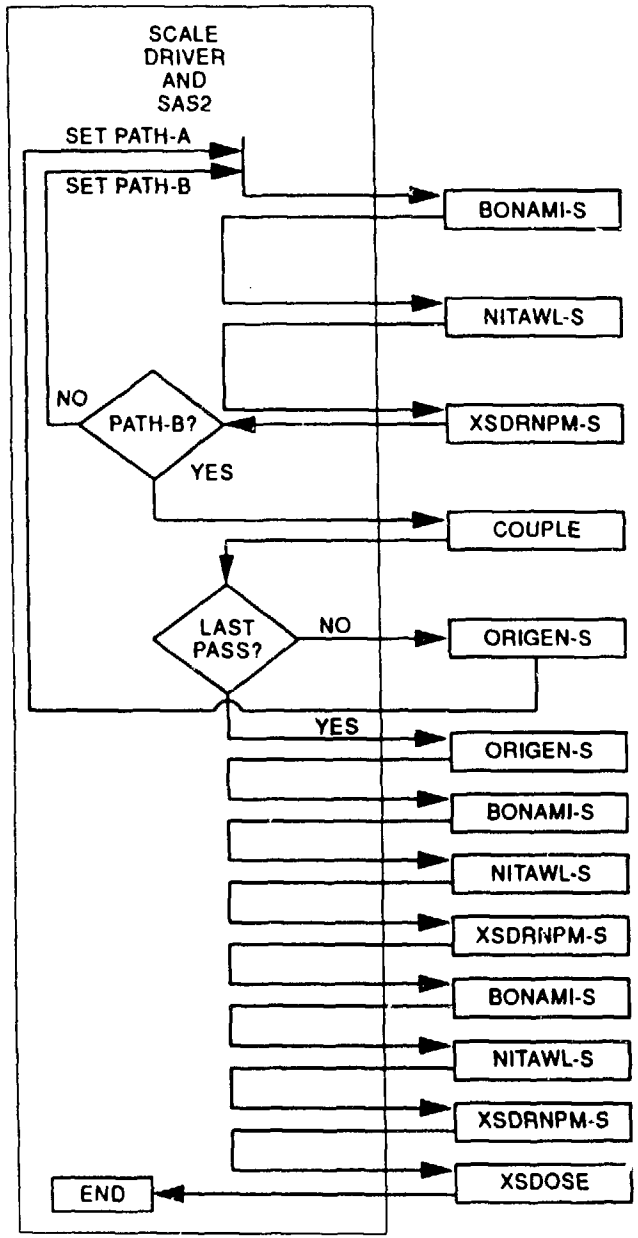
Assembly ID	Burnup, MWd/kgU	Initial ^{235}U wt %	Cooling time, d	Heat rate, watts		% difference	% difference
				Meas.	Calc.	$(\frac{\text{Calc}}{\text{Meas}} - 1)100\%$	assembly average
CZ102:	11.667	1.1	2565	62.3	78.9	26.6	
			2645	70.4	77.8	10.5	18.6
CZ205:	25.344	2.5	857	324.0	328.3	1.3	
			867	361.0	325.3	−9.9	
			871	343.5	324.1	−5.6	
			872	353.2	323.8	−8.3	
			886	331.8	319.8	−3.6	
			887	338.7	319.5	−5.7	
			892	327.5	318.1	−2.9	
			896	313.1	316.9	1.2	
			899	311.4	316.1	1.5	
			930	314.0	307.8	−2.0	
			936	331.2	306.2	−7.5	
			946	317.1	303.7	−4.2	−3.8
CZ209	25.383	2.5	891	279.5	290.1	3.8	3.8
CZ259:	26.466	2.5	1288	247.6	285.7	15.4	
			1340	288.5	278.5	−3.5	6.0
CZ331:	21.332	2.5	2369	162.8	161.6	−0.7	
			2457	180.1	158.2	−12.2	−6.5
CZ369	26.576	2.5	888	347.6	340.4	−2.1	−2.1
CZ429	27.641	2.5	889	385.6	366.5	−5.0	−5.0
CZ515:	25.737	2.5	1254	294.0	282.3	−4.0	
			1285	296.0	276.7	−6.5	−5.3
CZ526	27.596	2.5	864	395.4	374.7	−5.2	−5.2
CZ528	25.715	2.5	1286	297.6	275.4	−7.5	−7.5
Average						−1.4	−0.7
Std dev						±1.7	±2.6

[a] See Ref. 9.

Table 5. Comparison of various approximations for BWR fuel modeling

	k_∞ Values[a]		
	Top node	Middle node	Bottom node
Without Gd rods[b]			
DORT (2-D)	1.33	1.34	1.37
SAS2H (full assembly)	1.33	1.34	1.37
Pin cell	1.05	1.17	1.32
With Gd rods[c]			
DORT (2-D)	1.08	1.10	1.12
SAS2H (1/6 assembly)	1.12	1.14	1.17
DORT (actual pin-split enrichments ~~of Table 2~~)	–	–	1.10
DORT (maximum enrichments 4.15%)	–	–	1.20

[a] 3.4% initial average enrichment unless otherwise noted.
[b] KENO V.a (3-D) value is 1.35.
[c] KENO V.a (3-D) value is 1.12.



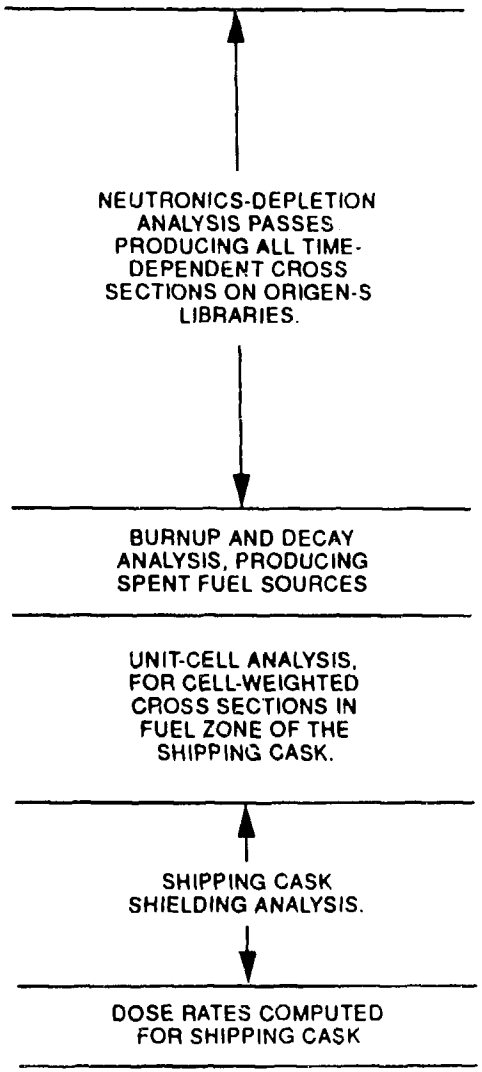


Fig 1
Flow path invoked by <A537H sequence.

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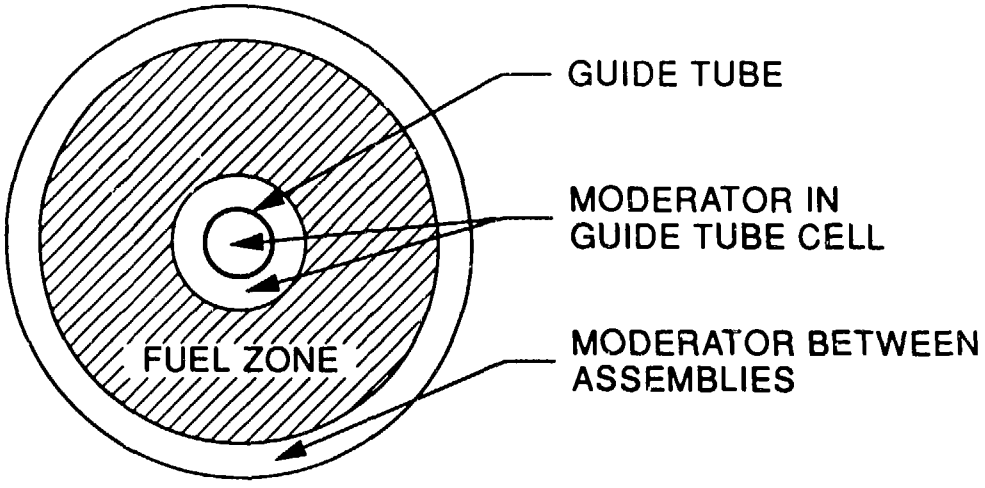
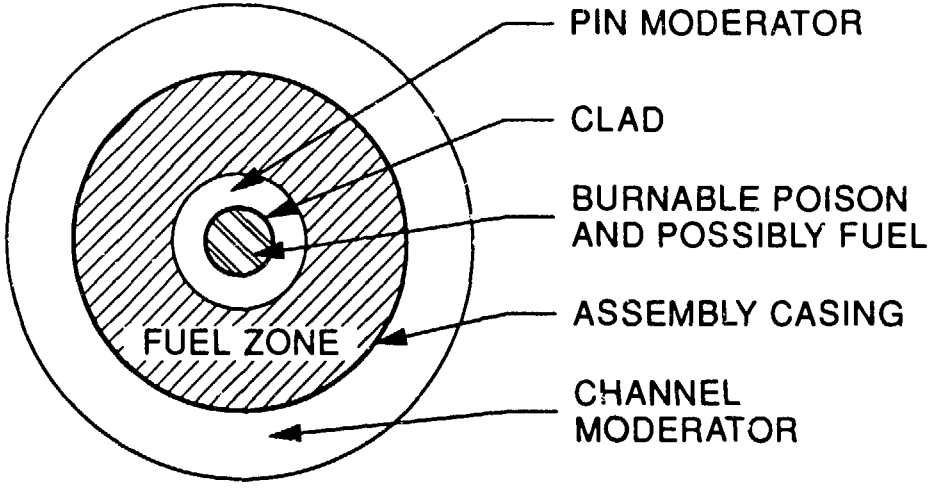
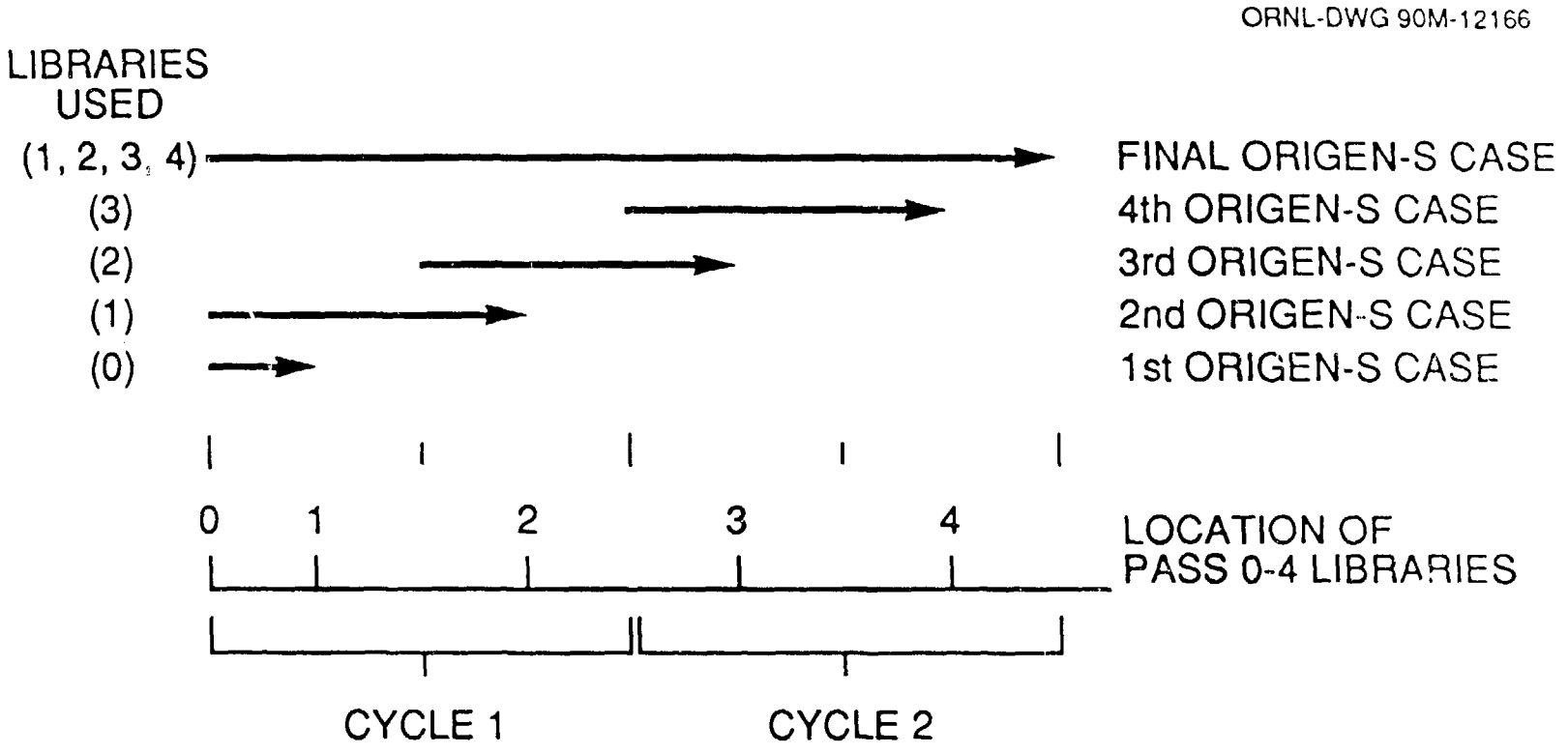


(a) FOR PWR CONTROL ROD ASSEMBLY, AFTER CONTROL RODS WITHDRAWN.



(b) FOR BWR BURNABLE POISON ASSEMBLY WITH LARGE CHANNEL ZONE.



[redacted].3. Schematic of successive ORIGEN-S cases used to produce the burnup-dependent number densities.

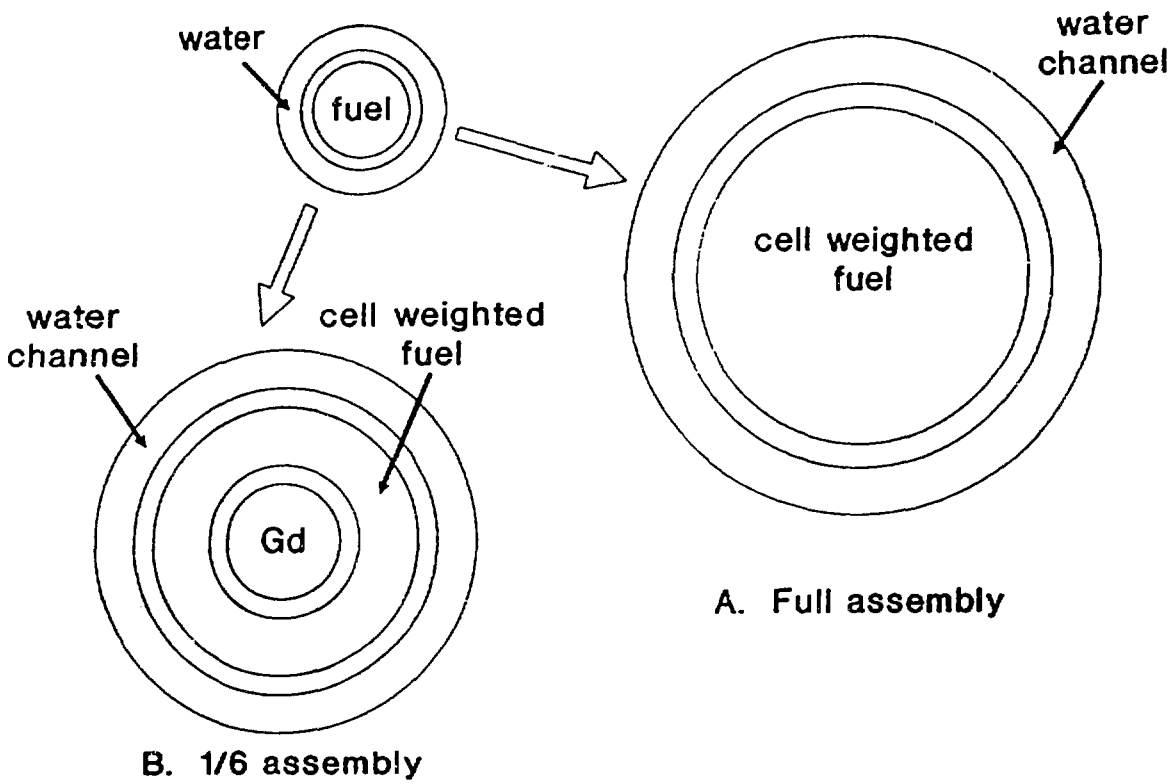


Fig. 4 BWR assembly models investigated with SAS2H.

Fig. 5 k_∞ versus burnup for constant axial power assumption and one-node case.