

ORIGAMI: A NEW INTERFACE FOR FUEL ASSEMBLY CHARACTERIZATION WITH ORIGEN

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I. INTRODUCTION

ORIGAMI (ORIGen AsseMbly Isotopics) is a new interface to the well-established ORIGEN code [1] to be distributed with the upcoming SCALE 6.2 release designed to enable simplified 3-D depletion and decay calculations for used nuclear fuel (UNF) assemblies. ORIGAMI calculates assembly characteristics through the use of discrete depletion “nodes,” corresponding to individual axial zones and pin locations. Using a nominal irradiation history, ORIGAMI calculates individual node isotopic compositions using axial and radial relative power distribution maps to create a zone-specific burnup, thereby enabling users to easily specify assembly-wide power distributions for depletion modeling.

ORIGAMI includes several useful capabilities for UNF assembly analyses, including visualization of key parameters by generating MeshView-compatible output files, generation of materials cards for MCNP and KENO for further source term analysis (for example, cask loading and dose studies for dry storage and transport [2] and simulation of full assemblies for NDA instrumentation studies [3, 4]). Additionally, ORIGAMI offers the ability to store individual depletion zone concentrations in an ORIGEN-compatible binary file for later re-evaluation (such as decay analysis of previously-depleted assemblies).

The ORIGAMI interface is not a new nuclear fuel depletion code; rather, it is a new convenience interface for ORIGEN designed to take advantage of the latest application program interface (API) layers within ORIGEN which were implemented as part of a recent code modernization effort [5]. Through this direct coupling with the ORIGEN API, it is therefore possible to provide a new “wrapper” interface around the ORIGEN code structure to provide convenient interfaces for new types of problems, such as evaluating assembly isotopics through combinations of axial and radial “zones” to form depletion “nodes” (as opposed to the traditional single-point depletion calculation performed by calling ORIGEN through the ORIGEN-ARP sequence).

Similar to the ORIGEN-ARP sequence, the ORIGAMI package relies upon one-group reactor data libraries produced previously through lattice physics methods such as TRITON. However, ORIGAMI also allows users to specify individual libraries for each pin or groups of pins, thereby capturing intra-lattice effects such as changes to the neutron spectrum due to proximity to water holes, burnable absorbers, or lattice edges.

Individual depletion calculations for each node are performed by ORIGEN via direct calls to the new ORIGEN application program interface (API); similarly, ORIGAMI automatically performs the appropriate node-level cross-section library interpolation based upon the node characteristics (i.e., cycle burnup, enrichment, etc.). In addition to leveraging ORIGEN’s

validated capabilities, this coupling also allows ORIGAMI to run in parallel using MPI (Message Passing Interface) over Linux clusters for very large assembly calculations [5].

The purpose of this paper will be to introduce the new ORIGAMI interface for ORIGEN, including an overview of key features of the interface and its application to UNF modeling problems, both for applications to used fuel disposition studies as well as safeguards applications involving nuclear fuel assembly modeling.

II. ORIGAMI CALCULATIONAL METHOD

The underlying depletion method employed by the ORIGAMI interface is identical to that employed by the ORIGEN-ARP sequence [1], given that ORIGAMI is simply a convenience interface to ORIGEN calculation engine [5]. For the default 0-D case (i.e., no axial/radial zones are specified by the user, or only one axial and radial zone are specified), the calculation is identical to that of the ORIGEN-ARP sequence, wherein the reactor data library is automatically interpolated for the problem-specific initial fuel enrichment, moderator void fraction, and mid-cycle burnups.

The following sections will describe how the ORIGAMI method is applied to multi-dimensional assembly models (i.e., 1-D axial models, 2-D lattice plane models, and 3-D nodal assembly models), including modeling power distributions through power shaping factors and the methods of normalizing the specific powers (in $\frac{\text{MW}}{\text{MTU}}$ and mass bases (in MTU) within the nodes to ensure that the total assembly power (in MW) is conserved.

II.A. 1-D, 2-D, and 3-D assembly modeling with power / burnup gradients

For the one-dimensional case (i.e., N_z axial zones across a single radial pin / zone), N_z separate ORIGEN cases are run for each of the axial zones. For such a case, axial power shaping factors are specified by the user (either in terms of the fractional axial power, wherein $\sum a_z = 1$, or in terms of relative powers, wherein $\frac{\sum a_z \Delta z}{\sum \Delta z} = 1$). These axial power shaping factors are used as modifiers to the nominal irradiation history. The net result is that an individual point depletion calculation is performed for each node (i.e., identical to the ORIGEN-ARP sequence once more), with an appropriate cross-section interpolation to the new effective burnup, thereby easily allowing users to model axial variations in assembly power for depletion calculations.

The spacing of the axial mesh need not be uniform; while the default behavior of ORIGAMI is to assume a uniformly-spaced axial mesh when no axial boundaries are specified (but a number of axial zones N_z has), users can also specify a series of $(N_z + 1)$ axial node boundaries, therefore allowing for

non-uniform axial node sizes (e.g., to accommodate tighter axial spacing at the assembly ends, where the shape of the axial power distribution typically changes more rapidly, falling precipitously as one reaches the edges, compared to the relatively “flat” profile near the center). Therefore, for a 1-D case the axial node specific powers (P_z^{SP} , in $\frac{\text{MW}}{\text{MTU}}$) are expressed as:

$$P_z^{SP} = P_A^{SP} \cdot a_z \quad (1)$$

Where P_A^{SP} is the nominal specific power of the assembly (i.e., the cycle specific power expressed in the nominal irradiation history).

For a non-uniform axial spacing, the **total** power in the axial node is:

$$P_z = P_A^{SP} \cdot \left(M_A \cdot \frac{\Delta Z}{Z} \right) \cdot a_z \quad (2)$$

Where $\frac{\Delta Z}{Z}$ is the fractional axial length of the node and M_A is the total mass of the assembly (in MTU). Two-dimensional cases can similarly be calculated (expressed as N_{xy} zones across a square lattice of $\sqrt{N_{xy}}$ pins; at present, ORIGAMI can only handle square-pitch lattice geometries). For this case, the power shaping factors (r_{xy}) are expressed as the relative radial power profile, which can equivalently be expressed as the fraction of the total lattice power (i.e., $\sum r_{xy} = 1$) or as a relative modifier from the nominal power. In either case, the individual specific pin powers (P_{xy}^{SP}) are thus:

$$P_{xy}^{SP} = P_A^{SP} \cdot r_{xy} \quad (3)$$

Finally, a three-dimensional case can be expressed by the user providing both axial and radial power shaping factors; individual node powers are calculated as the product of the axial and radial shaping factors, i.e.

$$P_{xy,z}^{SP} = P_A^{SP} \cdot a_z \cdot r_{xy} \quad (4)$$

Similar to before, the total power in an individual node is therefore simply:

$$P_{xy,z} = P_A^{SP} \cdot \left(M_A \cdot \frac{\Delta Z}{Z} \cdot \frac{1}{N_{xy}} \right) \cdot a_z \cdot r_{xy} \quad (5)$$

In each case, prior to the depletion calculation the cycle burnup is calculated by ORIGAMI to interpolate the specified one-group reactor library for the node to produce the most accurate problem-dependent cross-sections. In cases where users additionally specify individual pin enrichments (e.g., to model “zoned” enrichment, such as would be seen in BWRs or MOX assemblies) and/or individual reactor libraries for pins (i.e., to allow for higher-fidelity modeling of local spectral effects, such as proximity to burnable absorbers or water holes), these features are likewise folded into the reactor data library interpolation sequence; thus, the depletion calculation is tailored to each node through the appropriate cross-section library interpolation.

II.B. Power normalization

As eluded to in the previous section, ORIGAMI allows users to specify the assembly power distribution via axial and radial power shaping factors, allowing users to capture burnup gradients in both dimensions. In ORIGAMI, two types of power normalization can be employed; *absolute* normalization, in which power shaping factors are treated as giving the *fractional* assembly power (and thus, the *total* power for each node adds to the total assembly power), and *relative* normalization, wherein the power shaping factors are treated as modifiers to the *average* assembly power expressed by the nominal irradiation history.

To ensure consistency between calculations and to ensure conservation of total assembly power, ORIGAMI automatically normalizes the power shaping factors. For *absolute* shaping factors, this is accomplished by ensuring that the fractional powers in each node add up to the total assembly power, i.e.:

$$P_A = \sum P_A^{SP} \cdot \left(M_A \cdot \frac{\Delta Z_i}{Z} \right) \cdot a_z \quad (6)$$

For relative power shaping factors (R_z), the conversion to absolute power shaping factors for each node (a_z)_{*i*} is accomplished as follows:

$$(a_z)_i = \frac{(R_z)_i \cdot M_A \cdot \left(\frac{\Delta Z_i}{Z} \right)}{\sum (R_z)_i \cdot M_A \cdot \left(\frac{\Delta Z_i}{Z} \right)} = \frac{(R_z)_i \cdot \left(\frac{\Delta Z_i}{Z} \right)}{\sum (R_z)_i \cdot \left(\frac{\Delta Z_i}{Z} \right)} \quad (7)$$

Obviously, for a uniformly-spaced axial mesh, the use of relative axial power modifiers is identical to absolute power fractions, as $\left(\frac{\Delta Z_i}{Z} \right)$ simply becomes a constant. However, such a conversion to absolute power fractions is particularly important for non-uniform axial meshes in order to ensure a conservation of total assembly power.

For radial power shaping factors, given the assumption that the mass is uniformly distributed across each fuel pin (i.e., fuel pins are all assumed to be of the same volume and thus the same mass), it is simple to show that the absolute and relative power shaping factors are identical:

$$(r_{xy})_i = \frac{(R_{xy})_i \cdot \frac{M_A}{N_{xy}}}{\sum (R_{xy})_i \cdot \frac{M_A}{N_{xy}}} = \frac{(R_{xy})_i}{\sum (R_{xy})_i} \quad (8)$$

The logic of relative power modifiers comes from the assumption that users modeling assemblies would be obtaining burnup information from NDA techniques such as measurement of burnup indicators nuclides (such as the $^{134}\text{Cs} / ^{137}\text{Cs}$ ratio) to obtain axial and radial burnup profiles [6]; these measurements would therefore be obtained as *relative* burnup indicators (i.e., expressed as a ratio to an average gamma signature intensity or nominal calculated burnup value).

II.C. Physics basis of ORIGAMI depletion

As noted previously, the ORIGAMI sequence relies on the same solution method for solving the Bateman Equations to

calculate updated isotopic inventories as the ORIGEN-ARP sequence [1]. In the ORIGEN-ARP sequence, material depletion, transmutation, and decay is calculated through the use of collapsed, one-group reactor data libraries previously generated through a 2-D, multi-group lattice physics calculation by codes such as TRITON. At each depletion interval in the lattice physics transport method, the multi-group spectrum is collapsed to a one-group spectrum and corresponding flux-weighted effective one-group cross-sections and transition coefficients are calculated. Within TRITON, this collapse can be performed as a single lumped material over all fuel materials within the assembly or for individual pins or zones of pins, allowing the user to create reactor data libraries specific to particular “zones” of the assembly in order to capture local changes to the neutron spectrum (such as proximity to burnable absorbers, water holes, and other lattice features) that can produce substantial differences in the effective one-group cross-sections.

Additionally, as the TRITON sequence generates collapsed one-group cross-sections for fixed initial assembly configurations (i.e., initial enrichment, moderator void fraction, etc.) at fixed burnup points, the ORIGEN-ARP sequence likewise allows users to interpolate across a series of one-group libraries on both these initial parameters as well as the problem-specific cycle burnups in order to obtain one-group cross-sections that more accurately reflect the problem conditions without requiring computationally expensive lattice physics transport calculations each time a problem is run.

ORIGAMI extends this concept by allowing users to specify different reactor data libraries for individual pins, thus building on TRITON’s ability to create both “discrete” and “lumped” libraries for fuel lattices. Further, ORIGAMI automatically interpolates reactor data libraries for each depletion node based both on the initial assembly configuration (i.e., interpolating over the same parameters as the ORIGEN-ARP sequence, such as burnup, initial enrichment, and moderator void fraction) and on the effective node burnup for each cycle (i.e., based on nominal assembly power is scaled by the node-specific power shaping factor). Additionally, because ORIGAMI is capable of 1-D axial models and 3-D full assembly models, users are also able to specify an axially-varying moderator density (i.e., void fraction), therefore capturing an important moderator effect of BWR assemblies. Finally, ORIGAMI allows users to specify individual enrichments for each pin (similar to BWR and MOX assemblies), which are likewise factored into the automatic cross-section library interpolation component of the depletion calculation.

It should be stressed that ORIGAMI is **not** a lattice physics code; ORIGAMI simply performs depletion calculations across individual “nodes” as defined by a nominal irradiation power history, the node composition (whether it be through a single, globally-specified enrichment or individual pin enrichments), moderator density (if specified), and axial/radial power shaping factors. ORIGAMI therefore does not calculate interaction effects between pins (except that which is captured through the use of individual pin-level cross-section libraries previously generated from transport calculations); rather, each pin is a discrete depletion calculation identical to that which would be performed by a standalone ORIGEN-ARP depletion calculation.

III. OVERVIEW OF ORIGAMI FEATURES

III.A. User input and case specification

To facilitate maximum usability (particularly for scenarios involving the automated generation of a large number of assembly irradiation histories) and flexibility, the ORIGAMI input employs a newly-developed Standard Object Notation (SON)-based interface, allowing users to easily specify assembly characteristics including material compositions, power distribution maps, pin-level libraries, etc. The resulting tool offers a powerful, flexible capability for UNF assembly characterization appropriate for a wide variety of modeling applications.

The SON syntax is similar in nature to the JSON (JavaScript Standard Object Notation) standard [7], employing key-value pairs for defined keywords, allowing for array data enclosed in square brackets ([]), and object data enclosed in curly brackets ({ }). For example, an individual cycle history is expressed as a collection of key-value pairs (i.e., Figure 1):

```
cycle{ power=35.0 burn=300 nlibs=3 down=30 }
```

Fig. 1. An example of a power cycle specification block in ORIGAMI; here, the assembly is irradiated at 35 $\frac{\text{MW}}{\text{MTU}}$ for 300 days (with 3 interpolation sub-divisions) and then cooled for 30 days.

A collection of these objects can be assembled into an array to specify an entire cycle history, such as Figure 2:

```
hist[
  cycle{ power=35.0 burn=300 nlibs=3 down=30 }
  cycle{ power=38.2 burn=350 nlibs=6 down=30 }
  cycle{ power=30.0 burn=200 nlibs=4 }
  cycle{ down=10000 }
]
```

Fig. 2. A complete power history block in ORIGAMI, specifying three power cycles (at 35, 38.2, and 30.0 $\frac{\text{MW}}{\text{MTU}}$ for 300, 350, and 200 days, respectively, followed by a cooling time of 10,000 days.

III.A.1. Pin-level mapping features: power maps, enrichments, and libraries

ORIGAMI handles mapping power shaping factors as arrays (for axial power shaping factors) and *maps* (i.e., to map pin powers along an x-y grid); an example of this is given as Figure 3.

```
xy[ 0.2  0.3
    0.4  0.5 ]
ax[ 0.35  0.4  0.25]
```

Fig. 3. Radial and axial power shaping factor input in ORIGAMI; here, a 2x2 radial power grid is specified along with 3 axial zones.

Maps share an identical syntax to arrays but allow users to break lines across multiple rows to allow for an intuitive display of the x-y mapping; the ORIGAMI automatically converts these multi-line arrays (maps) into the appropriate 2-D mapping through the assumption that assemblies follow a square-pitch lattice design. Non-fuel pins (e.g., water holes, etc.) are simply specified as 0.0 in the radial power shaping arrays.

Additionally, for 1-D and 3-D calculations ORIGAMI allows users to specify an axial moderator density distribution (Figure 4). Note for this case that the number of moderator density zones must match the number of axial zones.

```
mod[ 0.73  0.715  0.710 ]
```

Fig. 4. An example of a user-specified axial moderator density distribution in ORIGAMI, specifying three axial zones with an average moderator density of 0.73, 0.715, and 0.710 $\frac{\text{g}}{\text{cm}^3}$.

In order to accommodate a wide range of assembly types, ORIGAMI includes a number of pin-level configurations options, such as specifying individual pin enrichments/compositions (e.g., facilitating modeling of zoned enrichments and gadolinia rods), specification of individual one-group cross-section libraries for each pin (enabling users to capture local spectrum effects such as pins adjacent to water holes, burnable absorbers, etc.) Users specify *maps* of these parameters to map configurations such as individual libraries, enrichments, etc. to pins, similar to power shaping factor maps. An example of this is provided as Figure 5.

```
enrich[ 3.21 3.43 3.57 ]
libs[ ce14x14 ce16x16 ]
pinmap[ 1 2
        2 1 ]
enrmap[ 1 2
        2 3 ]
```

Fig. 5. An example of mapping individual libraries and enrichment zones to pins in ORIGAMI.

In this case, the `enrich` array contains three enrichments; in the `enrmap` block, these enrichments are substituted in at each x-y location based on the index in the `enrich` array (starting at index 1, corresponding to 3.21% enrichment). Individual libraries are mapped similarly in the `pinmap` block.

For cases in which the radial power factor is 0.0, the library index is 0, or the enrichment index is 0, ORIGAMI therefore assumes the lattice entry is a non-fuel pin (and subsequently cross-checks the radial power, library, and enrichment maps for consistency to this effect). The net effect is that the entry is treated as having no fuel and therefore is skipped in the depletion calculation (and not factored into normalization calculations).

III.A.2. Non-fuel materials

ORIGAMI allows users to specify non-fuel compositions to be included in depletion calculations (e.g., cladding and other fuel hardware materials) in order to calculate the contribution

of the activation source term to the total assembly thermal and radiation output. Non-fuel materials are specified as pairs of data in the `nonfuel` array, pairing the chemical symbol (e.g., Zr, etc.) with the a relative mass (in kg per MTU); these masses can optionally be specified as a fraction of the total fuel mass. For non-fuel materials, elemental masses are specified; ORIGAMI automatically calculates isotopic masses from their elemental natural abundances using the ORIGEN data libraries. An example specification is shown as Figure 6.

```
nonfuel[ zr 520.3  sn 8.4 ]
```

Fig. 6. Example of non-fuel materials in ORIGAMI; here, 520.3 kg of zirconium (Zr) and 8.4 kg of tin (Sn) per MTU of fuel material are specified.

III.B. Assembly restart calculations

Additionally, ORIGAMI supports a “restart” analysis capability through the use of ORIGEN binary concentration files (automatically generated for each depletion node by ORIGAMI), i.e., to evaluate the effects of subsequent decay times on assembly isotopic and source term characteristics, etc. To perform the restart calculation, users provide an ORIGEN binary concentrations file containing the lumped axial zone concentrations and a number of axial zones (note that ORIGAMI does not currently support pin-by-pin restart calculations) along with a nominal power history (i.e., typically a decay time); ORIGAMI then updates the isotopic compositions for each axial zone and produces a new set of lumped concentrations files, axial decay heat maps (if requested), etc. Such a feature is particularly useful for evaluating the evolution of thermal-hydraulic characteristics of fuel assemblies placed in long-term storage in dry storage casks.

III.C. Output and data analysis options

ORIGAMI contains several output features designed to facilitate advanced analysis of irradiated nuclear fuel assemblies. These features include visualization of key nuclides, material cards for additional analysis in SCALE and MCNP, and other useful source terms for assembly-level analysis, including ORIGEN-compatible binary concentration files and thermal and radiological source terms.

III.C.1. Output visualization with MeshView

ORIGAMI’s visualization features include generating MeshView-compatible interactive 3-D plots of key assembly characteristics (such as the burnup distribution) as well as similar plots for key nuclides of interest, such as the major plutonium isotopes, key characteristic burnup indicator nuclides (such as ^{137}Cs , ^{134}Cs , ^{154}Eu , etc.), and other nuclides of interest (i.e., minor actinides such as Am, Cm, and Np). These plots are viewable with the Java-based MeshView utility distributed with SCALE; Figure 7 shows an example plot of the assembly axial and radial plutonium distributions.

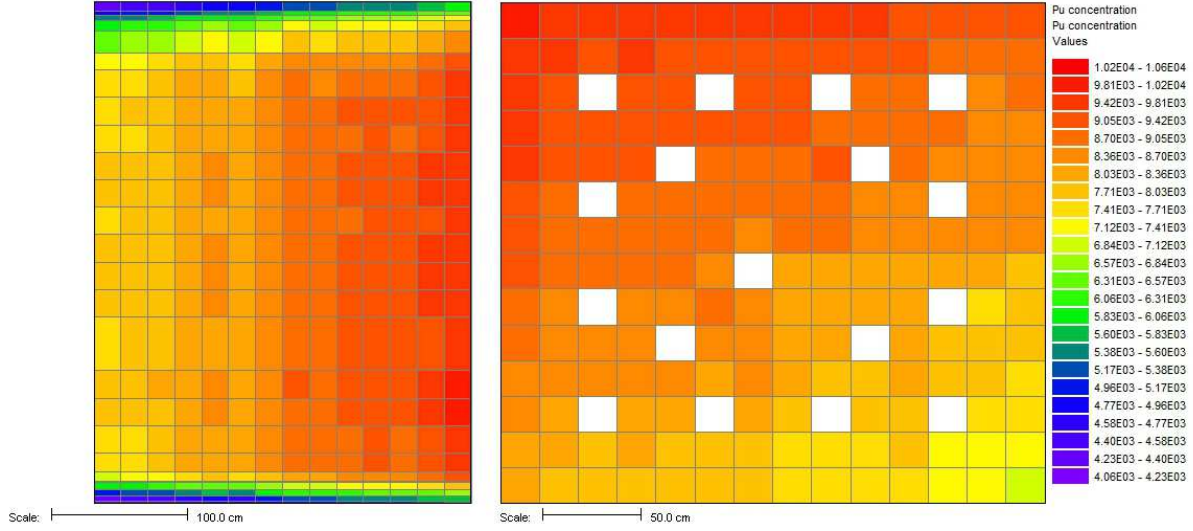


Fig. 7. Example MeshView plots for the calculated assembly plutonium content for a 14x14 fuel assembly with 26 axial zones and relative pin powers specified; (left) Vertical cut-away view; (right) Horizontal (axial plane) cut-away view. Concentration units in gram-atoms (moles).

III.C.2. Generation of MCNP and SCALE standard composition data files

ORIGAMI has the ability to generate material cards useful for MCNP and SCALE-based geometries, based on the discharge isotopic content of each depletion node. Such a feature is particularly useful when working with multi-dimensional models (such as 1-D axial models or 3-D full assembly models), allowing a user to populate a pre-defined geometry template with materials cards based on the individual burnup conditions of the assembly.

For MCNP material cards, ORIGAMI follows MCNP material ZAIID conventions, creating a material card for each depletion node with all available MCNP isotopes. Similarly, for SCALE standard composition files (used for KENO and any other SCALE-based tool requiring a composition block), a unique mixture number is assigned to each depletion node and the corresponding number densities of each nuclide (accounting for fuel density, etc.) are provided for each mixture ID.

III.C.3. Other ORIGAMI source term outputs

Finally, ORIGAMI also contains several source term output features for post-depletion assembly analyses. These features include radiation source term outputs by depletion zone (i.e., total gamma / neutron intensities, in particles/s) and decay heat (lumped by axial zone, in watts), and finally ORIGEN binary concentration files (.f71 format) for each depletion zone, as well as lumped concentrations files for each axial zone and finally a lumped concentration for the aggregate assembly, used for restart analyses (as discussed prior).

Decay heat for each axial zone is calculated from the sum of the decay energies of each isotope across each pin (for 3-D

calculations) for each axial zone, i.e.:

$$\begin{aligned}
 H_Z &= \sum_{i=1}^{i_{tot}} Q_i \lambda_i \frac{M_Z^{(i)}}{A^{(i)}} \cdot 1.602 \cdot 10^{-13} \cdot N_A \\
 &= 9.65 \cdot 10^{10} \sum_{i=1}^{i_{tot}} Q_i \lambda_i \frac{M_Z^{(i)}}{A^{(i)}}
 \end{aligned} \tag{9}$$

Here, H_Z is the total axial zone thermal power (in watts), Q_i is the decay energy of nuclide i (in MeV), λ_i is the decay constant of nuclide i (in s^{-1}), $1.602 \cdot 10^{-13}$ is the conversion factor between MeV to J, $M_Z^{(i)}$ is the total mass of nuclide i in the axial zone and $A^{(i)}$ is the molar mass of nuclide i , and N_A is Avogadro's number.

For radiation source term outputs (i.e., to be used in conjunction with MCNP materials cards), ORIGAMI calculates the total gamma/neutron intensity for each region (in particles/s) and produces separate output files for both the gamma and neutron source terms; the total intensities are matched to the depletion zones using the same material numbering convention used for dumping MCNP material concentrations.

For concentration dump files (.f71 format), ORIGAMI uses a similar convention to the MCNP materials file generation, wherein the dumpfile dumps starting at the first axial zone (i.e., bottom of the assembly, progressing upward) and the bottom-left pin in each axial plane, moving from left-to-right and restarting at each row until the top-right pin is dumped, repeating this process for each axial plane. ORIGAMI generates two separate concentrations files; one file containing each individual depletion zone and a second containing the lumped axial zone concentrations, the latter of which can be used for restart analyses in ORIGAMI.

III.D. Parallel execution on Linux-based computing clusters

A key feature of ORIGAMI, particularly for 3-D depletion models, is the ability of ORIGAMI to execute nodal depletion calculations in parallel across several processors and compute nodes on Linux-based clusters. For example, consider a 17x17 fuel array with 264 fuel pins modeled over 24 axial zones; the total calculation would span 6,336 discrete depletion nodes. Even assuming a relatively rapid time per depletion calculation (on the order of a few seconds), such a calculation would take several hours to complete if executed in serial. Given that the nodal depletion calculations are entirely independent of one another, the problem can be easily divided across a number of separate compute nodes and executed in parallel fashion, resulting in a near-linear scale-up factor [5].

IV. APPLICATIONS OF ORIGAMI TO HIGH-FIDELITY USED FUEL MODELING

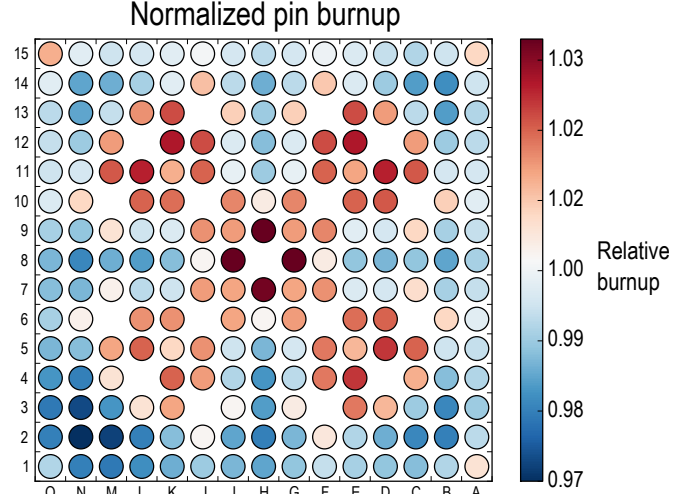
IV.A. High-fidelity fuel assembly modeling for safeguards development applications

A particular application ORIGAMI was designed to accommodate was in the ability to capture individual pin and axial node burnup features in order to develop high-fidelity models of irradiated fuel assemblies for safeguards development [3, 4]. Unlike typical lattice transport methods such as TRITON and Monte Carlo techniques such as KENO or MonteBurns, the ORIGAMI sequence allows one to directly reconstruct pin-level burnups given an assembly burnup distribution (i.e., obtained from NDA measurements and/or operator-supplied irradiation history data). Thus, for a well-characterized burnup distribution, ORIGAMI allows one to capture assembly isotopics both with greater fidelity and speed compared to traditional methods such as the aforementioned codes.

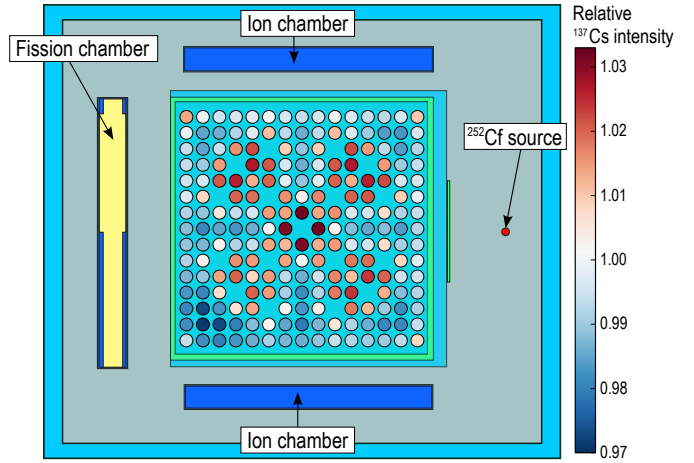
An example of this type of analysis is shown as Figure 8. For used fuel with relatively long cooling times (i.e., greater than 10 years, such as is shown in Figure 8), the gamma emission is dominated by ^{137}Cs , which is proportional to the fuel burnup. The good agreements between the burnup distribution (calculated based on user input, as shown in Figure 8(a)) and gamma source distribution (output by ORIGAMI, based on isotopic calculations and shown in Figure 8(b)) indicate that ORIGAMI performs burnup calculations consistently among all fuel pins.

Figure 8(b) also demonstrates the usefulness of ORIGAMI for nuclear safeguards applications [8]), especially when high-fidelity nuclide compositions and radiation source terms are needed to quantify the performance of advanced NDA instruments. In Figure 8(b), ORIGAMI was used to calculate detailed isotopic inventories for an assembly with well-characterized axial and burnup gradients (Figure 8); the resulting pin-level ^{137}Cs profile was then used to help model the ^{252}Cf Interrogation Prompt Neutron (CIPN) detector being developed by LANL for the NGSi project [8].

The Next Generation Safeguards Initiative (an NNSA-sponsored research initiative focused on the development of advanced NDA systems for UNF safeguards and accountancy)



(a) Assembly-normalized pin-level burnups (specified by user)



(b) Assembly-normalized ^{137}Cs source terms in a CIPN detector model

Fig. 8. An example of ORIGAMI-generated used fuel assembly isotopics and radiation source terms used in NDA instrument modeling to quantify the performance of the CIPN detector designed for nuclear safeguards applications [8].

has been employing ORIGAMI to generate spent fuel “reference libraries” (i.e., detailed MCNP assembly models for characterizing new detector systems) from nodal depletion calculations. This process employs well-characterized assemblies where both detailed operator information exists and where extensive NDA measurements have been performed to further characterize the burnup gradient among individual pins within the assembly and/or assembly-level burnup gradients, such as shown in Figure 8) where axial gamma scans of several fuel rods were used to characterize assembly burnup gradients.

Using this detailed burnup information, ORIGAMI was used to generate the corresponding MCNP materials cards for each depletion region, thereby enabling the rapid creation of a series of detailed MCNP-based assembly “reference libraries” (spanning a variety of fuel irradiation conditions) useful for development and prototyping of advanced NDA systems for spent fuel safeguards [9, 10].

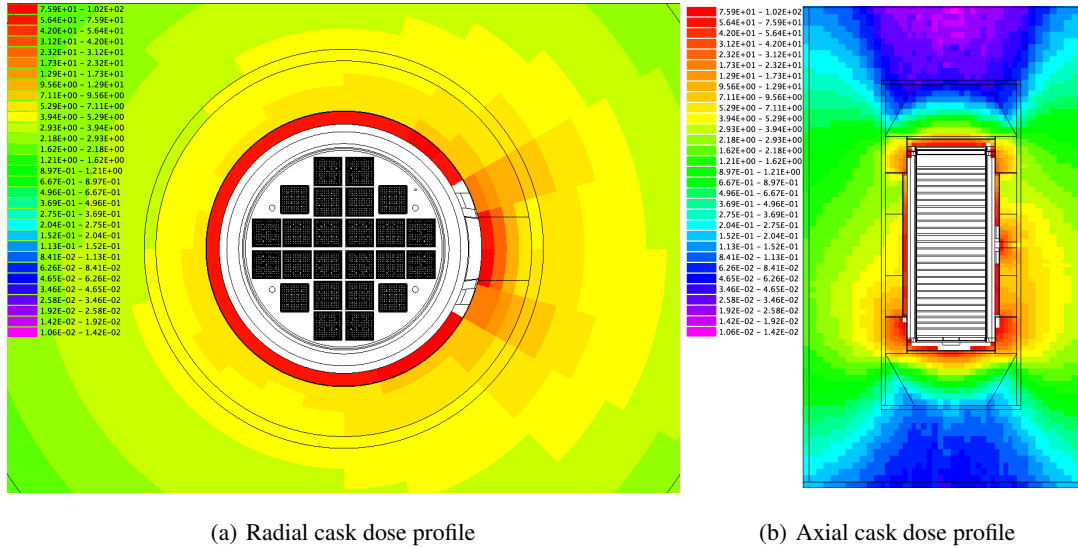


Fig. 9. Dose models for as-loaded dry storage casks for used nuclear fuel using source terms generated from the ORIGAMI tool; doses calculated in mrem/hr [2].

IV.B. 3-D nuclear fuel assembly depletion for UNF disposition analysis

The new ORIGAMI interface has also become a central component of the UNF ST&NDARDS (Used Nuclear Fuel Storage, Transportation, and Disposal Analysis Resource and Data System) tool for UNF disposition analysis [11]. The UNF ST&NDARDS Unified Database includes data on stored UNF assemblies from a variety of open literature sources, including the U.S. UNF discharge inventory through December 31, 2002 [12] as well as data on stored fuel at U.S. commercial reactors [2, 11].

UNF ST&NDARDS serves as an integrated workflow to comprehensively capture as-loaded UNF information from dry storage casks, calculate isotopic inventories from fuel assemblies, and from this calculate key information of interest to UNF management, including thermal analysis of as-loaded casks (e.g., thermal source terms and calculated temperatures of the clad and outer canister surface) as well as external radiation dose calculations based on the source term of fuel assemblies loaded within the cask [2]. An example of such an as-loaded dose analysis of casks using ORIGAMI source terms is presented as Figure 9.

In addition to dose analysis, ORIGAMI axial decay heat profiles have been integrated into the UNF ST&NDARDS tool to provide detailed decay heat source terms used to calculate anticipated peak clad temperatures in dry storage casks for long-term storage and transport analysis [13]. For these cases, ORIGAMI is used to create a time-dependent axial profile of the decay heat from each assembly loaded into the cask, based on available irradiation history information for each assembly. These decay heat profiles are combined with thermal-hydraulic models of the cask using COBRA-SFS to evaluate key parameters such as the peak clad temperature over time as well as realistic thermal conditions for the cask [13].

For each of these tasks, ORIGAMI plays an essential supporting role by affording rapid generation of the isotopic, radiological, and thermal source terms with ORIGEN [1] needed for further analysis of UNF storage conditions with codes such as MAVRIC [14] for shielding and dose analysis and COBRA-SFS for thermal analysis [13].

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REFERENCES

1. I.C. GAULD, G. RADULESCU, G. ILAS, B.D. MURPHY, M.L. WILLIAMS, and D. WIARDA. Isotopic Depletion and Decay Methods and Analysis Capabilities in SCALE. *Nuclear Technology*, 174(2):169–195, May 2011.
2. G. RADULESCU, D.E. PEPLow, M.L. WILLIAMS, and J.M. SCAGLIONE. Dose Rate Analysis of As-Loaded Spent Nuclear Fuel Casks. In *18th Topical Meeting of the Radiation and Shielding Division of ANS (RPSD 2014)*,

- Knoxville, TN, September 2014.
3. S.E. SKUTNIK, I.C. GAULD, C.E. ROMANO, and H.R. TRELLUE. Creating NDA “Working Standards” through High-Fidelity Spent Fuel Modeling. In *Proceedings of the Institute of Nuclear Materials Management, 53rd Annual Meeting*, Orlando, FL, July 2012.
 4. J. HU, I.C. GAULD, J. BANFIELD, and S. SKUTNIK. Developing Spent Fuel Assembly Standards for Advanced NDA Instrument Calibration – NGSF Spent Fuel Project. Technical Report ORNL/TM-2013/576, Oak Ridge National Laboratory, Oak Ridge, TN, USA, March 2014.
 5. S.E. SKUTNIK, F. HAVLÚJ, D. LAGO, and I.C. GAULD. Development of an Object-Oriented ORIGEN for Advanced Nuclear Fuel Modeling Applications. In *International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013)*, Sun Valley, ID, May 2013.
 6. J.R. PHILLIPS. Irradiated fuel measurements. In *Passive Nondestructive Analysis of Nuclear Materials*. Los Alamos National Laboratory, Los Alamos, NM, March 1991.
 7. ECMA international. The JSON Data Interchange Format. Technical Report ECMA-404, October 2013.
 8. J. HU, D. HENZLOVA, and S. TOBIN. Customized Design and Simulated Performance of the Californium Interrogation Prompt Neutron Detector for Spent Fuel Measurement at the Post Irradiation Examination Facility in the Republic of Korea. In *Proceedings of the Institute of Nuclear Materials Management, 53rd Annual Meeting*, Orlando, FL, 2012.
 9. H.R. TRELLUE, J.D. GALLOWAY, N.A. FISCHER, and S.J. TOBIN. Advances in Spent Fuel Libraries. In *Proceedings of the Institute of Nuclear Materials Management, 54th Annual Meeting*, Desert Springs, CA, July 2013.
 10. J.D. GALLOWAY, H.R. TRELLUE, M.L. FENSIN, and B.L. BROADHEAD. Design and Description of the NGSF Spent Fuel Library with Emphasis on the Passive Gamma Signal. *Journal of Nuclear Materials Management*, XL(3):25–34, Spring 2012.
 11. J.M. SCAGLIONE, K. BANERJEE, K.R. ROBB, and R.A. LEFEBVRE. The Used Nuclear Fuel Storage, Transportation, and Disposal Analysis Resource and Data System. In *Proceedings of the Institute of Nuclear Materials Management, 55th Annual Meeting*, Atlanta, GA, July 2014.
 12. U.S. Energy Information Administration (EIA). RW-859 Nuclear Fuel Data, October 2004.
 13. R.R. DEVOE and K.R. ROBB. COBRA-SFS Dry-Cask Modeling Sensitivities in High-Capacity Canisters. In *2015 International High-Level Radioactive Waste Management Conference (IHLRWM 2015)*, Charleston, SC, April 2015.
 14. D.E. PEPLOW. Monte Carlo Shielding Analysis Capabilities with MAVRIC. *Nuclear Technology*, 174(2):289–313, 2011.