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# Enhancing GADRAS Source Term Inputs for Creation of Synthetic Spectra

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## Abstract

The Gamma Detector Response and Analysis Software (GADRAS) team has enhanced the source term input for the creation of synthetic spectra. These enhancements include the following: allowing users to programmatically provide source information to GADRAS through memory, rather than through a string limited to 256 characters; allowing users to provide their own source decay database information; and updating the default GADRAS decay database to fix errors and include coincident gamma information.

## ACKNOWLEDGMENTS

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## NOMENCLATURE

| Abbreviation | Definition |
|---|---|
| **GADRAS** | Gamma Detector Response and Analysis Software |
| **ORNL** | Oak Ridge National Laboratory |
| **ORIGEN** | Oak Ridge Isotope Generator |
| **API** | Application Programming Interface |

# 1. INTRODUCTION

Gamma Detector Response and Analysis Software (GADRAS) is widely used for generating a gamma detector response to radiation sources [1]. Enhancements for creating synthetic spectra in GADRAS were introduced with GADRAS version 18.8. These enhancements include the ability to generate spectra for a source containing an unlimited number of nuclides, the ability to use user-created source databases, and updates to GADRAS's default source database. This document describes the enhancements that have been implemented in more detail. This effort was driven by needs from Oak Ridge National Laboratory (ORNL) in their efforts to generate synthetic spectra for burnup samples using output from Oak Ridge Isotope Generator (ORIGEN) as the input for GADRAS.

# 2. CREATING SPECTRA WITH UNLIMITED SOURCES

Before GADRAS 18.8, the source term for a synthetic spectrum was limited to a 256-character string. To generate a spectrum with more source terms, users would have to generate GAM files that incorporate 10-15 source nuclides each, then create a GAM file that concatenated all the generated GAM files. This method is tedious and subject to user errors, especially when creating a spectrum from a source that contains over 400 nuclides. As an alternative, a new method for generating the spectrum was created which allows for an unlimited number of source nuclides.

Instead of using a string to transfer the source term information, GADRAS can now accept a list of objects through memory transfer that contains all the necessary source information for each nuclide. The list does not have a size limit and is passed programmatically through the GADRAS Application Programming Interface (API). The source object defines the source name, shielding layers, activity, age, and 3D effects (translation and rotation). There is both a C# API function and a C API function exposed to the user. Both the C# and C API functionality can be used with the released version of GADRAS 18.8 in Windows. A version of the C API can be used with Linux operating systems. If the Linux API is needed, contact the development team at GADRAS@sandia.gov for more information.

Users can create a full-information source object or a minimal-information source object. The members of each source type are described in Figure 1, as well as how to specify shielding.

| | |
|---|---|
| struct Source | |
| char* Name | name of nuclide being plotted (e.g. Cs137) (eventually will also take calibration source, gam file, or 3dm file) |
| int ShieldCount | number of shield layers attenuating source (can be 0) |
| struct Shield* Shields | pointer to array of shield layers (NULL if ShieldCount is 0) – the Shield struct is described below |
| float Activity | activity of nuclide in Ci |
| int AgeSpecifiedFlag | 1 if age is specified, 0 if age is determined by RadionuclideList.txt file located in main GADRAS folder |
| float Age | age of source in years (only applies if AgeSpecifiedFlag is turned on) |
| | |
| struct FullSource | |
| char* OriginalString | unused variable - used to store original string passed by GADRAS GUI to backend |
| char* FormattedString | unused variable - used to store formatted source string passed to GADRAS GUI from backend |
| char* SourceName | name of nuclide being plotted (e.g. Cs137) (eventually will also take calibration source, gam file, or 3dm file) |
| int ShieldLayerCount | number of shield layers attenuating source (can be 0) |
| struct Shield* ShieldLayers | pointer to array of shield layers (NULL if ShieldCount is 0) |
| int ActivitySpecifiedFlag | 1 if activity is specified in Activity field, 0 if not |
| int CalibrationSourceFlag | unimplemented - 1 if source is calibration source (e.g. 137CS_1351202), SerialNumber must be populated, activity cannot be specified; 0 if not calibration source |
| int AgeSpecifiedFlag | 1 if age is specified, 0 if age is determined by RadionuclideList.txt file located in main GADRAS folder |
| int AtomicNumber | unused variable - parsed and populated from SourceName |
| int MassNumber | unused variable - parsed and populated from SourceName |
| int IsomerNumber | unused variable - parsed and populated from SourceName |
| char* SerialNumber | unimplemented - string containing calibratino source serial number (CalibrationSourceFlag must be turned on to use this field) |
| double Activity | activity of nuclide in Ci |
| int ActivityUnitsEnum | unimplemented - enumeration specifying units of activity |
| double X | horizontal displacement in cm of source relative to dead-center (positive is left from detector line-of-sight) |
| double Y | vertical displacement in cm of source relative to dead-center (positive is up from detector line-of-sight) |
| double Z | displacement in cm of source relative to specified detector distance (positive is away from detector) |
| double Theta | rotation of source in degrees about x-axis (only applies to 1dm and 3dm sources) |
| double Phi | rotation of source in degrees about y-axis (only applies to 1dm and 3dm sources) |
| double Psi | rotation of source in degrees about z-axis (only applies to 1dm and 3dm sources) |
| double SourceRangeStart | For moving sources (currently only used for areal surveys), where it starts relative to 0 in cm (usually negative) |
| double SourceRangeEnd | For moving sources (currently only used for areal surveys), where it ends relative to 0 in cm (usually positive) |
| double Age | Age of source in years (only applies if AgeSpecifiedFlag is turned on) |
| | |
| struct Shield | |
| double AN | average atomic number of shield (weighted by AD) |
| double AD | aerial density of shield (g/cm^2) |
| double AH | fraction of AD that is hydrogen (scattering cross sections are heavily skewed by hydrogen) |

**Figure 1. Members of each source type, as well as how to specify shielding.**

# 3. USER-DEFINED SOURCE DATABASE

There are many sources of radiation decay information. The source decay database distributed with GADRAS is based on ENSDF5 and has been modified to align with benchmark measurements that the GADRAS development team has observed. In previous versions, the only way users could modify the source database was to directly modify the xml file. This modification method is both time-consuming and prone to user errors. It also did not allow users to override any x-ray information. Users can now create a custom database that GADRAS can use. If GADRAS cannot find the decay information it is looking for in the custom database, it will use its default database to find the desired information.

Users can override the following information in the database:

- Nuclide information including:
    - Average atomic mass of a nuclide (used to generate the specific activity)
    - Half-life of a nuclide
    - Add metastable states
    - Add nuclides not in the default GADRAS database
        - Note: if users want to add a transition that includes a parent or daughter nuclide that is not included in the default database with a <nuclide> tag, users must include it in the user-defined database
- Transition information including
    - Branching ratio – the probability of a given parent decaying to the specified daughter
    - Add new transition
        - Note: if nuclides are introduced in the new transition as a parent or daughter that are not included in a <nuclide> tag in the database, the nuclide needs to be added
    - Particles emitted in a transition including:
        - Alpha
            - Energy
            - Intensity
            - Hindrance

- Beta / positron / electron capture
    - Energy
    - Intensity
    - Forbiddenness
    - Log ft. values
- Gamma
    - Energy
    - Intensity
    - Coincident Gamma information
        - Energy
        - Intensity of coincident gamma (provided that first gamma is emitted)
- X-Ray
    - Energy
    - Intensity

To create a custom database, users should create a new xml file called "sandia.decay.user.xml". The format should begin with the following tag/attribute: <document xmlns="sandia.decay.xsd">

The following excerpt, Figure 2, is an example of how to override the transition from B-12 to C-12:

```
  <transition branchRatio="1" child="C12" mode="b-"
parent="B12">
    <beta energy="3069.30" intensity="8.0000E-04"
logFT="4.200" />
    <beta energy="5715.00" intensity="1.5000E-02"
logFT="4.130" />
    <beta energy="8930.39" intensity="1.2300E-02"
logFT="5.126" />
    <beta energy="13369.30" intensity="9.7220E-01"
logFT="4.066" />
    <gamma energy="4438.0" intensity="0.0123" />
    <xray energy="0.277" intensity="5.4518e-12" />
  </transition>
```

**Figure 2. Example of how to override the transition from B-12 to C-12.**

By creating a custom database in the specified format, users can take any source database and use it with GADRAS. Future plans include creating an API function to create a custom decay database, allow users to select from multiple custom databases, and creating a GUI to compare different decay databases.

# 4. GADRAS DEFAULT DATABASE CORRECTIONS

When the current GADRAS decay database was created, there were some errors that had not been corrected up to version 18.8. The main errors are the decay branching ratios when metastable nuclide states are involved. If a nuclide decays to both a daughter's ground state and an excited metastable state, the GADRAS database stated that the nuclide decayed to the metastable state 100% of the time. Many of these errors have been manually corrected in previous databases, but many nuclides (including many fission products) were not corrected. The error in the database parser has been found and corrected, and a new GADRAS database was created and is included in version 18.8.

Another deficiency was the lack of coincident gamma information. This information is important when the detector measuring the sample encompasses a high solid angle around the source and the source emits a significant number of cascading gammas. Many coincident gammas were included manually in the decay database, but many coincidences important in analyzing fission products were not included. All coincident gammas that would influence typical measurements have been incorporated into the new default decay database. An example of a transition that includes a coincident gamma is shown in Figure 3 below:

```
    <transition parent="Co60" child="Ni60" mode="b-"
branchRatio="1">
    <beta energy="317.88" intensity="0.9988"
logFT="7.512"/>
    <beta energy="1492" intensity="0.0012" logFT="14.7"
forbiddenness="2u"/>
    <gamma energy="347.14" intensity="7.5E-05"/>
    <gamma energy="826.1" intensity="7.6E-05"/>
    <gamma energy="1173.228" intensity="0.9985"/>
    <gamma energy="1332.492" intensity="0.999826">
      <coincidentgamma energy="1173.228"
intensity="1.0"/>
    </gamma>
    <gamma energy="2158.57" intensity="1.2E-05"/>
    <gamma energy="2505.692" intensity="2E-08"/>
  </transition>
```

**Figure 3. Example of a transition that includes a coincident gamma.**

# 5. CONCLUSION

GADRAS version 18.8 has been updated to allow users greater flexibility when creating synthetic spectra from many nuclides. Users can now specify an unlimited number of nuclides through an API function in both C and C# to create a synthetic spectrum. Users can also create a custom source database that GADRAS will use when generating synthetic spectra. The default source database in GADRAS has been corrected for metastable branching ratios and significant coincident gamma information has been incorporated.

## REFERENCES

1. D. J. Mitchell, "Gamma Detector Response and Analysis Software (GADRAS)," Sandia National Laboratories, SAND88-2519, 1988.

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