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AN OVERVIEW OF THE QADS CODE

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ABSTRACT

QADS is a module that performs multidimensional point-kernel estimation of gamma transport through practically any type of shielding material via a simplified input scheme that follows the general input philosophy of the SCALE shielding sequences SAS1, SAS2, and SAS4. This paper presents a general overview of the theory and input requirements for QADS.

1. INTRODUCTION

QADS is a module that performs multidimensional point-kernel estimation of gamma transport through practically any type of shielding materials using a simplified input scheme that follows the general input philosophy of the SCALE [1] shielding sequences, SAS1, SAS2, etc. Conceptually, QADS was designed to capture the flexibility and power of the QAD technique [2] for problems amenable to point kernel solution while allowing for an efficient and user-friendly input interface. Functionally, the QADS module is called via the SCALE driver and first reads the free-form input values and then preprocesses the actual input for the QAD-CGGP code.[2] The driver then calls and executes QAD-CGGP automatically. For this version of QADS, QAD-CGGP was unchanged from the publicly distributed version to allow future updates of the QAD-CGGP code to be easily implemented into QADS. The SCALE standard composition library is used to allow simplified input of materials. The problem geometry is coded using the well-known MORSE combinatorial geometry package. Finally, the dose portion of the input follows similarly the XSDOSE input data in module SAS1 [1]. The combined use of the SCALE standard compositions and free-form input with the multidimensional geometry capabilities and generally short running time of point kernel techniques produces a very powerful procedure for shielding analysis of a wide variety of problems.

2. POINT-KERNEL DOSE ESTIMATION THEORY

2.1 POINT-KERNEL THEORY

Point-kernel techniques have been widely used in gamma-ray radiation shielding analyses through the years and the methods are well known. However, for completeness the discussion of the method in ref. 2 is repeated herein. For gamma-ray calculations the QADS module uses the point-kernel ray-tracing technique. In this method, the point kernel representing the transfer of energy by the uncollided flux along a line-of-sight path is combined with an appropriate buildup factor to account for the contribution from the scattered photons. With a distributed source, the point kernel is integrated over the source volume for each source energy considered. Expressed as an equation, the gamma-ray dose rate at any point due to an anisotropic source emitting s photons of energy E per second per unit volume is

$$D(\bar{r}) = \frac{K\int_v s(\bar{r}')B(\mu|\bar{r}-\bar{r}'|,E)\exp(-\mu|\bar{r}-\bar{r}'|)dv}{4\pi|\bar{r}-\bar{r}'|^2} \qquad (1)$$

where

$\bar{r}$ = point at which gamma dose rate is to be calculated,

$\bar{r}'$ = location of source in volume v,

v = volume of source region,

μ = total attenuation coefficient at energy E,

$|\bar{r}-\bar{r}'|$ = distance between source point and point at which gamma intensity is to be calculated,

K = flux-to-dose conversion factor.

2.2 BUILDUP FACTOR OPTIONS

Two buildup factor options are available in the QADS module. The first option is the use of the original QAD-P5A code [2] values based on the Goldstein and Wilkins moments method calculations for gamma-ray transporting infinite homogeneous media. This method uses Capo's fit to the Goldstein-Wilkins data with bivariant polynomial expressions to calculate the appropriate buildup factors as a function of the gamma-ray energy and the number of mean free paths (mfp) from the source to the detector. For high atomic number materials, the polynomial fit has the form

$$B(\mu|\bar{r}-\bar{r}'|,E) = \sum_{j=0}^{4}\sum_{i=0}^{3} C^{ij}(\mu|\bar{r}-\bar{r}'|)^i(E)^j , \tag{2a}$$

and for low atomic number materials it has the form

$$B(\mu|\bar{r}-\bar{r}'|,E) = \sum_{j=0}^{4}\sum_{i=0}^{3} C^{ij}(\mu|\bar{r}-\bar{r}'|)^i\left(\frac{1}{E}\right)^j , \tag{2b}$$

where the C^{ij}s are the coefficients of the expansion.

The second buildup factor method that can be selected is the geometrical progression approximation (GP method).[3] This method has recently received a lot of attention and appears to more closely reproduce more exact calculations than other methods. The buildup factors are approximated by the equations

$$\begin{aligned} B(X,E) &= 1 + (b-1)\frac{K^X-1}{K-1} \qquad (K \neq 1); \\ &= 1 + (b-1)X \qquad (K = 1); \end{aligned} \tag{3a}$$

$$K(X) = cX^a + d\cdot\frac{\tanh(X/X_k-2)-\tanh(-2)}{1-\tanh(-2)} ; \tag{3b}$$

where X is the source-detector distance in mfps of the medium, b is the value of the buildup factor at 1 mfp, and K represents the photon dose multiplication per mfp penetration. The parameters a, c, d, and X_k are fitting parameters and are allowed to vary with energy. A differing form of Eq. (3b) is used for penetrations greater than 40 mfp.

3. INPUT SPECIFICATIONS

3.1 INPUT OVERVIEW

The QADS module input can be broken into the following areas: (1) material component specification, (2) source specification, (3) problem geometry, and (4) selection of built-in data and detector options. A brief description of each input group follows.

3.1.1 Material Component Specification

The selection of the constituent material compositions is straightforward since the SCALE standard composition library and material input processor are utilized by QADS. Therefore the input specifications for QADS materials should be unchanged from those of the standard SCALE sequences. Unlike the SCALE shielding sequences, the QADS module does not call the BONAMI and NITAWL modules (see Sects. F2 and F3 of the SCALE manual) since the data in QADS are fixed and do not require any resonance processing.

3.1.2 Source Specification

The specification of a source in QADS allows for a great deal of flexibility to handle a large number of source situations ranging from a flat source to one that has a somewhat arbitrary shape in any of the three directions. The input is such that the description of most source situations is straightforward; however, as the source complexity increases so does the detail necessary to describe the given situation. This section is designed to give the user sufficient understanding to describe practically any given source configuration. The source description internal to the code includes an overall normalization, a spatial mesh and corresponding spatial distribution by mesh point, an energy structure and corresponding energy spectral shape, and a specified coordinate system. The source description can use a Cartesian, cylindrical, or a spherical coordinate system; however, the Cartesian system is recommended if the source is off-centered or if there are multiple sources. The technique utilized for off-centered or multiple sources is to describe one source geometry that encloses the origin and all sources, then selectively zero-out nonsource regions by use of zero weights [see Eq. (5).]

The use of keywords in the source geometry and shape, and defaults in the source mesh points, energy group structure, and in some cases the source spectrum, greatly simplifies the typical source description and will suffice for many practical applications. The source shape description for a flat (keyword FLATS) or a cosine (keyword COSIN) shape are handled internally by the following equation for the point variation in the source:

$$P(a,b,c) = \cos\{xiso(1,1)[a - xiso(2,1)]\} * \cos\{xiso(1,2)[b - xiso(2,2)]\} * \cos\{xiso(1,3)[c - xiso(2,3)]\}; \quad (4)$$

where a, b, and c are the coordinates of the point in the appropriate coordinate systems, and the *xiso* values are either calculated internally by the code or input by the user. For the FLATS and COSIN options the values of *xiso* are computed internally (e.g., all *xiso* values are zero for the flat option). For the COSIN options the values of *xiso* are computed such that the power or source strength peak occurs at the midplane and is equal to zero at the external boundary. Only for the Cartesian coordinates are COSIN specifications allowed in all three directions. As an option, the QADS module allows the user to input a unique set of *xiso* values.

The final option for specifying the source shape is to input the relative shape by mesh point along each axis. This option assumes separability in each of the three directions and the user inputs the power or source shape independently along each axis. The relative magnitudes of each different axis are not important since the code normalizes to the input value ASO. The overall normalization is performed (for cylindrical geometry) by using the input shapes P(r), P(z), and P(θ), to calculate the weights F_r, F_z, and F_θ:

$$F_l = \int_{r_l}^{r_{l+1}} rP(r)dr;$$
$$F_m = \int_{z_m}^{z_{m+1}} P(z)dz; \qquad (5)$$
$$F_n = \int_{\theta_n}^{\theta_{n+1}} P(\theta)d\theta.$$

The F_n value is primed to allow overall normalization to be performed as follows:

$$A = \frac{ASO}{\left(\sum_{l=1}^{L} F_l\right)\left(\sum_{m=1}^{M} F_m\right)\left(\sum_{n=1}^{N} F_n'\right)}; \qquad (6)$$
$$F_n = A\, F_n'.$$

Thus, the total power and the input value ASO can be equated.

$$P = ASO = \left(\sum_{l=1}^{L} F_l\right)\left(\sum_{m=1}^{M} F_m\right)\left(\sum_{n=1}^{N} F_n\right), \qquad (7)$$

and the power at any point is given by

$$P_{lmn} = F_l F_m F_n. \qquad (8)$$

In this manner the correct normalization is given regardless of the relative magnitudes of the individual coordinates.

3.1.3 Problem Geometry Specification

The problem geometry input uses the MORSE combinatorial geometry description. The input includes first a description of each body, where the nine different body types are defined in ref. 4. The user then defines the corresponding combination of bodies for each zone and, finally, the mixtures numbers for each zone. The input geometry description should be obvious to MORSE combinatorial geometry users; for those unfamiliar with MORSE geometry input the user is referred to Sect. F9 in the SCALE manual (ref. 1).

3.1.4 Built-In Database Description

QADS contains a large database of built-in quantities, which simplifies the user input for most problems of interest. This built-in data consists of (1) buildup factors for both the standard and GP techniques; (2) dose factors that can be user input, read from a SCALE library or internally computed using the ANSI-standard description [5]; and (3) mass attenuation coefficients for any element.

3.2 INPUT DESCRIPTION

The user input to QADS is designed to be very similar to other SCALE sequences. Thus, with minimal effort a problem set up for another sequence can be rerun using the QADS sequence. Also, a user who is familiar with SCALE input and execution should have little problem becoming

proficient in the operation of QADS. The following is a condensed input description for QADS (for a complete description see ref. 4).

3.2.1 Sequence Specifier

When installed under the SCALE driver, QADS is invoked by the use of the sequence specifier "=QADS" and corresponding data shown in Table I. For stand-alone versions of the code, the sequence specifier is not necessary. The input sections following the sequence specifier consist of a title; cross-section library name; calculation type; standard composition data; QADS source specification; QADS problem geometry specification; QADS dose and detector specifications; and, finally, a QADS input terminator.

3.2.2 Title Card

The sequence specifier card is followed by an 80-character title card. Any descriptive title containing 80 or fewer characters is allowed.

3.2.3 Cross-Section Library Name

The input value for the cross-section library name has four options: 27N-18COUPLE, 22N-18COUPLE, ORIGENGP-SRC, and READINGP-SRC. The first two options specify that the problem group structure will be read from the corresponding SCALE library, while the input source spectrum will be read in the job input stream. Note that the cross sections on the SCALE library are not used, since QADS has built-in attenuation coefficients. The third option, ORIGENGP-SRC, signals the code to read both the problem group structure and the source spectrum and magnitude from the ORIGEN-S output saved on disk. This is a useful option for coupling ORIGEN-S source calculations and QADS shielding calculations. The final option, READINGP-SRC, directs the code to read both the problem group structure and source spectrum from the job input stream. While more cumbersome in preparing the input, this option provides flexibility in that any group structure can be used and it gives QADS the option of easily specifying gamma line sources. This is accomplished by specifying narrow energy bins with the mid-point energy equal to the gamma line source energy.

3.2.4 Calculation Type

The next input value, the calculational type, is included simply to minimize changes to existing decks that have been used in other SCALE sequences. The only value that is acceptable for this input is INFHOMMEDIUM. QADS does not perform any resonance processing on the cross sections since it uses built-in attenuation coefficients.

3.2.5 Standard Composition Data

The QADS standard composition data input is exactly like that of the standard SCALE input; thus, problem input descriptions should be easily transported from other applications to QADS. For more detailed explanations of each input value see the description given in the SCALE manual (Sect. M7.4, ref. 1 or ref. 4).

3.2.6 QADS Source Specification

A description of the QADS source specification input follows and is summarized in Table II. Following selection of the appropriate source geometry, the user enters the source strength, normally in units of photons/s. This is the value ASO discussed in Sect. 3.1.2. For the ORIGENGP-SRC option this value should be entered as zero, since the overall normalization is read directly from the ORIGEN-S output (see Sect. F7 of the SCALE manual). If a number other than zero is entered, the value from ORIGEN-S is discarded and the new value is used as the normalization. The use of eight different keyword inputs describes the spatial shape of the source within the defined source body. The first six options give a simple definition of the spatial variation of the source and no further information is needed to describe this variation. If either XISOS or WEIGHTS are specified, then a more detailed description of the spatial shape of the source is given in the More Data array parameters, XIS or WAT, respectively. Specifying XISOS directs the code to read the six values of XIS [*xiso* values of Eq. (4)] in the following order:

$$XIS=XIS(1,1),XIS(2,1),XIS(1,2),XIS(2,2),XIS(1,3),XIS(2,3).$$

If the user specifies WEIGHTS, then the relative shapes for each mesh point for each coordinate axis should follow the WAT=keyword in the More Data array. The order of weights by axis is R, Z, θ for cylindrical; X, Z, Y for Cartesian; and ρ, θ, ψ for spherical. The optional fields of group structure and particle spectrum are read in next; the option is determined by the value of the cross-section library name specified previously. The group structure array is read in only if the cross-section library input value READINGP-SRC is specified. Similarly, the particle spectrum array is read in only if the cross-section library input value is specified as either READINGP-SRC or one of the SCALE libraries (27N-18COUPLE or 22N-18COUPLE).

The More Data array contains seven different keywords that in many instances will not have to be changed from their default values; however, using the keyword options increases the module's flexibility. This is easily illustrated by the first keyword, NZS. The value of NZS defaults to 1 and describes the body number corresponding to the source body. In many instances, the source will be the central body in the problem description and a common convention is to number the innermost body as 1. However, in some instances the source may incorporate several boundaries and simply specifying the body number for the outermost body will effectively spread the source out over all intermediate boundaries. This is an important parameter since the source mesh is generated from the body data corresponding to the body number specified. The procedure used internally is to determine, based on the data for the specified body number, the innermost and outermost dimensions of the source body and then construct the mesh based on the specified number of equally spaced meshes (determined by the MSH= parameter). If MSH=0, then the number of mesh intervals is set to 30 for the R, X, Y, Z, and ρ axes and 20 for the θ and ψ axes. These values can be changed by specifying MSH= and entering the new number of mesh intervals for each of the three coordinate axes in the same order as previously given for the weights. Should changes from the defaults be attempted, care should be exercised in the selection of an appropriate number of mesh cells. Since the source representation is completely described by the source mesh, the mesh should be fine enough to adequately model the source body. This is particularly important for surface or near-surface doses where errors can occur if the mesh size is larger than the surface-to-detector distance. Alternately, if the value of MSH is entered as a negative number, the actual mesh can then be entered immediately after each MSH value has been input (e.g., MSH= -15, then enter 16 R mesh values; -10, enter 11 Z mesh values; -5, enter 6 θ mesh values). This will allow for special situations when the intermediate boundaries, not just the endpoints, need to be specified.

The NSO and NPS parameters give the ORIGEN-S unit number and source position for the ORIGEN-S data saved to disk in an earlier run. Only in a few instances should values other than the defaults have to be entered. The XIS and WAT parameters allow the user to enter their own set of source shapes. The last optional parameter is INU. Specifying INU greater than 0 allows the user to perform a neutron calculation. This document assumes that a gamma only calculation is the intent of most users and further information on the neutron capabilities is given in the original QAD document [2].

3.2.7 QADS Problem Geometry Specification

Tables 4 and 5 of ref. 4 outline the user input for the QADS problem geometry input. This input is very similar to that of the MORSE-SGC. See Sect. F9 in the SCALE manual for more detailed information.

3.2.8 QADS Dose and Detector Specification

The description of the final input section, QADS detector and buildup factor specification, is given in Table III. This section consists of buildup factor selection followed by two optional inputs: the number and type of flux-to-dose conversion factors and the number and position of detectors for the problem. The first 8 options for the buildup factors given in Table III correspond to the standard buildup factors [Eq. (2)], while the 43 additional options are available corresponding to the GP buildup factor data [Eq. (3)]. For the standard buildup factor data, the DOSE keyword indicates that the buildup factors are for an air exposure response with penetration through the given material and the ENG keyword indicates a response of the energy absorbed in the material itself. Similarly for the GP buildup factor data, the ABS keyword indicates a response of the energy absorbed in the material, while the keyword EXP indicates the air exposure response with penetration through the given material.

The next input parameter is NFACTR, which specifies the number and/or type of flux-to-dose conversion factors. For all but a very few cases, the default value is sufficient. If the default value is used, ANSI-standard dose factors are either read from the SCALE library or calculated internally. The user can optionally specify other dose IDs from the SCALE library if that option is being utilized in the problem. Lastly, the user can input dose response values by specifying a number between 0 and 9000. This allows NFACTR sets of conversion factor sets to be read from the job input stream. The default for the number of detectors is four, NDETEC=0, and the detectors are located at 0, 1, 2, and 4 m from the outermost edge of the outermost nonvoid cylinder along the midplane of the cylinder. This default option is valid only for cylindrical source geometries. For other geometries and/or other detector locations the user enters the number of detectors desired, NDETEC=number of detectors, followed by the location of each detector. The default detector geometry is cylindrical and need not be entered unless the user desires another geometry for the detector.

3.2.9 Terminate QADS Sequence

An END card should be included to terminate the user input to QADS. No built-in mechanisms for stacking several cases within a QADS sequence exist. The use of the SCALE driver provides such an option since additional cases can be stacked by simply respecifying the entire QADS sequence input following the END card (i.e., including an =QADS as the card following the END card).

4. SAMPLE PROBLEMS

QADS was developed largely to provide a simplified input scheme to expedite shielding analyses of spent fuel shipping casks. Of course, many other applications are well suited for analysis using the QADS module. The two sample problems and their corresponding outputs given in ref. 4 are examples of how QADS could be used in shipping cask analysis. The examples were designed to use as many options as possible, in some cases more than are actually necessary, to give the user insight into how the particular options can be best utilized.

5. SUMMARY

The QADS module as described herein allows the user to utilize the point kernel technique as implemented in the QAD-CGGP code in an efficient, user-friendly manner. The built-in attenuation and build-up data for a wide range of materials, combined with the automatic generation of flux-to-dose conversion factors and source mesh descriptions make the QADS package extremely flexible.

5. REFERENCES

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(2) "QAD-CGGP: A Combinatorial Geometry Version of QAD-P5A, A Point Kernel Code System for Neutron and Gamma-Ray Shielding Calculations Using the GP Buildup Factor," available from Radiation Shielding Information Center at Oak Ridge National Laboratory as CCC-493/QAD-CGGP.

(3) Harima, Y., Sakamoto, Y., Tanaka, S., and Kawai, M., "Validity of the Geometrical Progression Formula in Approximating Gamma-Ray Buildup Factors," Nucl. Sci. Eng. 94, 24-35 (September 1986).

(4) Broadhead, B. L., "QADS: A Multidimensional Point Kernel Analysis Module," NUREG/CR-5468, ORNL/CSD/TM-270, U.S. Nuclear Regulatory Commission (May 1990).

(5) "Neutron and Gamma-Ray Flux-to-Dose-Rate Factors," ANSI/ANS-6.1.1-1977, American Nuclear Society (1977).

Table I. Outline of material information processor data for QADS

Data position	Type of data	Data entry	Comments
1	Sequence specifier	=QADS	Begin in column 1. PARM=CHK beginning in column 11 checks the input for errors
2	Title	Enter a title	80 characters
3	Cross-section library name	27N-18COUPLF 22N-18COUPLE ORIGENGP-SRC READINGP-SRC	These keywords are used to select the problem group structure only. QADS has built-in cross sections
4	Calculation type	INFHOMMEDIUM	This is only valid option for QADS calculation
5	Standard composition data	Enter the appropriate data	Terminate this data block with END COMP
6	QADS source specification	Enter the appropriate data	End this data block with END SOURCE. See Table II for more information
7	QADS problem geometry specification	Enter the combinatorial geometry data	End this data block with END GEOM
8	QADS dose and detector specification	Enter the appropriate data	Terminate this block with an END DOSE card. See Table III for explanation of input
9	Terminate QADS sequence	END	Must begin in column 1

Table II. Input data description for QADS source specification

Data position	Type of data	Data entry	Comments
1	Source geometry	CYLINDRICAL CARTESIAN SPHERICAL	Select the appropriate source geometry
2	Source strength	Enter the appropriate data	Enter the number of source particles/s. Enter 0 for source read from ORIGEN-S
3	Source shape	FLATS COSINX COSINY COSINZ COSINR COSINRHO XISOS WEIGHTS	Terminate with an END card
4	Group structure (optional)	Enter number of groups, then group bounds (high-to-low in eV)	Input only if READING-SRC is specified
5	Particle spectrum (optional)	Enter value for each group	Input only if READINGP-SRC or SCALE library is specified
6	More Data array (optional)	NZS= INU= NSO= NPS= XIS= MSH= WAT=	[1] - body # for source [0] - neutron calculation if > 0 [71] - ORIGEN-S unit number [0] - source position number, 0=last [0] - xiso values (6 values) [0] - number of mesh intervals[a] (values for each coordinate direction) [0] - weights read in[a]
7	End source array	END SOURCE	Terminate source input

[a]The mesh intervals and weights for each axis are input in the following order: Cartesian (X,Z,Y), cylindrical (R,Z,θ), and spherical (ρ,θ,ψ).

Table III. Input data description for QADS detector specification

Data position	Type of data	Data entry	Comments
1	Buildup factors	WATE DOSE or ENG ALUM ENG IRON DOSE or ENG LEAD DOSE or ENG CONC DOSE	These buildup factors correspond to the standard exponential buildup factor data. For GP values see Table 7 of ref. 4
2	Number/type flux-to-dose conversion factor (optional)	NFACTR=[0] NFACTR > 9000 0 < NFACTR < 9000 END	Use ANSI-Standard Dose Use ID from SCALE Read NFACTR responses from input[a] Terminate with END
3	Number of detectors (optional)	NDETEC = [0]	Defaults of 0, 1, 2, 4 m from midplane (valid only for CYLINDRICAL source)
4	Detector data (NDETEC ≠ 0)	RRC ZRC PHIRC NRCOP for each detector	R, X, or ρ value Z, Z, or θ value θ, Y, or ψ value CYLINDRICAL CARTESIAN SPHERICAL (defaults to source geometry)
5	Terminate input	END DOSE	Terminate dose input

[a]NFACTR for values between 0 and 9000 is the number of response sets, not the total number of values entered. After the value of NFACTR is entered, response values are entered by group for each of the NFACTR responses.