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INTERNAL DOSIMETRY VERIFICATION AND VALIDATION DATABASE

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Simulated-data internal dosimetry cases for use in intercomparison exercises or as a software verification and validation tool have been published on the internet (www.lanl.gov/bayesian/software Bayesian software package II). A user may validate their internal dosimetry code or method using this simulated bioassay data. Or, the user may choose to try out the Los Alamos National Laboratory codes ID and UF, which are also supplied. A Poisson–lognormal model of data uncertainty is assumed. A collection of different possible models for each nuclide (e.g. solubility types and particle sizes) are used. For example, for ^{238}Pu, 14 different biokinetic models or types (8 inhalation, 4 wound and 2 ingestion) are assumed. Simulated data are generated for all the assumed biokinetic models, both for incidents, where the time of intake is known, and for non-incidents, where it is not. For the dose calculations, the route of intake, but not the biokinetic model, is considered to be known. The object is to correctly calculate the known true dose from simulated data covering a period of time. A 'correct' result has been defined in two ways: (1) that the credible limits of the calculated dose include the correct dose and (2) that the calculated dose is within a factor of 2 of the correct dose.

INTRODUCTION

The IDEAS 2005[1] project and predecessor intercomparison exercises had as their goal the harmonisation of internal dosimetry methods, through cross-checking and discussion by participants of results obtained for a given set of test cases. To this end also we have web-published the verification and validation (VV) test cases used for the internal dosimetry programme at Los Alamos National Laboratory (LANL)[2] for the nuclides ^{3}H, ^{234}U and ^{238}Pu. Etherinton *et al.*[3] discuss something similar in principle to what is done here (the HPA method), where simulated data are used to test a particular internal dosimetry algorithm. The advantages of these types of tests are that all aspects of the correct answer are known, which allows detailed checking of the mathematical calculation. Of course, scientific questions remain about possible biokinetic behaviours outside of the imagined scope of possibilities.

A Poisson–lognormal model of data uncertainty is assumed[4,5] in order to simulate as accurately as possible the actual measurement process. As discussed in Doerfel *et al.*[6], two sources of uncertainty can be identified: type-A or measurement uncertainty, which is related to the Poisson uncertainty of the counting measurement, and type-B or normalisation uncertainty, which is related to uncertainty or variability of the normalisation factor applied to the measured net counts to obtain the quantity of interest (e.g. excretion rate). There is experimental evidence, e.g. Moss *et al.*[7], that normalisation factors are described by lognormal distributions, and this is a standard assumption (e.g. it is the basis of the lognormal model discussed in Doerfel *et al.*[6]).

METHOD

A collection of different possible models for each nuclide (e.g. solubility types and particle sizes) are used. In Bayesian terminology, the collection of biokinetic models used to generate the data constitutes a 'biokinetic prior'. The situation described here is favourable for a Bayesian interpretation of the data, i.e. the same biokinetic prior is used to analyse the data as was used to generate the data, although this need not be the case.

For example, for ^{238}Pu, 14 different biokinetic models are assumed: 8 inhalation, 4 wound and 2 ingestion. The two ingestion models correspond to choosing the gut absorption factor f_1 as the recommended value for ICRP66-type S or M[8,9]. These models are denoted by the three-character symbols GIS and GIM. Six of the inhalation models are ICRP66-type M and S, with particle sizes (AMAD) of 1, 5 and 10 μm. These are denoted by three-character symbols such as IS0, for inhalation, type S, 10 μm AMAD, etc. The other two inhalation models and the wound models are defined in Table 1, using ICRP66[9] terminology.

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Table 1. LANL-specific biokinetic models.

Route of intake	Three-character symbol	LANL incident date	Nuclide	Comment
Inhalation	IEE	31 July 1971	^{238}Pu	'Wing-9' incident, $s_p = 1 \times 10^{-8}$ d^{-1} $s_{pt} = 1.8 \times 10^{-4}$ d^{-1} $s_t = 4 \times 10^{-3}$ d^{-1} $f_l = 1 \times 10^{-8}$ d^{-1} AMAD = 0.5 μm
Inhalation	ICD	16 March 2000		$s_p = 10$ d^{-1} $s_{pt} = 90$ d^{-1} $s_t = 5 \times 10^{-4}$ d^{-1} $f_l = 1 \times 10^{-4}$ d^{-1} AMAD = 0.8 μm
Wound	WIN			Immediate injection
Wound	WND			Durbin wound model: 67% 500 d 33% 7 d
Wound	WTA	14 March 1989	^{239}Pu	Wound with excision: 80% 1000 d 20% 60 d
Wound	WDT	24 August 1994	^{239}Pu	Wound with excision: 70% 20 d 30% 0.5 d

Simulated data are generated for all the assumed biokinetic types, both for incidents where the time of intake is known and for non-incidents where it is not. For the dose calculations, the route of intake, but not the biokinetic model, is considered to be known. The object is to correctly calculate the known true dose from simulated data covering a period of time. A 'correct' result has been defined in two ways (other definitions could be used): (1) that the credible limits of the calculated dose include the correct dose, and (2) that the calculated dose is within a factor of 2 of the correct dose. Credible limits are the Bayesian nomenclature for the interval of the quantity of interest such that the probability is some specified small amount (usually 5%) that the quantity is less than the lower limit or greater than the upper limit. For a general discussion of Bayesian terminology, see Miller *et al.*[10].

There are two types of errors that need to be checked, false negatives and false positives[10]. The false-negative database, which is discussed here, contains simulated data from intakes producing the smallest $E(50)$ doses of regulatory interest in the USA. For plutonium and uranium, these are assumed to be 1 mSv for incident-related intakes and 5 mSv for non-incident-related intakes. A simple per cent-correct score can be given (% correct out of total number of cases). A false-positive database would contain a very large number of cases generated from zero true intake, a small fraction of which might be falsely interpreted as intakes. This database is not discussed further here.

As an example, consider a non-incident-related case for ^{238}Pu where the biokinetics are chosen to be IS5. The bioassay data to be generated consist of routine urine samples taken every 6 months over a total work history of 10 years (20 samples in all). In the interval between the first and second data points, a time of intake is generated from a uniform distribution. The intake amount corresponding to a 5 mSv $E(50)$ dose is calculated from the biokinetic model. Then using this intake amount and the time of intake, the urine excretion (the 'signal') is calculated for all data points. As explained in Miller[5], the measurement situation under consideration is a counting measurement that detects N gross counts coupled with a sample-blank background measurement that detects N_B background counts (in R counting periods). There is assumed to be an additional lognormally distributed background b in actual samples that does not show up in the sample blanks, e.g. the uranium environmental background often present in uranium urine bioassay samples. This background is assumed to be known from other measurements. The counts are assumed to have Poisson distributions

$$\begin{aligned} \text{gross counts} &= N \sim \text{Poisson}(\mu + \mu_B + \mu_b), \\ \text{background} &= N_B \sim \text{Poisson}(\mu_B), \end{aligned} \tag{1}$$

where μ is the mean number of counts from the decays of interest, and μ_B and μ_b are the mean numbers of counts from sample-blank background and real background. The quantity of interest ν (the

'signal', e.g. 24-h urine excretion rate) is assumed to be related to μ by a lognormally distributed normalisation factor F,

$$\nu = \mu F = \mu f_n f_m.$$

Uncertainty or variability of F is assumed to arise from two sources: (1) f_n, the basic normalisation uncertainty associated with the measurement type, assumed to have logarithmic standard deviation S_n (e.g. biological variability, sample collection variability) and (2) f_m, the normalisation uncertainty associated with the measurement itself, assumed to have logarithmic standard deviation S_m (e.g. uncorrected variability of radiochemical yield).

In this way, the counts and background counts are generated for each data point using the value of ν calculated from the intake, time of intake and biokinetic model. Sometimes, e.g. for ^{238}Pu and certain times after intake and certain biokinetic models, the gross counts are approximately equal to the background counts. Since in this study the true dose is always positive, if the calculated final determination of dose comes out to be zero, this would be an example of a false-negative error.

ORGANISATION OF THE SIMULATED DATA

The software contains the VV test cases for ^{238}Pu, ^{234}U and ^{3}H for the LANL internal dosimetry programme. In the spirit of harmonisation of worldwide internal dosimetry, these cases are made available for others to use with codes and methods of their choice. The user can make detailed comparisons of results using their method with both the known correct result and with those obtained using the LANL ID[11] and UF[12] codes, which are also supplied.

Each test case is in its individual subfolder. For example, the file/BayesII/calcdata/id/pu238/wrk/PIS0R3/bioassay.in contains the bioassay data for the case denoted by PIS0R3. The structure of the BIOASSAY.IN file is explained in the Windows help file ID.CHM.

The case labelling system is as follows, using the case PIS0R3 as an example.

- The first character 'P' denotes plutonium.
- The characters 'IS0' (inhalation, type S, 10 μm AMAD) denote a biokinetic model or type as explained in the help file /BayesII/progs/id/ID.CHM. The biokinetic types correspond to biokinetic interpolation table files in the folder/BayesII/dfs/pu238/icrp60.
- 'R' denotes a non-incident-related intake detected through routine bioassay, where the date of intake is unknown, rather than an intake associated with an incident (I), where the date of intake as well as some information about the magnitude of intake is known.
- '3' is a sequence number that indicates the random number seed and the data treatment (1–3 exact Poisson, 4–6 Gaussian approximation, 7–9 censored data, 1 4 7 have same seeds, etc).

For tritium (^{3}H), multiple intakes are generated using the alpha prior[13] with $\alpha = 1.9\ y^{-1}$ and $E(50)$ from $E_{min} = 0.5$ to $E_{max} = 50$ μSv. The number of intakes has a Poisson distribution with mean number $= \alpha \ln(E_{max}/E_{min}) = 8.7\ y^{-1}$. The label H13R03 means there are thirteen ('13') non-incident-related intakes, and '03' is a sequence number labelling the random number seed. Simulated and actual LANL ^{3}H data are shown in Figure 1.

For ^{234}U, the label UIM508 implies a single non-incident-related intake with biokinetic type 'IM5' (inhalation, type M, 5 μm AMAD), and '08' is a sequence number labelling the random number seed. There is a lognormally distributed environmental urine background, determined empirically from LANL data to have whole population median of

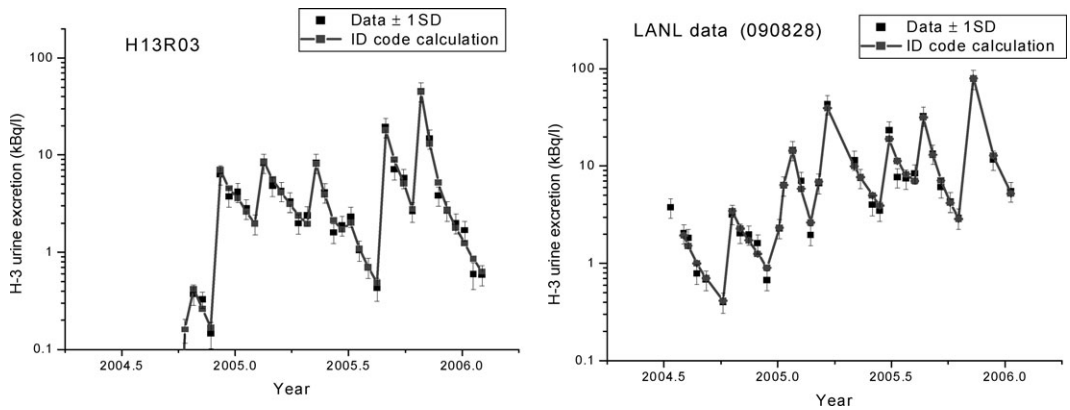

Figure 1. Simulated and actual LANL ^{3}H urine bioassay data.

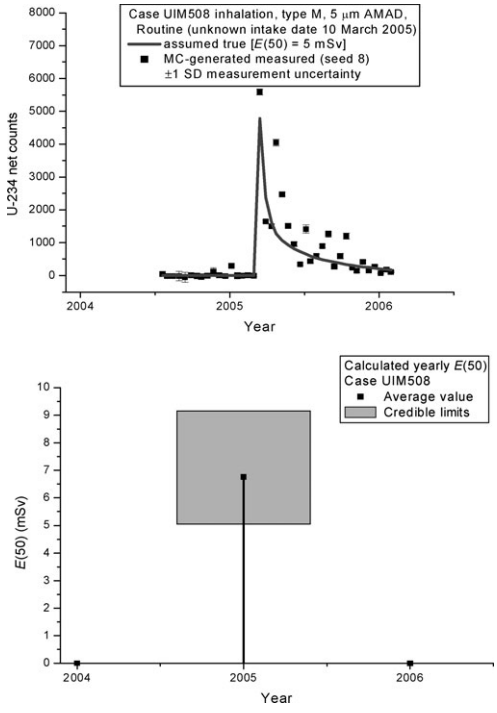

Figure 2. Simulated ^{234}U urine bioassay data and calculated yearly $E(50)$ using the ID code. This case is 'missed' with $E(50)$ credible limits not including the correct result of 5 mSv. Note the large numbers of net counts in the uranium case and the corresponding small measurement uncertainties represented by the error bars. The obvious scatter of the data in this case is caused by the environmental background.

3 mBq/d and lognormal standard deviation of $S = 1.3$ ($\sigma_g = 3.67$). Simulated ^{234}U data are shown in Figure 2.

SUMMARY OF RESULTS USING LOS ALAMOS CODES ID AND UF

A summary of results using the Los Alamos Codes ID and UF is shown in Table 2. The quantity $E(50)$ is the 50-year committed effective dose.

Table 2 illustrates some aspects of such a VV exercise using simulated data.

- Different data treatments are possible, and they yield different results. At one end of the spectrum considered is the use of actual measured count quantities that are used to calculate the exact Poisson–lognormal likelihood functions describing the data. Such a data treatment in practice depends on count quantities being provided by the analytical laboratory. Sometimes, only the result and measurement uncertainty standard deviation are provided. The Gaussian approximation of the likelihood function might be used in these cases, incorporating both measurement (type A) and estimated normalisation (type B) uncertainties into a single uncertainty quantity as described by Miller[5]. Alternatively, a lognormal model might be used as advocated by Doerfel *et al.*[6]; however, such a model will not accommodate small or negative data. With a lognormal model, data less than a few standard deviations positive are sometimes censored, meaning that such a measurement result is designated 'less than limit of detection' and no further information reported. The data treatment labelled 'censored' is essentially this approach.
- Whether or not an incident has occurred is important, and an incident-related internal dosimetry case is distinct from a non-incident case. When an incident has occurred, the time of intake is known and additional bioassay samples are collected. Since more information is available and there is only a single intake, intakes are generally easier to detect.
- The dose quantity needs to be defined. Total $E(50)$ for all years generally has smaller uncertainty than the $E(50)$ for any given year.
- The criterion defining 'correct' needs to be defined. Two reasonable but arbitrary choices are illustrated.
- Different algorithms, such as ID and UF, produce different results. The reason for having more than one algorithm is that one method (ID) is meant to be definitive, a straightforward evaluation of Bayes theorem using Markov Chain Monte Carlo without approximations, whereas the other method (UF) is a faster approximation using 1-D numerical integration and summation. For single-intake situations, the two methods are mathematically equivalent, even though numerically they are quite different. So, the comparisons serve as a check for the mathematical approximations and the numerical techniques.
- And, since these are complex computer algorithms, the use of different computation platforms needs to be checked. The desktop platform is a Windows workstation, whereas the supercomputer platform[14] is a Linux cluster.

Examples of ^{3}H-simulated and actual data are shown in Figure 1. Simulated ^{234}U and ^{238}Pu data are shown in Figures 2 and 3.

MISSED CASES

The cases that are outside of Bayesian credible limits ('missed', i.e. 10 of 93 cases) using most effective method (ID code, exact Poisson likelihood) are

Table 2. Summary of results.

Code	Nuclide	Incident/non-incident	Data treatment	Platform	Missed	Total	Score (%)	Quantity	Criterion
ID	^{3}H	Non-incident	Exact Poisson	Desktop	1	18	94.4	2005 *E*(50)	Within credible limits
		Non-incident	Exact Poisson	Supercomputer	1	18	94.4	2005 *E*(50)	Within credible limits
	^{234}U	Non-incident	Exact Poisson	Desktop	2	9	77.8	2005 *E*(50)	Within credible limits
		Non-incident	Exact Poisson	Supercomputer	2	9	77.8	2005 *E*(50)	Within credible limits
	^{238}Pu	Non-incident	Exact Poisson	Desktop	4	24	83.3	Total *E*(50)	Within credible limits
		Non-incident	Exact Poisson	Supercomputer	3	24	87.5	Total *E*(50)	Within credible limits
		Non-incident	Gaussian	Desktop	11	24	54.2	Total *E*(50)	Within credible limits
		Non-incident	Gaussian	Supercomputer	11	24	54.2	Total *E*(50)	Within credible limits
		Non-incident	Censored	Desktop	16	24	33.3	Total *E*(50)	Within credible limits
		Non-incident	Censored	Supercomputer	16	24	33.3	Total *E(*50)	Within credible limits
		Incident	Exact Poisson	Desktop	3	42	92.9	Total *E*(50)	Within credible limits
		Incident	Exact Poisson	Supercomputer	3	42	92.9	Total *E*(50)	Within credible limits
		Incident	Gaussian	Desktop	6	42	85.7	Total *E*(50)	Within credible limits
		Incident	Gaussian	Supercomputer	6	42	85.7	Total *E*(50)	Within credible limits
		Incident	Censored	Desktop	6	42	85.7	Total *E*(50)	Within credible limits
		Incident	Censored	Supercomputer	6	42	85.7	Total *E*(50)	Within credible limits
UF	^{3}H	Non-incident	Gaussian	Desktop	3	18	83.3	2005 *E*(50)	Within credible limits
	^{234}U	Non-incident	Gaussian	Desktop	4	9	55.6	2005 *E*(50)	Within credible limits
	^{238}Pu	Non-incident	Gaussian	Desktop	15	24	37.5	Total *E*(50)	Within credible limits
		Non-incident	Censored	Desktop	20	24	16.7	Total *E*(50)	Within credible limits
		Incident	Gaussian	Desktop	15	42	64.3	Total *E*(50)	Within credible limits
		Incident	Censored	Desktop	17	42	59.5	Total *E*(50)	Within credible limits
ID	^{3}H	Non-incident	Exact Poisson	Desktop	0	18	100	2005 *E*(50)	Within factor of 2
		Non-incident	Exact Poisson	Supercomputer	0	18	100	2005 *E*(50)	Within factor of 2
	^{234}U	Non-incident	Exact Poisson	Desktop	2	9	77.8	2005 *E*(50)	Within factor of 2
		Non-incident	Exact Poisson	Supercomputer	2	9	77.8	2005 *E*(50)	Within factor of 2
	^{238}Pu	Non-incident	Exact Poisson	Desktop	5	24	79.2	Total *E*(50)	Within factor of 2
		Non-incident	Exact Poisson	Supercomputer	5	24	79.2	Total *E*(50)	Within factor of 2

Continued

Table 2. *Continued*

Code	Nuclide	Incident/non-incident	Data treatment	Platform	Missed	Total	Score (%)	Quantity	Criterion
		Non-incident	Gaussian	Desktop	13	24	45.8	Total $E(50)$	Within factor of 2
		Non-incident	Gaussian	Supercomputer	13	24	45.8	Total $E(50)$	Within factor of 2
		Non-incident	Censored	Desktop	13	24	45.8	Total $E(50)$	Within factor of 2
		Non-incident	Censored	Supercomputer	13	24	45.8	Total $E(50)$	Within factor of 2
		Incident	Exact Poisson	Desktop	12	42	71.4	Total $E(50)$	Within factor of 2
		Incident	Exact Poisson	Supercomputer	12	42	71.4	Total $E(50)$	Within factor of 2
		Incident	Gaussian	Desktop	12	42	71.4	Total $E(50)$	Within factor of 2
		Incident	Gaussian	Supercomputer	12	42	71.4	Total $E(50)$	Within factor of 2
		Incident	Censored	Desktop	9	42	78.6	Total $E(50)$	Within factor of 2
		Incident	Censored	Supercomputer	9	42	78.6	Total $E(50)$	Within factor of 2
UF	^{3}H	Non-incident	Gaussian	Desktop	0	18	100	2005 $E(50)$	Within factor of 2
	^{234}U	Non-incident	Gaussian	Desktop	3	9	66.7	2005 $E(50)$	Within factor of 2
	^{238}Pu	Non-incident	Gaussian	Desktop	13	24	45.8	Total $E(50)$	Within factor of 2
		Non-incident	Censored	Desktop	15	24	37.5	Total $E(50)$	Within factor of 2
		Incident	Gaussian	Desktop	14	42	33.3	Total $E(50)$	Within factor of 2
		Incident	Censored	Desktop	16	42	61.9	Total $E(50)$	Within factor of 2

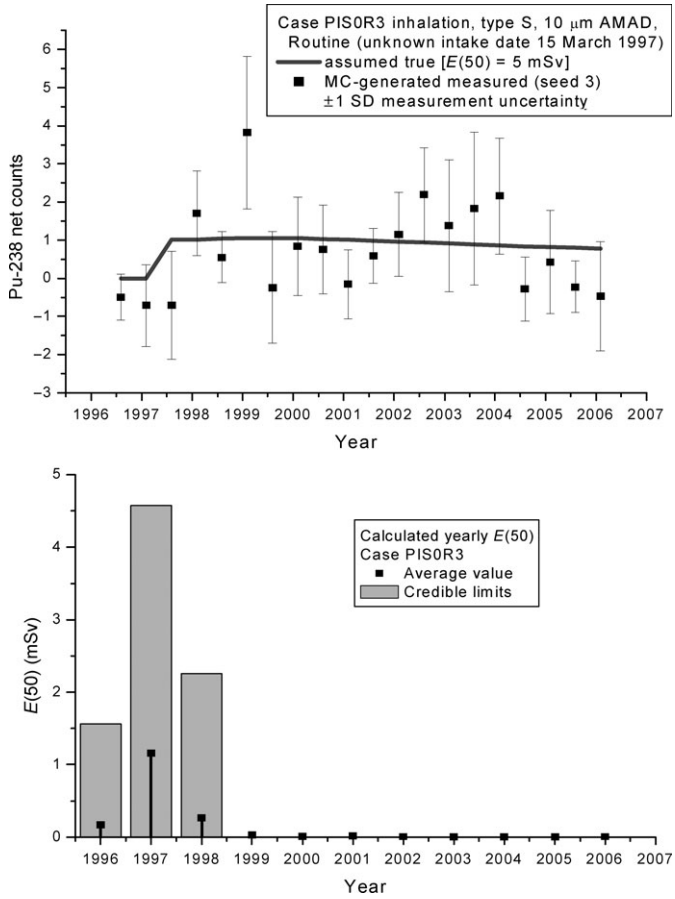

Figure 3. Simulated ^{238}Pu urine bioassay data and calculated yearly $E(50)$ using ID code. This case is 'missed' with $E(50)$ credible limits not including the correct result. Even though all data are less than 2 standard deviations positive, the calculation indicates an intake at approximately the correct time.

shown in Table 3. Two of the missed cases are also shown in Figures 2 and 3.

In Table 3, the 'number of chain iterations per potential intake' is the number of Markov Chain Monte Carlo iterations divided by the number of intakes, as discussed in Miller *et al.*[11]. Each chain iteration involves a forward biokinetics calculation (table lookup), and the number of chain iterations is a rough indicator of the computation time required. For incident-related cases, the number of potential intakes is 1. For non-incident-related cases, the number of potential intakes is 19 (1 intake in each interval between bioassay measurements), so the number of chain iterations was 19 times larger than the quantity given in the table for non-incident cases. The quantity χ^2/Ndata uses χ^2 calculated from the Poisson–lognormal model, as discussed in Miller [5]. If this quantity were much larger than 1, it would indicate a statistical inconsistency, where the Bayesian expectation values of the bioassay data (the 'fit') are not, on average, within a standard deviation from the data. The 'probability of intake' is defined by Miller *et al.*[15]. When the data are indistinguishable from zero, this probability is about 0.5. As it becomes more and more certain that the data are not consistent with 0, this probability approaches 1.

The tritium case is missed because the rather narrow credible limits marginally exclude the true value. There are no missed cases using the 'factor of 2' definition of correct.

Type M uranium is missed for a similar reason. However, type S 10 μm AMAD uranium does not provide enough 'signal' to be detected.

For plutonium, two 5 mSv non-incident cases are missed. One is a LANL-specific biokinetic model (ICD) describing an inhalation intake intermediate between types M and S. The intake is detected with high probability, but the dose is missed because of misidentification of biokinetic type for two out of

Table 3. All cases missed using most effective approach (ID code, exact likelihood calculation).

Nuclide	Incident/non-incident	Case	Platform	Chain iterations per potential intake	χ^2/Ndata	Probability of intakes	$E(50)$ (mSv), true	$E(50)$[a] (mSv), calculated	Year(s)	Ratio
^{3}H	Non-incident	H05R17	Desktop	1 000 000	0.62	1	0.03	0.04 (0.03, 0.05)	2005	1.32
	Non-incident	H05R17	Supercomputer	1 000 000	0.62	1	0.03	0.04 (0.03, 0.05)	2005	1.32
^{234}U	Non-incident	UIM508	Desktop	10 000 000	0.91	1	5	6.4 (5.01,8.8)	2005	1.28
	Non-incident	UIS003	Desktop	3 000 000	0.09	0.52	5	0.08 (0, 0)	2005	0.02
	Non-incident	UIS003	Supercomputer	1 000 000	0.09	0.52	5	0.05 (0, 0)	2005	0.01
^{238}Pu	Non-incident	PICDR1	Desktop	3 000 000	0.59	1	5	14.3 (7.7, 22.6)	All	2.87
	Non-incident	PICDR1	Supercomputer	10 000 000	0.59	1	5	14.3 (7.5, 22.5)	All	2.85
	Non-incident	PICDR3	Desktop	1 000 000	0.73	1	5	3.8 (2.7, 4.9)	All	0.77
	Non-incident	PICDR3	Supercomputer	1 000 000	0.73	1	5	3.8 (2.7, 4.9)	All	0.77
	Non-incident	PIS0R3	Desktop	1 000 000	0.57	0.77	5	1.3 (0, 4.6)	All	0.27
	Non-incident	PIS0R3	Supercomputer	1 000 000	0.57	0.77	5	1.3 (0, 4.7)	All	0.27
	Non-incident	PIEER1	Desktop	1 000 000	0.74	0.74	5	1.2 (0, 4.96)	All	0.24
	Incident	PIEEI2	Desktop	1 000 000	0.43	0.17	1	0.19 (0, 0.86)	All	0.19
	Incident	PIEEI2	Supercomputer	1 000 000	0.43	0.17	1	0.19 (0, 0.86)	All	0.19
	Incident	PIS1I3	Desktop	1 000 000	0.36	0.29	1	0.27 (0, 0.97)	All	0.27
	Incident	PIS1I3	Supercomputer	1 000 000	0.36	0.29	1	0.27 (0, 0.97)	All	0.27
	Incident	PWTAI1	Desktop	1 000 000	0.36	0.12	1	0.05 (0, 0.25)	All	0.05
	Incident	PWTAI1	Supercomputer	1 000 000	0.36	0.12	1	0.05 (0, 0.25)	All	0.05

[a]The calculated $E(50)$ is given as mean (5% CL, 95% CL).

three cases. The other case has been discussed and is shown in Figure 3. The 1 mSv plutonium incident cases that are missed involve two LANL-specific biokinetic models: IEE, delayed onset biokinetics for ^{238}Pu and WTA, a wound model having two long-time retention compartments. In addition, type S 1 μm AMAD biokinetics is also missed. These cases simply do not provide enough signal to be distinguishable from background.

DISCUSSION

The effectiveness of exact likelihood calculations, particularly in relation to data censoring at 2 standard deviations (87.5 versus 33% correct for ^{238}Pu case), shows the importance of the analytical laboratory reporting count quantities and use of the exact likelihood calculation for a situation such as plutonium. Data censoring here means that the likelihood function used is that corresponding to a 'less than limit of detection' measurement. All the data are used. Another approach, widely used but not considered here, is to simply ignore all data below the limit of detection.

The missed case for plutonium shown in Figure 3 is a good illustration of the problem of data censoring. For this case, all of the data are less than 2 standard deviations positive (measurement divided by measurement uncertainty standard deviation <2 for all data points). The censored data are therefore equivalent to data from zero true result. Even though outside of the Bayesian credible limits, the ID code result for these same data detects an intake with probability 0.77 and has calculated credible limits of (0, 4.7) mSv, a little off the correct result of 5 mSv.

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