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Uncertainty in compartmental models for hazardous materials — a case study

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Abstract

Performing uncertainty analysis on compartmental models is the main topic of this article. Elements of the methodology developed during a joint CEC/USNRC accident consequence code uncertainty analysis are introduced. The uncertainty is quantified using structured expert judgment. Experts are queried about physically observable quantities. Many code input parameters of the accident consequence codes are not physically observable but are used to predict observable quantities. Therefore, a probabilistic inversion technique was developed which 'transfers' the uncertainty from the physically observable quantities to the code input parameters. The probabilistic inversion technique is illustrated using the compartmental model of systemic retention of Sr in the human body. The article is concluded with a discussion on capturing uncertainty via compartmental models.

Keywords: Uncertainty analysis; Expert judgment; Compartmental models; Probabilistic inversion; Maximum entropy

1. Introduction

The 'hazardousness' of a given material is typically expressed in terms of size of response in humans per unit exposure. Choosing the proper hazard dimensions for a given substance is hardly a trivial task, but even when these dimensions have been selected, substantial uncertainty may remain. Direct experimental data on humans is usually scarce, and indirect data, e.g. involving animal experiments, are often difficult to interpret. Therefore, in environmental studies, the dose response models associated with

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hazardous materials are often a dominant contributor to uncertainty in the predicted results.

As decision makers learn to appreciate the substantial uncertainties in environmental transport or compartmental models, they typically request a quantification of these uncertainties. This in turn requires quantification of the uncertainties over input parameters in the dose response models of the hazardous substances.

This article discusses an element of the methodology for quantifying uncertainty in environmental models for hazardous substances developed in a joint research project with the Commission of the European Communities (CEC) and the United States Nuclear Regulatory Commission (USNRC) (see Refs. [3–8]). The method aims at quantifying the uncertainty in accident consequence codes for commercial nuclear power plants using structured expert judgment. One compartmental model for one substance, namely the acyclic compartmental model describing systemic retention of Strontium in the human body, is taken to illustrate the methodology.

Section 2 briefly describes relevant features of the joint research project. Section 3 describes the acyclic compartmental model for systemic retention of Strontium. Section 4 discusses how the uncertainty has been quantified and Section 5 discusses probabilistic inversion. Section 6 discusses uncertainty modeling from a general perspective.

2. Joint CEC / USNRC project

To estimate the risks and consequences of hypothetical accidents with commercial nuclear power plants, the CEC and USNRC separately developed Probabilistic Accident Consequence Codes (PACCs), COSYMA and MACCS, respectively. Since many modeling parameters in the codes are uncertain, these organizations decided jointly to establish a methodology and provide a base of information in order to perform uncertainty analysis on the calculations of PACCs. Available data are sparse and, as both organizations wanted to allow for a diversity of viewpoints, formal expert judgment elicitation was used to quantify the uncertainties. The goal of elicitating expert judgments is to encode degrees of belief into probability distributions.

Research institutes in Europe (TU Delft, National Radiological Protection Board, Energiecentrum Nederland, Forschungszentrum Karlsruhe) and in the USA (SANDIA National Laboratories, U. of Hawaii at Hilo, U. of Arizona) formulated the objectives for this joint effort. The broad objectives are stated in Ref. [5]: (1) to formulate a generic, state-of-the-art methodology for uncertainty estimation which is capable of finding broad acceptance. (2) To apply the methodology to estimate the uncertainties associated with the predictions of PACCs designed for assessing consequences of accidents at commercial nuclear power plants. (3) To better quantify and obtain more valid estimates of the uncertainties associated with the PACCs, thus enabling more informed and better judgments to be made in the areas of risk comparison and acceptability and therefore to help set priorities for future research. (4) To systematically develop credible and traceable uncertainty distributions for the respective code input variables using formal expert judgment elicitation process.

Expert panels were formed for the following areas of the PACCs: atmospheric dispersion, deposition, external doses, foodchain, early health effects, late health effects and internal dosimetry. The case study discussed in this article is taken from the uncertainty analysis on the internal dosimetry module of the codes.

3. Compartmental model for Sr

In this project, systemic retention of Sr in the human body is described by the acyclic compartmental model shown in Fig. 1.

The transfer coefficient k_{ij}, represents the proportion of material in compartment i moved to compartment j in a small time interval. The compartmental model determines a set of first order linear differential equations which, with the appropriate conditions, fully specify the movement of material between the compartments.

Although the transfer coefficients cannot be measured directly, the following relationships are assumed to hold on the basis of physical considerations.

(1) The transfer coefficients from compartment i to Bladder are modeled as:

$$k_{i6} = U{:}F * k_{i5} \tag{1}$$

with $i \in \{1,\ldots,4\}$ and $U{:}F$ the Urine-to-Faeces ratio for Sr. The $U{:}F$-ratio for Sr was set to 3.3.

(2) It was assumed that the transfer coefficient from Blood to Trabecular Bone, k_{12} is fully correlated to the transfer coefficient from Blood to Cortical Bone, k_{13} in the following manner:

$$k_{12} = \mathrm{tc} * k_{13} \tag{2}$$

where tc is the Trabecular-to-Cortical factor, tc and k_{13} are considered uncertain.

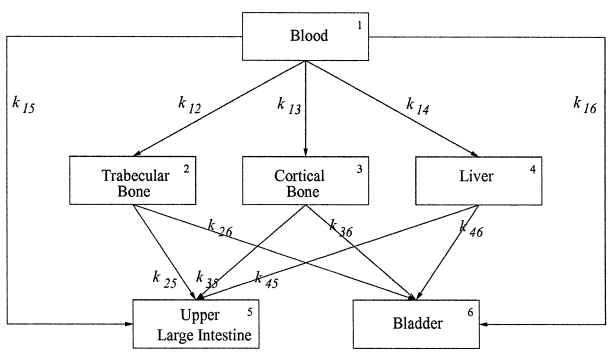

Fig. 1. Acyclic compartmental model for the systemic retention of Sr.

Based on the compartmental model shown in Fig. 1, Eqs. (1) and (2) and initial conditions [1] the equation describing the proportion of the amount of Sr at time t, for example, in the Skeleton (Trabecular Bone and Cortical Bone) and Liver is:

$$\begin{aligned} m_{\text{Skeleton+Liver}} &= m_2(t) + m_3(t) + m_4(t) \\ &= \text{tc}\, k_{13} \frac{e^{-4.3k_{25}t} - e^{-(k_{13}(1+\text{tc})+k_{14}+4.3k_{15})}}{k_{13}(1+\text{tc}) + k_{14} + 4.3k_{15} - 4.3k_{25}} \\ &\quad + k_{13} \frac{e^{-4.3k_{35}t} - e^{-(k_{13}(1+\text{tc})+k_{14}+4.3k_{15})}}{k_{13}(1+\text{tc}) + k_{14} + 4.3k_{15} - 4.3k_{35}} \\ &\quad + k_{14} \frac{e^{-4.3k_{45}t} - e^{-(k_{13}(1+tc)+k_{14}+4.3k_{15})}}{k_{13}(1+\text{tc}) + k_{14} + 4.3k_{15} - 4.3k_{45}}. \end{aligned} \tag{3}$$

Besides calculating the amount of Sr retained in any compartment at any time, the compartmental model is used in calculating the dose per unit intake (dose coefficient) of any compartment. These dose coefficients are used in further calculations of health effects.

From this point on we will refer to the acyclic compartmental model describing systemic retention of Sr in the human body, as shown in Fig. 1, as the Sr-model.

4. How to quantify uncertainties?

The Sr-model in Fig. 1 is typical of models used by international bodies charged with setting standards for radiation exposure for the general public and for radiological workers [9].

We have seen that the Sr-model can be used to compute dose coefficients. Compartmental models, like the Sr-model make strong assumptions, in particular: (a) These and only these compartments are involved in the transfer of material. (b) The rates of transfer from a source-compartment to a sink-compartment are proportional to the amount of material in the source compartment, and independent of all other physical variables.

The model itself is not derived from underlying physical laws, nor can it be verified by direct observation, most of the transfer coefficients cannot be measured by experiment.

The uncertainty analysis team is tasked with quantifying the uncertainty attending the use of such models in a traceable and defensible way. If these models were derived from accepted physical laws, and if the transfer coefficients could be measured, subject to measurement error, then the quantification of uncertainty would be straightforward. The transfer coefficients would be regarded as drawn from a sampling distribution reflecting

[1] Initial conditions for systemic retention of *Sr* are $m_1(t=0)=1$ and $m_i(t=0)=0$, where $i=2,\ldots,6$.

measurement error, and the uncertainty attending the use of such models would be obtained by propagating the sampling distribution through the model.

The above remarks make it clear that this straightforward method of quantifying uncertainty is not available for compartmental models like the Sr-model. The method by which these models are chosen and quantified cannot form the basis for a quantification of uncertainty. Indeed, the uncertainty analysis team did not encounter any generic method for choosing and subsequently quantifying such models. The type of arguments leading to a choice of a given model are peculiar to the species in question. Once a compartmental model is chosen, the method for determining the values of the transfer coefficients is also highly specific to the problem at hand and involves a great deal of qualitative reasoning.

The absence of direct physical measurements of transfer coefficients means that the uncertainty cannot be determined by objective statistical methods, rather the relevant uncertainty takes the form of subjective uncertainty of experts. The uncertainty must be quantified using structured expert judgment. At the same time, the lack of validation for the models themselves entails that we cannot simply ask experts ''what is your uncertainty in transfer coefficient k_{13} of the Sr-model'' as the uncertainty analysis team may not make any assumption regarding the model the experts should use.

4.1. Target variables and elicitation variables

At the inception of the joint project, the project team adopted the position that experts would be queried only about the results of possible measurements. Physically feasible measurement set-ups would be specified, values of all variables would be specified to the degree that they are read by the PACCs. Values of variables which are not read into the PACCs are left unspecified, and uncertainty over these values must be folded into the uncertainty over the measurement outcomes by the experts. Experts are then asked to state their uncertainty distributions over the possible outcomes of the measurements. By configuring the expert elicitations in this way, the experts' uncertainty is conditionalized on the knowledge that the user of the PACC possess during any given application.

The uncertain code input parameters for which an uncertainty distribution has to be determined will be called *target variables*. The quantities for which the experts have to provide assessments will be called *elicitation variables*. The target variables in the Sr-model are (k_{13}, k_{14}, k_{15}, k_{25}, k_{35}, k_{45}, tc). From the discussion earlier, it is clear that they cannot serve as elicitation variables. Elicitation variables were formulated on the amount of Sr retained in certain regions of the human body at certain times, after being administered intravenously as a single injection. The regions of the human body for which the experts were queried are the Skeleton + Liver and the Skeleton as a percentage of Skeleton + Liver. The elicitation questions are listed in Appendix A. Experts were asked to consider two populations: adults and 5-year-old children. In this article, we focus on adults only. For all elicitation variables, the experts were asked to state the 5%, 50% and 95% quantiles of their subjective distribution.

The elicitation variables cover important contributions to uncertainty in calculating doses from radionuclides reaching blood. Factors omitted in the Sr-model that might also contribute significantly to uncertainties are the location of sensitive cells in Bone

Table 1
Quantile information of aggregated experts based on equal weights for the two types of elicitation questions for adults

Question	Quantile (%)	1 day	1 week	1 month	1 year	10 years	50 years
Skel + Liver	5	0.17	0.12	0.1	6.74e − 2	1.8e − 2	1.1e − 3
	50	0.32	0.23	0.21	0.14	6.5e − 2	1.8e − 2
	95	0.58	0.48	0.35	0.24	0.14	8.9e − 2
Skel/Skel + Liver	5	0.85	0.82	0.85	0.77	0.68	0.64
	50	0.96	0.96	0.98	0.99	0.99	0.99
	95	0.998	0.998	0.999	0.999	0.999	0.999

and absorbed fractions for alpha- and beta-emitting Bone seekers, and tissue mass and geometric considerations. Experts are encouraged to take these factors into account in their uncertainty distributions.

4.2. Aggregated expert results

Once the expert uncertainty distributions are obtained, these uncertainties must be aggregated to form one uncertainty distribution, and this distribution must be used to derive an uncertainty distribution over the transfer coefficients of the Sr-model. The method of aggregation is not the focus of this article, for more detailed information see Ref. [2] and references therein. For the data analysed here, a simple arithmetic average of the experts' uncertainty distributions has been used. Aggregated expert results for the elicitation variables are given in Table 1.

In looking at the written rationales of the experts [6], it became clear that every expert used the ICRP 67 model for Sr (comparable to Fig. 1) in determining their median values. They stated that Sr is the best understood element of the Alkaline Earth Elements. Furthermore, they all consider the retention in the Liver to be negligible compared to the retention in the Skeleton.

Section 5 explains how the aggregated expert results are used to determine an uncertainty distribution on the target variables for the Sr-model.

5. Probabilistic inversion

Suppose we had a distribution over the transfer coefficients of the Sr-model. We could then push this distribution through the compartmental model and obtain a distribution over, for example the retention at various times in the Skeleton and Liver using Eq. (3). The problem at hand involves reversing this procedure: we have quantiles of distributions over retention in certain compartments at certain times, namely the aggregated expert uncertainty distributions (as in Table 1); and we seek a distribution over the transfer coefficients which, when pushed through the compartmental model, yields quantiles over retentions agreeing with those from the experts. Hence, our problem is one of probabilistic inversion: we must invert the compartmental model so as

to 'pull back' the distribution over the retention in certain compartments at certain times onto the transfer coefficients of the model.

Let H represent a distribution over retention in given compartments at given times. Let F represent a distribution over transfer coefficients in the Sr-model, and let $G(F)$ represent the distribution over retention in the given compartments at the given times, obtained by pushing the distribution F through the model G. Then our problem may be represented as: Find F such that $G(F) \sim H$, where ' $\sim$ ' means 'has the same distribution as', or equivalently, $F \sim G^{-1}(H)$.

Note that a probabilistic inverse $G^{-1}(H)$ may not exist, and if it exists it will be in general not unique. Therefore, we must have a method of selecting a preferred distribution in case of non-uniqueness and a method of choosing a best fitting distribution in case of non-existence.

Note also that probabilistic inversion is not restricted to expert judgment only. Distributions obtained from a series of experiments under similar conditions can also be used as input in the probabilistic inversion technique.

5.1. PREJUDICE

The acronym PREJUDICE stands for PRocessing Expert JUDgment Into Code paramEters. We will illustrate the different steps using the following compartmental model, see Fig. 2.

Suppose we want to perform an uncertainty analysis on the compartmental model shown in Fig. 2. The equations describing the retention in the different compartments are:

$$m_{\mathrm{A}}(t) = \mathrm{e}^{-(k_{\mathrm{AB}}+k_{\mathrm{AC}})t} \tag{4}$$

$$m_{\mathrm{B}}(t) = \frac{k_{\mathrm{AB}}}{k_{\mathrm{AB}}+k_{\mathrm{AC}}}(1-\mathrm{e}^{-(k_{\mathrm{AB}}+k_{\mathrm{AC}})t}) \tag{5}$$

$$m_{\mathrm{C}}(t) = \frac{k_{\mathrm{AC}}}{k_{\mathrm{AB}}+k_{\mathrm{AC}}}(1-\mathrm{e}^{-(k_{\mathrm{AB}}+k_{\mathrm{AC}})t}). \tag{6}$$

In performing the uncertainty analysis, a joint distribution over $(k_{\mathrm{AB}}, k_{\mathrm{AC}})$is required, i.e., $(k_{\mathrm{AB}}, k_{\mathrm{AC}})$ are the target variables. From the discussion above, it was concluded that the transfer coefficients cannot serve as elicitation variables. Therefore, the elicitation variables are on the retention of material in compartments B and C at certain times t_i $(i=1,\ldots,n)$ after a unit deposit in compartment A, represented by Y_i and Z_i

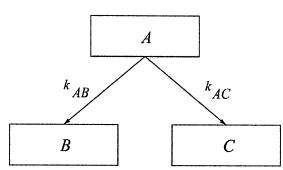

Fig. 2. Compartmental model.

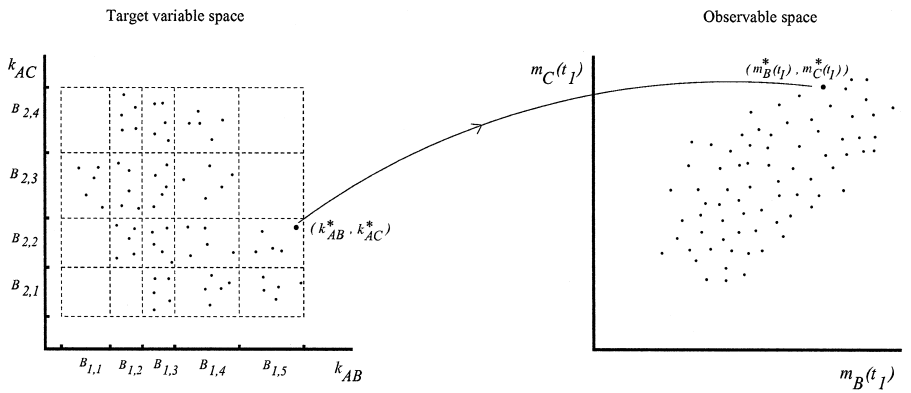

Fig. 3. Propagation of samples.

$(i = 1, \ldots, n)$. Figs. 3–5 depict the probabilistic inversion for $n = 1$. In determining the distribution over the target variables all elicitation variables are used.

Step 1 Support of Distribution: In this step, the support of the distribution over the target variables is determined.

For each i, $i = 1, \ldots, n$, an elicited quantile is chosen for Y_i and Z_i, say y_{i,j_i} and z_{i,k_i}, where j_i, $k_i \in \{1, 2, 3\}$. The set:

$$s = (y_{1,j_1}, z_{1,k_1}, \ldots, y_{n,j_n}, z_{n,k_n}) \tag{7}$$

is called a scenario. Let S be the set of all scenarios. Next, each scenario is tested for physically admissibility; in this example $(m_B(t), m_C(t))$ are increasing functions of t. Therefore, $s \in S$ is admissible only if $y_{i,j_i} < y_{i+1,j_{i+1}}$ where $i = 1, \ldots, n-1$, and similarly for z. Let S^* denote the set of admissible scenarios.

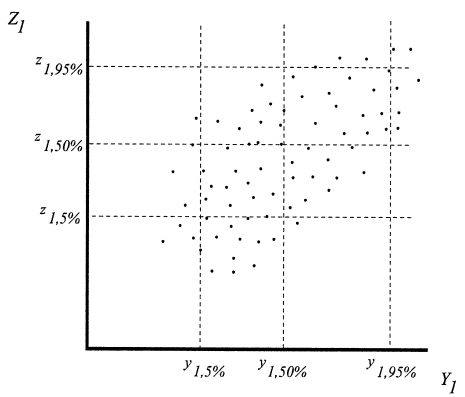

Fig. 4. Observable hypercubes.

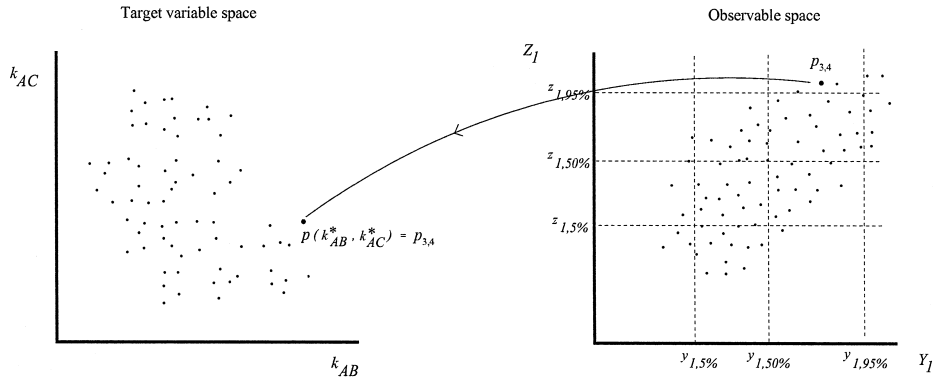

Fig. 5. 'Pullback'-distribution.

For each scenario $s \in S^*$, estimates $(k^s_{\mathrm{AB}},\ k^s_{\mathrm{AC}})$ for the target variables are determined, such that the quadratic difference between model output and scenario s is minimized.

$$\sum_{i=1}^{n}\left(\frac{k^s_{\mathrm{AB}}}{k^s_{\mathrm{AB}}+k^s_{\mathrm{AC}}}\left(\left(1-\mathrm{e}^{-(k^s_{\mathrm{AB}}+k^s_{\mathrm{AC}})t_i}\right)-y^s_i\right)\right)^2 + \sum_{i=1}^{n}\left(\frac{k^s_{\mathrm{AC}}}{k^s_{\mathrm{AB}}+k^s_{\mathrm{AC}}}\left(\left(1-\mathrm{e}^{-(k^s_{\mathrm{AB}}+k^s_{\mathrm{AC}})t_i}\right)-z^s_i\right)\right)^2 \tag{8}$$

For each target variable, intervals are determined which are (1) mutually exclusive and (2) whose union covers all estimates. In this way, each estimate $(k^s_{\mathrm{AB}},\ k^s_{\mathrm{AC}})$ falls in one hypercube of the target variable space. A number of samples are taken uniformly from each such hypercube and propagated through the model using Eqs. (5) and (6) for $t = t_1, \ldots, t_n$. This generates a set of points in the observable space. The samples taken in the target variable space will be the support of the distribution over the target variables and will be indicated by I. See Fig. 3 for a graphical illustration, the pair $(k^*_{\mathrm{AB}},\ k^*_{\mathrm{AC}})$ is sampled uniformly from the rectangle $B_{1,5} \times B_{2,2}$ and mapped into the observable pair $(m^*_{\mathrm{B}}(t_1),\ m^*_{\mathrm{C}}(t_1))$.

Step 2 Determination of Distribution: Note that the axis of the observable space, in which the propagated samples are defined, can be associated with elicitation variables Y_i and Z_i, $i = 1, \ldots, n$. 5%, 50% and 95% quantiles of the distributions of each elicitation variables are available.

Briefly, a joint distribution over the propagated samples in the observable space is determined, which has maximum entropy with respect to the uniform background measure and such that for each elicitation variable Y_i and Z_i, the quantile information of the marginal distribution complies with the quantile information of the distribution of Y_i

and Z_i.Each propagated sample in the observable space thus receives a probability and each point in I is assigned the probability associated with its image in the observable space. In this way, a distribution over I is determined. Details are given in Section 5.2.

5.2. Determination of distribution

The number of distributions over the propagated samples which will satisfy the constraints on the quantile information on Y_i and Z_i, as described in **Step 2**, may be large. From this set of distributions, we want to select *one* distribution: the distribution which has maximum entropy with respect to the uniform background measure [10,12]. Determining the joint distribution which has maximum entropy with respect to the uniform background measure can be formulated as a constrained Non-Linear Programming (NLP) problem.

To describe the NLP problem, we introduce a set of hypercubes in the observable space. For elicitation variable Y_i, we distinguish four intervals:

$$(-\infty, y_{i,5\%}], \ (y_{i,5\%}, y_{i,50\%}], \ (y_{i,50\%}, y_{i,95\%}], \ (y_{i,95\%}, \infty)$$

In the same way we distinguish four intervals for elicitation variable Z_i. Taking the product of all such intervals, for all elicitation variables, we generate a set of ''observable hypercubes'', indexed as $i_1 \ldots i_{2n}$, where $i_j \in \{1, 2, 3, 4\}$. Thus, $i_j = 3$ means that we consider interval $(y_{j,50\%}, y_{j,95\%}]$ for elicitation variable Y_j. For two elicitation variables, Y_1 and Z_1, the observable hypercubes are shown in Fig. 4.

The NLP problem may be formulated as follows:

$$\text{maximize} - \sum_{i_1=1}^{4} \sum_{i_2=1}^{4} \cdots \sum_{i_{2n}=1}^{4} c_{i_1 \ldots i_{2n}} p_{i_1 \ldots i_{2n}} \ln p_{i_1 \ldots i_{2n}} + C \tag{9}$$

$$\sum_{i_2=1}^{4} \cdots \sum_{i_{2n-1}}^{4} c_{1 i_2 \ldots i_{2n}} p_{1 i_2 \ldots i_{2n}} = 0.05 \qquad \ldots \qquad \sum_{i_1=1}^{4} \cdots \sum_{i_{2n-1}=1}^{4} c_{i_1 \ldots i_{2n-1} 1} p_{i_1 \ldots i_{2n-1} 1} = 0.05$$

$$\sum_{i_2=1}^{4} \cdots \sum_{i_{2n-1}}^{4} c_{2 i_2 \ldots i_{2n}} p_{2 i_2 \ldots i_{2n}} = 0.45 \qquad \ldots \qquad \sum_{i_1=1}^{4} \cdots \sum_{i_{2n-1}=1}^{4} c_{i_1 \ldots i_{2n-1} 2} p_{i_1 \ldots i_{2n-1} 2} = 0.45$$

$$\sum_{i_2=1}^{4} \cdots \sum_{i_{2-1}}^{4} c_{3 i_2 \ldots i_{2n}} p_{3 i_2 \ldots i_{2n}} = 0.45 \qquad \ldots \qquad \sum_{i_1=1}^{4} \cdots \sum_{i_{2n-1}=1}^{4} c_{i_1 \ldots i_{2n-1} 3} p_{i_1 \ldots i_{2n-1} 3} = 0.45$$

$$\sum_{i_2=1}^{4} \cdots \sum_{i_{2-1}}^{4} c_{4 i_2 \ldots i_{2n}} p_{4 i_2 \ldots i_{2n}} = 0.05 \qquad \ldots \qquad \sum_{i_1=1}^{4} \cdots \sum_{i_{2n-1}=1}^{4} c_{i_1 \ldots i_{2n-1} 4} p_{i_1 \ldots i_{2n-1} 4} = 0.05$$

$$p_{i_1 \ldots i_{2n}} \geq 0$$

where $c_{i_1 \ldots i_{2n}}$ represents the number of propagated samples falling in observable hypercube $i_1 \ldots i_{2n}$, and C is the constant ln. NLP problem (Eq. (9)) is solved for $p_{i_1 \ldots i_{2n}}$. The $p_{i_1 \ldots i_{2n}}$ represent the probability of each sample in observable hypercube $i_1 \ldots i_{2n}$. It is easy to see that Eq. (9) is a convex optimization problem. The interior point solver for large-scale convex problems [1] avoids problems with $p_{i_1 \ldots i_{2n}} = 0$ and gave excellent performance. In Fig. 5, the highlighted point receives probability $p_{3,4}$ and the probability is assigned to the pre-image of this point (k^*_{AB}, k^*_{AC}) in the target variable space.

5.3. Dealing with infeasibilities

The above NLP problem may not be feasible. In this case, we reduce the dimension of the observable space. Still considering the simple model of Fig. 2, with $2n$ elicitation variables, suppose the NLP problem (Eq. (9)) is infeasible. The idea is to look at $\binom{2n}{2n-1}$ problems of dimension $2n-1$. For each of the $\binom{2n}{2n-1}$ problems, **Step 1** and **Step 2** are carried out. Because all steps of the solution scheme are carried out for each problem, the support associated with the different problems will likely be different. Let N ($N \leq \binom{2n}{2n-1}$) denote the number of NLP problems for which a distribution in **Step 2** can be determined. Assuming that $N > 0$, we have obtained N distributions over the target variables on their specific supports. We are now confronted with the problem of finding a distribution over the target variables which ''best fits'' the N distributions. For the solution of this problem, we refer to Ref. [11].

If $N = 0$, we will reduce the dimension of the problem once more, and perform **Step 1** and **Step 2** for $\binom{2n}{2n-1}$ problems of dimension $2n-2$.

The details are omitted here; the NLP problem for the Sr-model was feasible.

5.4. Compartmental model for Sr: results

The dimension of the target variable space for the Sr-model is 7 and the dimension of the observable space is 12. The Sr-model was probabilistically inverted to determine a distribution over (k_{13}, k_{14}, k_{15}, k_{25}, k_{35}, k_{45}, tc). There were 1269 admissible scenarios and these were used to generate 1,269,000 samples in the target variable space as described in **Step 1**. The samples were propagated through the appropriate model predictors.

Quantile information for the marginal distributions and the rank correlation matrix among the target variables are given in Tables 2 and 3, respectively.

To determine how well the probabilistic inversion technique performs, the aggregated expert quantiles in Table 1 are compared to quantiles obtained by ''pushing'' the distribution over the target variables through the appropriate model predictors. Thus, we regard $m_{\text{Skeleton+Liver}}(t_i)$ (Eq. (3)), as a function of random variables (k_{13}, k_{14}, k_{15}, k_{25},k_{35}, k_{45}, tc) for 1 day, 1 week, 1 month, 1 year, 10 years and 50 years (see Table 1). The columns headed with Agg. Exp. give the aggregated expert assessments, the columns headed with Pred. give the 'push-through' results based on the distribution over the target variables as determined with PREJUDICE. For performing a large uncertainty

Table 2
Quantile information for the target variables

Quantile (%)	k_{13}	k_{14}	k_{15}	k_{25}	k_{35}	k_{45}	tc
5	6.89e−2	7.7e−4	5.54e−2	1.45e−5	2.63e−5	7.33e−6	0.29
50	2.18e−1	9.57e−4	2.68e−1	2.74e−2	5.48e−5	4.09e−5	2.03
95	6.97e−1	7.25e−2	3.53e−1	1.22e−1	7.41e−2	7.41e−2	2.35

Table 3
Rank correlations among target variables

	k_{13}	k_{14}	k_{15}	k_{25}	k_{35}	k_{45}	tc
k_{13}	1	−0.04	0.42	−0.61	−0.46	−0.45	−0.62
k_{14}	−0.04	1	−0.45	0.12	−0.27	−0.03	0.04
k_{15}	0.42	−0.45	1	−0.20	0.27	0.17	−0.25
k_{25}	−0.61	0.12	−0.20	1	−0.85	0.12	0.60
k_{35}	−0.46	−0.27	0.27	−0.85	1	0.01	−0.87
k_{45}	−0.45	−0.03	0.17	0.12	0.01	1	−0.02
tc	−0.62	0.04	−0.25	0.60	−0.87	−0.02	1

analysis, it is often necessary to represent the joint distribution in terms of marginal distributions and rank correlation coefficients. The columns ''Marg. Rank.'' give the 'push-through' results based on the distribution over the target variables which has maximum entropy satisfying the marginal distributions and rank correlation matrix given by PREJUDICE. Note that PREJUDICE fits the aggregated expert results quite well, and that the Marg. Rank. is poor for the 5% quantiles for (Skel)/(Skel + Liver).

6. Uncertainty capture

Physical models like the compartmental model discussed above are traditionally used with 'best estimates' of the transfer coefficients to predict phenomena. When we cannot infer the models from accepted laws and cannot measure the values of the transfer coefficients, then the predictions of the models are uncertain. Straightforward use of the model with 'best estimates' does not give any picture of the uncertainty attending model predictions. We suggest that these models can be legitimately employed to capture uncertainty. This employment differs in fundamental ways from straightforward prediction.

Capturing uncertainty in observable phenomena via distributions over transfer coefficients involves:

(i) using structured expert judgment to quantify uncertainty on measurable quantities predicted by the compartmental model.

(ii) performing probabilistic inversion to pull this uncertainty back onto the transfer coefficients of the model.

(iii) comparing the uncertainty pushed through the model with the experts' uncertainty.

If there is an imperfect fit in step (iii), the conclusion is not that the model is wrong; rather, the conclusion is that we are unable to capture the experts' uncertainty via a joint distribution over its model parameters. There may be several reasons for this.

(1) Although experts believe that the model is 'roughly right', their uncertainty may involve departures from the assumptions of the model. Thus, with regard to Fig. 1, experts may believe recirculation may occur from, for example Cortical Bone to Blood: under certain circumstances, a portion of material in the Cortical Bone may be

transferred back to the blood. In this case, the amount transferred to the Cortical Bone in a unit time would not be proportional to the amount in the blood. It may be impossible to capture the experts' uncertainty via a distribution over the transfer coefficients in Fig. 1.

(2) Although the experts each represent their uncertainties via distributions over the parameters of the ICRP 67 model for Sr, it may be impossible to represent their combined distribution in this way, taking account of physical constraints. For example, suppose each expert believes in the model of Fig. 1 and believes that Eq. (2), $k_{12} = \text{tc} * k_{13}$, is correct, but they do not agree on the value of tc. If Eq. (2) is interpreted as a physical constraint with tc a constant (i.e. assuming a single value with probability one), then it may be impossible to capture the combined expert distribution via a distribution over model parameters satisfying Eq. (2), even though this is possible for each expert individually.

(3) The mathematical processing may itself impose simplifications which cause a discrepancy in step (iii). Thus, in Table 4 we see that representing the joint distribution over transfer coefficients as a maximal entropy distribution under marginal and rank correlation constraints introduces significant discrepancies.

Assuming that the fit in step (iii) is good, the use of models to capture uncertainty may involve features which are unfamiliar to experts and decision makers alike, and which deserve special attention.

(1) The combined expert distribution will not, in general, agree with the distribution of any one expert. Typically, the uncertainty in the distributions obtained by averaging

Table 4
Comparison Aggregated Expert result (Agg. Exp.) vs. PREJUDICE (Pred.) vs. Marginals and Rank correlation (Marg. Rank.)

Time		Skel + Liver			Skel/Skel + Liver		
		Agg. Exp.	Pred.	Marg. Rank.	Agg. Exp.	Pred.	Marg. Rank.
1 day	5%	0.17	0.17	0.12	0.85	0.85	0.77
	50%	0.32	0.32	0.31	0.96	0.96	0.98
	95%	0.58	0.58	0.53	0.998	0.998	0.999
1 week	5%	0.12	0.12	0.11	0.82	0.82	0.67
	50%	0.23	0.23	0.26	0.96	0.96	0.97
	95%	0.48	0.48	0.55	0.998	0.998	0.998
1 month	5%	0.1	0.10	5.8e−2	0.85	0.85	0.58
	50%	0.21	0.21	0.2	0.98	0.98	0.96
	95%	0.35	0.35	0.49	0.999	0.999	0.999
1 year	5%	6.74e−2	6.74e−2	1.1e−2	0.77	0.77	4.4e−5
	50%	0.14	0.14	0.18	0.99	0.99	0.95
	95%	0.24	0.24	0.43	0.999	0.999	0.999
10 years	5%	1.8e−2	1.8e−2	4.8e−3	0.68	0.68	0
	50%	6.5e−2	6.45e−2	0.11	0.99	0.99	0.95
	95%	0.14	0.14	0.25	0.999	0.999	0.999
50 years	5%	1.1e−3	1.1e−3	2.1e−4	0.64	0.64	0
	50%	1.8e−2	1.85e−2	1.3e−2	0.99	0.99	0.97
	95%	8.9e−2	8.86e−2	7.4e−2	0.999	0.999	0.999

the uncertainties of several experts will be larger than the uncertainties of each individual expert.

(2) The distribution of model parameters may involve strong correlations, either positive or negative, which complicate the ways experts traditionally think about the models. Thus, experts like to think of transfer coefficients in terms of 'retention half times'. In Fig. 1, if we consider the Cortical Bone and ULI compartments in isolation, then the time at which half of a unit deposit to Cortical Bone is transferred to the ULI is $(\ln(2))/(k_{35})$ and is called the retention half time for Cortical Bone. Similarly, $(\ln(2))/(k_{25})$ is the retention half time for Trabecular Bone. These expressions suggest that k_{25} and k_{35} have a meaning independent of the model in which they are considered. This is not the case however as may become glaringly evident when k_{25} and k_{35} are assigned distributions as given in Table 2. Note from Table 3 that these variables have a strong negative correlation. A ''representative value'' for k_{25} (e.g. the median) together with a ''representative value'' for k_{35} may not yield representative values for simple functions of (k_{25}, k_{35}). Consider the following simple example: X and Y are uniformly distributed on $[0, 2]$ and completely negative correlated, so that $Y = 2 - X$. The median of X and Y is 1. Hence, the product of the medians is 1, but 1 is also the *maximum* of XY; the product of medians is not the median of the product.

(3) If uncertainty over observable phenomena can be captured via a distribution over model parameters, then this can, in general, be captured in more than one way. In other words, if the probabilistic inverse of a distribution over observables exists, then it is generally not unique. Hence, two uncertainty analysts using different search algorithms and different heuristics might come up with two different distributions over the transfer coefficients in Fig. 1, both of them adequately reproducing the uncertainty over observable phenomena.

7. Conclusions

The use of environmental models to capture uncertainty involves mathematical and conceptual problems. The probabilistic inversion techniques currently available cannot handle models much larger than that of Fig. 1. Research is in progress to develop new solution algorithms and new heuristics for dealing with larger models. To date, the choice of elicitation variables has been driven by heuristics and practical constraints. For example, elicitation variables must be familiar to the experts and the number of elicitation variables must remain relatively small. Finally, the use of models to capture uncertainty rather than to make simple predictions requires experts and decision maker to think about these models in new and different ways.

In spite of the above-problems, the approach to uncertainty modeling described above has been broadly successful within the context of the joint CEC/USNRC uncertainty analysis, and can, in principle, be applied to a wider range of problems.

Appendix A. Elicitation questions

These questions cover important contributions to uncertainty in calculating doses from radionuclides reaching blood. Factors omitted that might also contribute signifi-

cantly to uncertainties are the location of sensitive cells in Bone and absorbed fractions for alpha- and beta-emitting bone-seekers, and tissue mass and geometric considerations.

Considering the total amount reaching blood (as if administered intravenously as a single injection). Percentage retained in Liver and Skeleton (Bone + Bone marrow), as a function of time after entry into blood?

Considering the total amount reaching blood (as if administered intravenously as a single injection). % retained in Liver and Skeleton (Bone+Bone marrow), as a function of time after entry into blood?

	5 year old children			Adults		
	5%	50%	95%	5%	50%	95%
Skeleton and Liver, 1 day						
Sr						
Skeleton and Liver, 1 week						
Sr						
Skeleton and Liver, 1 month						
Sr						
Skeleton and Liver, 1 year						
Sr						
Skeleton and Liver, 10 years						
Sr						
Skeleton and Liver, 50 years						
Sr						

Retention in the Skeleton, % total retention in Liver + Skeleton (Bone+Bone marrow), as a function of time after entry into blood

	5 year old children			Adults		
	5%	50%	95%	5%	50%	95%
Skeleton, 1 day						
Sr						
Skeleton, 1 week						
Sr						
Skeleton, 1 month						
Sr						
Skeleton, 1 year						
Sr						
Skeleton, 10 years						
Sr						
Skeleton, 50 years						
Sr						

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