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Uncertain Numbers and Uncertainty in the Selection of Input Distributions – Consequences for a Probabilistic Risk Assessment of Contaminated Land

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Risks from exposure to contaminated land are often assessed with the aid of mathematical models. The current probabilistic approach is a considerable improvement on previous deterministic risk assessment practices, in that it attempts to characterize uncertainty and variability. However, some inputs continue to be assigned as precise numbers, while others are characterized as precise probability distributions. Such precision is hard to justify, and we show in this paper how rounding errors and distribution assumptions can affect an exposure assessment. The outcome of traditional deterministic point estimates and Monte Carlo simulations were compared to probability bounds analyses. Assigning all scalars as imprecise numbers (intervals prescribed by significant digits) added uncertainty to the deterministic point estimate of about one order of magnitude. Similarly, representing probability distributions as probability boxes added several orders of magnitude to the uncertainty of the probabilistic estimate. This indicates that the size of the uncertainty in such assessments is actually much greater than currently reported. The paper suggests that full disclosure of the uncertainty may facilitate decision-making in

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opening up a negotiation window. In the risk analysis process, it is also an ethical obligation to clarify the boundary between the scientific and social domains.

KEYWORDS: Distribution assumptions; interval analysis; imprecise numbers; Monte Carlo analysis; probability bounds analysis

1. INTRODUCTION

Risk assessment practice relies heavily on mathematical models.[1] Uncertainty arises from choice and structure of these models,[2] as well as model parameterization.[3] Uncertainty in empirical quantities is often separated into several types (e.g., measurement error, systematic error, linguistic imprecision, subjective judgment, variability, and inherent randomness).[4,5] Although some authors would question such a separation of uncertainty,[6] it seems to be generally agreed that uncertainty arising from variability and inherent randomness in the systems under study should be separated from uncertainty due to lack of knowledge.[3,7] In this paper, knowledge uncertainty (epistemic uncertainty) will be denoted simply as 'uncertainty.'

Assigning intervals rather than precise numbers to model parameters (inputs) is a simple approach to carry uncertainties through all the steps of a calculation.[8] When the model inputs are assigned as scalars, without additional uncertainty estimates, the precision is given by the number of significant digits. For example, consider a conservative point estimate for soil intake by children given as 150 mg/d.[9] This scalar has two significant digits and can thus be bound to an interval between 145 and 155, by outward rounding.[10] This interval may of course be expanded further to obtain a more realistic estimate of both uncertainty and variability, but already the number of significant digits implies a minimum level of uncertainty that cannot be ignored. This contribution to uncertainty may seem unimportant, but due to multiplicative effects, the difference between the bounding estimates for the outcome can easily exceed an order of magnitude in an exposure model of reasonable complexity (>20 input variables).

Despite the simplicity, intervals are usually not optimal in assigning uncertainty to the model inputs, since additional knowledge about central tendency, percentiles, distribution shape, etc. is not used.(8) Probabilistic methods provide a framework for using this additional information, and many applications have been reported for exposure from contaminated land.(2,11,12) In a probabilistic risk assessment, the inputs are normally described by parametric or empirical distribution functions.(3) The parametric distribution functions are obtained by fitting to the observed data, from surrogate information, or by purely theoretical considerations.(13,14) Empirical distributions may be preferable when large data sets are available, but they cannot be assumed to represent the high and low percentiles well if the sample size is small or if the measurement errors are substantial.(15) In this paper, we will only discuss the use of parametric distributions.

The selection of input distributions is critical for any probabilistic model and guidelines often stress that this selection should be justified.(2,16-19) The choice of input distributions may be of even greater importance for the outcome than dependencies between the input variables.(20) The selection process should preferably be based on observation data, and standard distributions for the use in risk assessment have been recommended.(21,22) However, it should be noted that the selection can be site-specific and the use of expert judgment is then unavoidable.(23)

Input distributions are difficult to characterize when data are sparse or missing – expert judgment then becomes increasingly important.[3,24] Different elicitation protocols have been developed to minimize biases in distribution selection, but it is well known that this uncertainty is often underestimated.[4,8,25] Even with an extensive database available, investigators may choose different distribution shapes to approximate the same data.[26] A standardized procedure for developing input distributions for well-researched exposure factors has been suggested.[27] Such standardization would undoubtedly reduce subjectivity, but the impact on the overall uncertainty is still limited by the lack of well-characterized data.

The uncertainty in the distribution shape is seldom evaluated, mainly because of the difficulty of including it in the standard Monte Carlo (MC) framework. One alternative to explore this uncertainty is to evaluate the outcomes from a series of model simulations, with different distribution assumptions or/and different parameter settings.[28-31] However, this approach becomes impractical as model complexity increases and it does not account for all possible distribution shapes.

Probability bounds analysis (PBA) has been introduced as a method of investigating the full extent of uncertainty, including the selection of input distributions.[7,10,32,33] PBA is founded on the use of probability boxes (p-boxes) rather than probability distributions to describe model inputs. A p-box encloses all possible distributions that meet certain constraints, for example a maximum, a minimum, and a median. These p-boxes can then be used in the arithmetic of expressing models for transport, exposure, and effects.[34] The potential for use in risk analysis seems promising and a growing number of applications are appearing in the environmental field (e.g., climate change, extinction risks, and persistent organic pollutants).[35-39] PBA has also been shown to be a useful tool for risk assessment of contaminated land.[40]

A PBA will enclose the best estimate of the outcome; it has therefore been suggested as a quality assurance procedure for MC analysis to give a broader perspective on the uncertainty involved.[37] In particular, the uncertainty in the selection of input distributions deserves more attention. Here it is our intention to investigate how distribution assumptions have affected a previously reported probabilistic exposure assessment.[41] We also wish to evaluate the effect of rounding errors for scalars used in both the deterministic and probabilistic assessments.

2. METHODS

An environmental exposure model developed by the Swedish EPA was applied to a site contaminated by a metallurgical industry over two centuries. The surface water exposure route had minor influence and was not included. The complete exposure assessment encompassed several contaminants, [41] but here we focus only on cadmium to illustrate the different calculations. The point estimate for the intake of cadmium was similar to the tolerable daily intake (TDI) and differences between estimation methods can therefore be of importance for a remediation decision.

2.1 The exposure model

A sensitive land use scenario was evaluated encompassing all types of land use, e.g., residential, kindergarten, agriculture, and ground water extraction. Minor adjustments were made to the exposure model to conform to the latest draft now published for comment by the Swedish EPA.[42] All exposure routes were dominated by the long-term exposure of children and estimates are therefore based on this group alone. The previously used model was further simplified by disregarding differences between sexes and only considering surface contamination (except for the drinking water pathway). The exposure routes included are summarized in Fig. 1.

Transport of cadmium to the groundwater (C_{gw}) is calculated from the average total concentration in the soil (C_t), the distribution coefficient between soil and water (K_d), the soil water content (θ_w), the dry soil bulk density (ρ_b), and the dilution-factor (DF_{gw}). This dilution-factor is calculated from mathematical expressions that contain several repeated parameters, which always pose a problem in interval and probability bounds analysis (PBA).[10] Here, this problem was circumvented by calculating a point estimate for the dilution-factor (0.08) and using numerical optimization to estimate an interval (0.022-0.27), as prescribed by the significant digits for the other factors in those expressions.

$$C_{gw} = C_t \cdot \left[K_d + \frac{\theta_w}{\rho_b} \right]^{-1} \cdot DF_{gw}$$

Transport of cadmium to plants is described by the plant concentration factor between fresh plant and dry soil (K_{pl}), calculated from the bioconcentration factors (BCF), the fractional consumption of stem and leaf vegetables (f_{stem}) and root vegetables (f_{root}), and the dry weight to fresh weight ratios (r_{stem} and r_{root})

$$K_{pl} = BCF_{stem} \cdot f_{stem} \cdot r_{stem} + BCF_{root} \cdot f_{root} \cdot r_{root}$$

The direct oral intake from soil (I_{is}) is determined by the average surface soil concentration (C_s), the average daily soil intake (SI), and the exposure time (t_{is}).

$$I_{is} = \frac{C_s \cdot SI \cdot t_{is}}{365}$$

The dermal uptake (I_{du}) is determined by the surface soil concentration, the dermal soil exposure (SE), the exposed skin area (A), the relative dermal absorption factor (f_{du}), and the exposure time (t_{du}).

$$I_{du} = \frac{C_s \cdot SE \cdot A \cdot f_{du} \cdot t_{du}}{365}$$

The inhalation uptake from respirable dust (I_{id}) is determined by the surface soil concentration, the concentration of respirable dust indoors ($C_{d,in}$), the fraction of dust indoors originating from contaminated area ($f_{d,in}$), the fraction of time spent indoors ($f_{t,in}$), the fraction of dust outdoors originating from contaminated area ($f_{d,out}$), the fraction of time spent outdoors ($f_{t,out}$), the breathing rate (BR), the lung retention (LR), and the exposure time (t_{id}).

$$I_{id} = \frac{C_s \cdot (C_{d,in} \cdot f_{d,in} \cdot f_{t,in} + C_{d,out} \cdot f_{d,out} \cdot f_{t,out}) \cdot BR \cdot LR \cdot t_{id}}{365}$$

The intake from vegetables (I_{ig}) is determined by the surface soil concentration, the plant concentration factor (K_{pl}), the average daily consumption of vegetables (R_{ig}), the fraction of consumed vegetables grown on site (f_h) , and the exposure time (t_{ig}).

$$I_{ig} = \frac{C_s \cdot K_{pl} \cdot R_{ig} \cdot f_h \cdot t_{ig}}{365}$$

The intake with drinking water (I_{iw}) is determined by the concentration in ground water (C_{gw}), the average daily water consumption (WC), and the exposure time (t_{iw}).

$$I_{iw} = \frac{C_{gw} \cdot WC \cdot t_{iw}}{365}$$

The total intake is calculated as the sum divided by the body weight (BW) and expressed in mg/kg/day.

$$I_{tot} = \frac{I_{is} + I_{du} + I_{id} + I_{ig} + I_{iw}}{BW}$$

The calculations of I_{is}, I_{du}, I_{id}, and I_{ig} were coordinated to avoid repetition of the soil concentration variable. The bioavailability was assumed to be one for all exposure routes. Except for dermal uptake, exposure was assumed to occur every day. Thirty-two input variables and constants were retained in this simplified exposure model, of which 18 were characterized by parametric probability distributions (8 lognormal, 6 triangular, 3 normal, and 1 uniform) or p-boxes, Table I.

2.2 Calculation methods

Initially, a deterministic calculation was performed as a baseline for the probabilistic analyses to follow. The concentration of cadmium was estimated at the 95% upper confidence limit of the mean using bootstrapping (resampling with replacement). Rounding errors in the deterministic estimate were explored further after assigning the input variables and constants as imprecise numbers (intervals prescribed by significant digits). These calculations were performed with the software Risk Calc v4.0 (Applied Biomathematics, Setauket, NY).

Subsequently, variability and uncertainty were propagated together in a Monte Carlo (MC) simulation of exposures. The uncertainty in the average soil contamination was described by fitting lognormal distributions to the bootstrapped data. Settings and distributions for the other input variables and constants were chosen from the documentation of the Swedish model, the US EPA Exposure Factors Handbook,[(23)] the Exposure Factors Sourcebook for European Populations,[(43)] the revised CSOIL parameter set,[(44)] and from statistics provided by the SCB (Statistics Sweden) and the Swedish National Food Administration. A two-dimensional (2D) MC analysis was deemed inappropriate since it was not possible, with the data available, to separate variability and uncertainty for most of the inputs. The average daily soil intake or bioconcentration factors for vegetables are two examples were such a separation is difficult if not impossible. Both of these inputs are characterized by a substantial variability, between individuals and between species, but both inputs are also characterized by uncertainty due to the limited availability of data. The MC simulations (10,000 iterations) were run with the software Crystal Ball 2000 Standard Edition v5.2.2 (Decisioneering, Denver, CO).

Finally, two PBA evaluations were carried out and probability boxes (p-boxes), with the same defining parameters, then replaced the parametric distributions. However, the uncertainty in the concentration term for cadmium continued to be characterized by a lognormal distribution (cf. the recommendation by the US EPA in ref. 2). Other variables and constants were assigned both as specific values and as imprecise numbers (to evaluate the effect of rounding errors). These calculations were also run with the software Risk Calc v4.0. In this study, all distributions and p-boxes with infinite ranges were truncated at the 0.5th and 99.5th percentiles respectively.

The use of PBA for risk assessment has been extensively discussed by Ferson et al.[10,34] The main difference between PBA and a 2D MC simulation is in the treatment of uncertainty. In the 2D MC simulation, variability and uncertainty are separated by running the computations iteratively in two loops, one inner and one outer. Variability and uncertainty are then both described by probability distributions, although it is questionable whether uncertainty can be assumed to vary randomly.[7,45,46] In a PBA, variability may continue to be characterized by probability distributions, whereas uncertainty is described by intervals. P-boxes are used to generalize both these characteristics by placing interval bounds on cumulative probability distributions. A p-box is the class of distribution functions $F(x)$ bounded by two cumulative distribution functions $F_1(x)$ and $F_2(x)$ such that $F_1(x) \leq F(x) \leq F_2(x)$ for all x.[47] An example is shown in Fig. 2, where a normal distribution of body weight with a mean of 70 kg and standard deviation of 10 kg is compared to a p-box where these parameters are rounded outward into intervals of 65-75 kg and 5-15 kg, respectively.

When the precise input distribution is unknown, other available pieces of information may be put together as constraints for the class of possible distributions. The intake of soil by children can be used as an example. Statistics given by ECETOC suggest 50th and 95th percentiles at 40 and 200 mg/d respectively.[43] These statistics can be used to define a lognormal probability distribution truncated at 200 mg/d (reasonable maximum exposure). A p-box can similarly be defined to only have positive values, an arithmetic mean of 65, a standard deviation of 82, and a max value of 200 mg/d, Fig. 3. It is readily inferred from both Figs. 2 and 3 that the uncertainty due to the choice of distributions can be particularly pronounced at the low and high percentiles.

3. RESULTS AND DISCUSSION

This investigation compared five different sets of input definitions for the environmental exposure model: point estimates, point estimates with rounding errors, probability distributions, probability boxes (p-boxes), and p-boxes with rounding errors, Table I. The first two sets of point estimates were parameterized directly with data from the exposure model used by the Swedish EPA. The three following sets of probabilistic input definitions were partly based on supplementary data (see Methods); this should be taken into account when comparing results between the different sets. However, it should also be observed that the deterministic and interval approaches cannot use this extra information.

3.1 Deterministic calculation and rounding errors

The deterministic point estimate of the cadmium intake, with a sensitive land use scenario, was 1.8×10^{-3} mg/kg/day. The tolerable daily intake (TDI) applied for cadmium by the Swedish EPA is 1.0×10^{-3} mg/kg/day, thus indicating a potential for negative health effects.

The uncertainty in any exposure estimate depends on many factors. Scenario and conceptual model uncertainty affect any type of exposure modeling, and can often be assumed to have a dominant role. Here, however, the focus is on the characterization of the chosen model variables and constants. In a deterministic model these are assigned as precise numbers. A few examples from the Swedish exposure model can be used as illustration: the dry soil bulk density is assigned a value of 1.5 kg/dm^3, the proportion of vegetables grown at the site is specified as 0.3, and the bioconcentration factor for cadmium to stem vegetables is given a value of 0.7. Taking the rounding errors expressed by the significant digits into account, these numbers can be specified as 1.45-1.55, 0.25-0.35, and 0.65-0.75, respectively. If all constants and variables are assigned as imprecise numbers in an equal manner, then the estimated intake of cadmium will vary between 6.9×10^{-4} to 1.1×10^{-2} mg/kg/day. Thus, already the rounding of numbers in the deterministic estimate has a substantial influence on the outcome and appraisal of the potential for health effects. The intake seemingly could be anything between 31% below to 1000% above the TDI.

The reported interval represents the best possible estimate given the uncertainty embodied by the significant digits.

3.2 Probabilistic Monte Carlo simulation

The MC simulation, with probability distributions assigned to most input variables and constants, indicates an intake of cadmium in the interval 1.6×10^{-4} to 1.3×10^{-3} mg/kg/day, with a median value at 4.7×10^{-4} mg/kg/day. The interval equals the 5th and 95th percentiles of the output probability distribution, Fig. 4.

A sensitivity analysis was performed by evaluating the Spearman rank correlation coefficient (r_s) between the different input variables and the estimated total intake. The most important inputs were the total soil concentration of cadmium (r_s=0.54), the average daily water consumption (r_s=0.37), the fraction of consumed vegetables grown on site (r_s=0.33), followed by three other variables related to the intake from vegetables, the surface soil concentration and the body weight (eight variables in all). Ten input variables, assigned with a probability distribution, were of less importance. Not surprisingly, the most important exposure routes were ingestion of vegetables and drinking water, with estimated contributions at the 50th percentile of 47% and 50%, respectively.

Here it is interesting to note that the uncertainty and variability described by the MC simulation is less than the previously investigated rounding errors. This could indicate that the probabilistic approach alone cannot fully capture the uncertainty present.

3.3 Probability bounds analysis (PBA)

The uncertainty in selecting the correct probability distribution for an input may be evaluated by running the MC simulations repeatedly with different distribution selections. However, already with a small or medium-sized exposure model this task quickly becomes practically impossible. The model used here initially had 18 parametric distributions assigned, and testing of only two different distribution assumptions for each would require the evaluation of 2^18 or 262,144 combinations.

P-boxes, as previously described, provide a convenient approach to represent all probability distributions meeting a set of specified constraints. To evaluate the uncertainty in the distribution assignments, all parametric distributions were supplemented by p-boxes applying the previously used parameters (min, max, mean, mode, and standard deviation) as constraints. Symmetric shape was added as an additional constraint for variables previously assigned a normal distribution (body weight and the average daily consumption of vegetables and drinking water). Variables previously assigned as lognormal distributions were constrained to have values above zero. Other constraints, such as assigning specific distributions with uncertainty in the parameters, could have been considered if more were known about the site and its future population. Inputs held constant in the MC simulation were also assigned as precise numbers in this analysis.

The PBA indicates an intake of cadmium in the interval 1.0×10^{-4} to 1.6×10^{-3} mg/kg/day for the 50th percentiles, and in the interval 1.7×10^{-5} to 6.2×10^{-3} mg/kg/day for the lower 5th and upper 95th percentiles, Fig. 5. The two cumulative distribution functions, as depicted in the figure, circumscribe the uncertainty for estimated total intake of cadmium.

The PBA shows that the choice of input distributions is critical for both the lower and upper estimates of intake; interestingly, however, the largest deviation is for the lower bound, thus indicating that the risks may be grossly overestimated. The explanation for this difference between the MC simulation and the PBA is to be found in our frequent use of lognormal distributions, which are highly skewed, to define inputs in the exposure model.

Sensitivity analyses are more cumbersome with the PBA method. The partial derivatives can be computed and evaluated, but ‘pinching’ the input variables is a more robust approach. Each probability box was replaced in turn by a corresponding deterministic value and the reduction in the range of uncertainty was evaluated. The same eight input variables as in the MC simulation were important together with one additional variable related to the intake of vegetables (f_{stem}). Both the MC simulation and the PBA thus indicate that half of the input variables assigned with probability distributions or p-boxes could be substituted with scalars, without influence on the outcome. The direct oral, dermal and inhalation exposure pathways could actually have been eliminated altogether from this example without making much of a difference.

3.4 Probability bounds analysis (PBA) with rounding errors added

A substantial number of inputs were assigned a precise value in the previous intake estimations, except for the evaluation of rounding errors in the deterministic calculation. In a similar manner, imprecise numbers can be added to the probability bounds analysis. Here we limit the use of imprecise numbers to the previously constant inputs, although it would also be possible to apply imprecise numbers to defining parameters for distributions and constraints of p-boxes. A PBA with rounding errors added indicates an intake of cadmium in the interval 3.1×10^{-5} to 3.9×10^{-3} mg/kg/day for the 50th percentile, and in the interval 4.8×10^{-6} to 1.8×10^{-2} mg/kg/day for the lower 5th and upper 95th percentiles, Fig. 6.

The probability bounds of the output distribution are wide when all this uncertainty is taken into account. Some inputs could possibly be specified with greater precision in the future, while uncertainty should be added to others since the defining parameters/constraints are imprecise. Dependencies between input variables are an additional source of uncertainty. In this evaluation we have so far assumed complete independence to facilitate the comparison between the methods and intake estimates. The last PBA calculation was, however, repeated without assuming independence between:

transport to stem, leaf and root part of plants; dermal soil exposure, exposed skin area and exposure time; respirable dust indoors and outdoors from contaminated area; breathing rate and lung retention; average daily consumption of vegetables and fraction of consumed vegetables grown on site; intake for each exposure route and body weight. This PBA, with major independence assumptions removed, indicates an intake of cadmium in the interval 1.3×10^{-5} to 9.4×10^{-3} mg/kg/day for the 50th percentile, and in the interval 1.7×10^{-6} to 6.7×10^{-2} mg/kg/day for the lower 5th and upper 95th percentiles. The probability bounds widen substantially, but less than an order of magnitude. Our results thus seem to corroborate the previously cited observation, that the choice of input distributions may be more important for the outcome.(20)

3.5 Comparison of the different intake estimates

The deterministic approach appears to be simple and straightforward, but this is true only superficially. The assignment of the values for input variables and constants is inevitably uncertain, with some values given as best estimates and others as conservative estimates. In addition, we have demonstrated that the rounding errors add more than an order of magnitude to this uncertainty, further complicating the evaluation.

A varying proportion of the uncertainty is accounted for when applying the different probabilistic approaches. With the MC analysis the risk assessor needs to know which input distributions to apply, while the PBA approach is possible also when the exact shapes of the distributions are unknown. The consequences of selecting one approach over another can be visualized with Box-Whisker type plots, Fig. 7.

The difference between the deterministic estimate and the median of the Monte Carlo simulation is mainly due to the substitution of conservative point estimates by probability distributions with realistic centers of gravity. A striking observation is that the uncertainty due to rounding errors is greater than the difference between the high (95th) and low (5th) percentile in the MC simulation of variability and uncertainty. However, it should be noted that the span in simulation results could be even wider if all variables and constants were supplemented with probability distributions.

The span between high and low estimates can be overwhelming when p-boxes describe the inputs.[37] It is therefore reasonable to ask if uncertainty may be overstated. The PBA method allows the specification of p-boxes with a varying degree of detail. Here we have used p-boxes that are free of distribution assumptions, but a p-box can also be described by a parametric probability distribution with uncertainty regarding the values of the defining parameters. If there is no uncertainty, then this p-box converges to the corresponding probability distribution and the outcome will be the same as for a MC simulation. Hence, the methodology itself does overstate or understate uncertainty. Instead it is the information supplied by the analyst that may be too precise or imprecise. Extensive studies over the last 25 years seem to suggest that former is more common, i.e. the knowledge about the problem is overstated and uncertainty is understated.[25]

The uncertainty in distribution assumptions is seldom shown in probabilistic risk assessments and could have profound implications for risk management decisions. It is not surprising that the upper-bound intake estimate increases and a simplistic interpretation would be, without further consideration, to call for even more stringent clean up targets. However, the wide span between the high and low uncertainty bounds suggests that an approach that focuses only on the high percentiles and upper confidence limits is biased and potentially misleading. Risk management decisions, risk communication, and stakeholder involvement should provide full disclosure by also describing the uncertainty in the other direction. Disregarding this part of the information could otherwise lead to a distortion of risk management priorities.

4. CONCLUSIONS

The problem of excessive precision is not new in risk analysis, and a recent review has called for a more explicit consideration of uncertainty.[(48)] The probabilistic approach is a considerable improvement on previous deterministic risk assessment practices, in that it attempts to characterize uncertainty and variability. However, some inputs continue to be assigned as precise numbers, while others are characterized as precise probability distributions. Such precision is hard to justify, as is the subjective assignment of probability distributions to characterize uncertainty. In this paper, we have highlighted the consequences of recognizing this lack of precision, in numbers and in probability distributions, in a standard environmental exposure model for soil contaminants. We have not evaluated structural uncertainty and the uncertainty due to dependencies between input variables, but already this limited assessment clearly demonstrates that error bounds of exposure estimates are substantial, comprising several orders of magnitude.

Probability bounds analysis (PBA) seems to provide a straightforward and flexible approach to include all available information, without making any unfounded assumptions. PBA offers an interesting alternative to two-dimensional Monte Carlo (MC) simulations, and especially so if intervals are seen as more reliable than probability distributions for the bounding of uncertainty. The main problem with this technique is that it does not give a best estimate or probability density within the probability box. However, this does not limit the use of PBA as a quality assurance and bounding technique to improve the standard MC analyses. PBA can thus be applied to all kinds of advanced risk assessments involving empirical quantities, with similar implications for the decision-making.

The practice of selecting the best fitting distribution and characterizing its parameter uncertainty will obviously not disclose the full range of uncertainty. It therefore seems reasonable to require that probabilistic risk assessments should address this issue by actually evaluating a whole range of reasonable distribution assumptions. This evaluation should encompass most, if not all, input variables assigned with a probability distribution. Input variables assigned as numbers should at a minimum be evaluated for rounding errors.

In risk assessments, the usual practice is to focus on the upper-bound estimate or the high percentiles.(2) This is in accordance with the precautionary principle, but may become difficult to defend when the full range of uncertainty is exposed. In addition to the upper-bound estimate, a PBA also supplies a lower-bound estimate. We think it is reasonable to provide the complete set of information, as a framework for evaluation by decision-makers and stakeholders, to avoid the selection of overly-cautious risk management strategies. We should not be afraid to acknowledge that science can sometimes provide only very imprecise answers or no answer at all. In fact, such a demarcation is an important prerequisite for a continued reliance on scientific methods, where decision-making needs to be risk-informed rather than risk-based.(49) Scientific uncertainty could then be treated as knowledge, not ignorance, to develop our understanding and finding solutions to some of the urgent problems of modern society.[(50)] Not acknowledging the full degree of scientific uncertainty will blur the boundary between science and policy, is potentially misleading, and may damage the credibility of the risk analysis profession.[(4)]

The benefits of a full disclosure of the uncertainty in risk estimates were eloquently discussed recently.[(8)] There is an ethical obligation to communicate honestly the full extent of uncertainty,[(4)] but it may also provide an advantage in the decision-making process since it opens up a negotiation window. With precise point estimates, or a strictly regulated procedure using probabilistic information in a similar manner, this possibility for a meaningful risk dialogue would certainly diminish.

In summary, this paper has attempted to explore different approaches to quantify uncertainty and discuss its implications for risk-informed decisions. It seems that the uncertainty is often underestimated since distribution assumptions and rounding errors are not fully evaluated. We suggest, as a future practice, that such information should be included in advanced risk assessments and also be fully disclosed.

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REFERENCES

1. Kammen, D. M. & Hassenzahl, D. M. (1999). *Should we risk it? exploring environmental, health, and technological problem solving.* Princeton, NJ: Princeton University Press.

2. U.S. EPA. (2001). *Risk assessment guidance for Superfund: Volume III - Part A, Process for conducting probabilistic risk assessment.* Report EPA/540/R-02/002. Washington, DC: U.S. Environmental Protection Agency.

3. Cullen, A. C. & Frey, H. C. (1999). *Probabilistic techniques in exposure assessment: a handbook for dealing with variability and uncertainty in models and inputs.* New York, NY: Plenum Press.

4. Morgan, M. G., Henrion, M. & Small, M. (1990). *Uncertainty: a guide to dealing with uncertainty in quantitative risk and policy analysis.* Cambridge, UK: Cambridge University Press.

5. Regan, H. M., Colyvan, M. & Burgman, M. A. (2002). A taxonomy and treatment of uncertainty for ecology and conservation biology. *Ecological Applications, 12,* 618-628.

6. Winkler, R. L. (1996). Uncertainty in probabilistic risk assessment. *Reliability Engineering and System Safety, 54,* 127-132.

7. Ferson, S. & Ginzburg, L. R. (1996). Different methods are needed to propagate ignorance and variability. *Reliability Engineering and System Safety*, 54, 133-144.

8. Burgman, M. A. (2005). *Risks and decisions for conservation and environmental management.* Cambridge, UK: Cambridge University Press.

9. Elert, M., Jones, C. & Norman, F. (1996). *Development of generic guideline values - Model and data used for generic guideline values for contaminated soil in Sweden.* Report 4639. Stockholm, Sweden: Swedish Environmental Protection Agency.

10. Ferson, S. (2002). *RAMAS Risk Calc 4.0 software: Risk assessment with uncertain numbers.* Boca Raton, FL: Lewis Publishers.

11. Öberg, T. & Bergbäck, B. (2005). A review of probabilistic risk assessment of contaminated land. *Journal of Soils and Sediments, 5,* 213-224.

12. Finley, B. & Paustenbach, D. (1994). The benefits of probabilistic exposure assessment: Three case studies involving contaminated air, water, and soil. *Risk Analysis, 14,* 53-73.

13. Vose, D. (2000). *Risk analysis: a quantitative guide.* Chichester, UK: Wiley.

14. Thompson, K. M. (1999). Developing univariate distributions from data for risk analysis. *Human and Ecological Risk Assessment, 5,* 755-783.

15. Stanek III, E. J. (1996). Estimating exposure distributions: A caution for Monte Carlo risk assessment. *Human And Ecological Risk Assessment, 2,* 874-891.

16. Haas, C. N. (1997). Importance of distributional form in characterizing inputs to Monte Carlo risk assessments. *Risk Analysis, 17,* 107-113.

17. U.S. EPA. (1997). *Guiding principles for Monte Carlo analysis.* Report EPA/630/R-97/01. Washington, DC: U.S. Environmental Protection Agency.

18. Burmaster, D. E. & Anderson, P. D. (1994). Principles of good practice for the use of Monte Carlo techniques in human health and ecological risk assessments. *Risk Analysis, 14,* 477-481.

19. U.S. EPA. (1999). *Report on the Workshop on selecting Input Distributions for Probabilistic Assessments.* Report EPA/630/R-98/004. Washington, DC: U.S. Environmental Protection Agency.

20. Bukowski, J., Korn, L. & Wartenberg, D. (1995). Correlated inputs in quantitative risk assessment - The effects of distributional shape. *Risk Analysis, 15,* 215-219.

21. Finley, B., Proctor, D., Scott, P., Harrington, N., Paustenbach, D. & Price, P. (1996). Recommended distributions for exposure factors frequently used in health risk assessment. *Risk Analysis, 14,* 533-551.

22. Hope, B. K. (1999). Distributions selected for use in probabilistic human health risk assessments in Oregon. *Human and Ecological Risk Assessment, 5,* 785-808.

23. U.S. EPA. (1997). *Exposure factors handbook.* Report EPA/600/P-95/002F. Washington, DC: U.S. Environmental Protection Agency.

24. Moore, D. R. J. (1996). Using Monte Carlo analysis to quantify uncertainty in ecological risk assessment: Are we gilding the lily or bronzing the dandelion? *Human and Ecological Risk Assessment, 2,* 628-633.

25. Bier. V. (2004). Implications of the research on expert overconfidence and dependence. *Reliability Engineering and System Safety, 85.* 321-329.

26. Binkowitz, B.S. & Wartenberg, D. (2001). Disparity in quantitative risk assessment: A review of input distributions. *Risk Analysis, 21,* 75-90.

27. Maddalena, R. L., McKone, T. E. & Sohn, M. D. (2004). Standardized approach for developing probabilistic exposure factor distributions. *Risk Analysis, 24,* 1185-1199.

28. Lessmann, K., Beyer, A., Klasmeier, J. & Matthies, M. (2005) Influence of distributional shape of substance parameters on exposure model output. *Risk Analysis, 25,* 1137-1145.

29. Frey, H. C. & Rhodes, D. S. (1998). Characterization and simulation of uncertain frequency distributions: Effects of distribution choice, variability, uncertainty, and parameter dependence. *Human and Ecological Risk Assessment, 4,* 423-468.

30. Brattin, W.J., Barry, T.M. & Chiu, N. (1996). Monte Carlo modeling with uncertain probability density functions. *Human and Ecological Risk Assessment, 2,* 820-840.

31. Hamed, M. M. (2000). Impact of random variables probability distribution on public health risk assessment from contaminated soil. *Journal of Soil Contamination, 9,* 99-117.

32. Williamson, R.C. & Downs, T. (1990). Probabilistic arithmetic I: numerical methods for calculating convolutions and dependency bounds. *International Journal of Approximate Reasoning, 4,* 89-158.

33. Frank, M. J., Nelsen, R. B. & Schweizer, B. (1987). Best-possible bounds for the distribution of a sum - problem of Kolmogorov. *Probability Theory and Related Fields, 74,* 199-211.

34. Ferson, S. & Hajagos, J. G. (2004). Arithmetic with uncertain numbers: rigorous and (often) best possible answers. *Reliability Engineering and System Safety, 85,* 135-152.

35. Kriegler, E. & Held, H. (2005). Utilizing belief functions for the estimation of future climate change. *International Journal of Approximate Reasoning, 39,* 185-209.

36. Ferson, S. & Burgman, M. A. (1995). Correlations, dependency bounds and extinction risks. *Biological Conservation, 73,* 101-105.

37. Regan, H. M., Hope, B. Y. & Ferson, S. (2002). Analysis and portrayal of uncertainty in a food-web exposure model. *Human and Ecological Risk Assessment, 8,* 1757-1777.

38. Ricci, P. F., Rice, D., Ziagos, J. & Cox, L. A. (2003). Precaution, uncertainty and causation in environmental decisions. *Environment International, 29,* 1-19.

39. Hart, A. (Ed.) (2001). Probabilistic Risk Assessment for Pesticides in Europe: Implementation & Research Needs. Sand Hutton, UK: Central Science Laboratory.

40. Regan, H. M., Sample, B. E. & Ferson, S. (2002). Comparison of deterministic and probabilistic calculation of ecological soil screening levels. *Environmental Toxicology and Chemistry, 21,* 882-890.

41. Sander, P., Öberg, T. (2006). Comparing deterministic and probabilistic risk assessments. A case study at a closed steel mill in southern Sweden. *Journal of Soils and Sediments, 6,* 55-61.

42. Back, P.-E., Starzec, P., Wik, O., Elert, M. & Jones, C. (2005). *Calculation model for guideline values for soil. Draft version* (In Swedish: Beräkningsmodell för riktvärden för mark. Remissversion). Stockholm, Sweden: Swedish Environmental Protection Agency.

43. ECETOC. (2001). *Exposure factors sourcebook for European populations (with focus on UK data).* Brussels, Belgium: European Centre for Ecotoxicology and Toxicology of Chemicals.

44. Otte, P. F., Lijzen, J. P. A., Otte, J. G., Swartjes, F. A. & Versluijs, C. W. (2001). *Evaluation and revision of the CSOIL parameter set.* Bilthoven, The Netherlands; National Institute for Public Health and the Environment.

45. Vasquez, V. R. & Whiting, W. B. (2005). Accounting for both random errors and systematic errors in uncertainty propagation analysis of computer models involving experimental measurements with Monte Carlo methods. *Risk Analysis, 25,* 1669-1681.

46. Shlyakhter, A. I. (1994). An improved framework for uncertainty analysis: Accounting for unsuspected errors. *Risk Analysis, 14,* 441-447.

47. Ferson, S., Nelsen, R. B., Hajagos, J., Berleant, D. J., Zhang, J., Tucker, W. T., Ginzburg, L. R. & Oberkampf, W. L. (2004). *Dependence in probabilistic modeling, Dempster-Shafer theory, and probability bounds analysis.* Report SAND2004-3072. Albuquerque, NM: Sandia National Laboratories.

48. Hassenzahl, D. M. (2006). Implications of excessive precision for risk comparisons: Lessons from the past four decades. *Risk Analysis, 26,* 1-12.

49. Apostolakis, G. E. (2004). How useful is quantitative risk assessment? *Risk Analysis, 24,* 515-520.

50. Bradshaw, G. A. & Borchers, J. G. (2000). Uncertainty as information: Narrowing the science-policy gap. *Conservation Ecology, 4,* 7. [online] URL: http://www.consecol.org/vol4/iss1/art7/

Table I. Characterization of the input variables affecting the long-term exposure of children to cadmium using different estimation approaches: deterministic (det), Monte Carlo (MC), or probability bounds analysis (PBA), with or without rounding errors (err). Normal (N) and lognormal distributions (LN) are characterized by the arithmetic mean and the standard deviation. Intervals are shown with square brackets around and the nomenclature for p-boxes is adapted from ref. 10.

Variables	**Symbol**	**Det.**	**Det. with error**	**Monte Carlo**	**PBA**	**PBA with error**
General						
Concentration in soil 0-1 m, mg/kg	C_s	4.95	4.95	LN(3.1,1.0)	LN(3.1,1.0)	LN(3.1,1.0)
Concentration in soil total, mg/kg	C_t	17.4	17.4	LN(6.9,5.7)	LN(6.9,5.7)	LN(6.9,5.7)
Body weight child, kg	BW	15	[14.5,15.5]	N(18,2.66), min=5, max=25	symmeanstddev(18,2.66), min=5, max=25	symmeanstddev(18,2.66), min=5, max=25
Transport to groundwater						
Distribution soil-water, dm^3/kg	K_d	100	[50,150]	100	100	[50,150]
Soil water content, dm^3/dm^3	θw	0.3	[0.25,0.35]	triangular(0.05,0.3,0.5)	minmaxmode(0.05,0.5,0.3)	minmaxmode(0.05,0.5,0.3)
Soil bulk density, kg/dm^3	ρ_b	1.5	[1.45,1.55]	triangular(0.25,1.2,1.6)	minmaxmode(0.25,1.6,1.2)	minmaxmode(0.25,1.6,1.2)
Dilution soil-groundwater	DF_{gw}	0.08	[0.022,0.27]*	0.08	0.08	[0.022,0.27]*
Transport to plants						
Bioconcentration stem and leaf, (mg/kg dry)/(mg/kg soil)	BCF_{stem}	0.7	[0.65,0.75]	LN(0.85,0.61)	posmeanstddev(0.85,0.61)	posmeanstddev(0.85,0.61)
Fractional consumption, stem and leaf	f_{stem}	0.5	[0.45,0.55]	LN(0.38,0.13), max=1	posmeanstddev(0.38,0.13), max=1	posmeanstddev(0.38,0.13), max=1
Dry to fresh weight stem and leaf, kg/kg	r_{stem}	0.117	0.117	0.117	0.117	0.117
Bioconcentration root, (mg/kg dry)/(mg/kg soil)	BCF_{root}	0.15	[0.145,0.155]	LN(0.35,0.33)	posmeanstddev(0.35,0.33)	posmeanstddev(0.35,0.33)
Fractional consumption, root	f_{root}	$1- f_{stem}$	$1- f_{stem}$	$1- f_{stem}$	$1- f_{stem}$	$1- f_{stem}$
Dry to fresh weight root, kg/kg	r_{root}	0.202	0.202	0.202	0.202	0.202
Direct oral intake						
Daily soil intake, mg/kg	SI	150	[145,155]	LN(65,82), max=200	posmeanstddev(65,82), max=200	posmeanstddev(65,82), max=200
Exposure time, day	t_{is}	365	365	365	365	365

<u>Dermal uptake</u>						
Dermal soil exposure, $mg/m^2/day$	SE	5100	[5050,5150]	LN(2000,990), max=7400	posmeanstddev(2000,900), max=7400	posmeanstddev(2000,900), max=7400
Exposed skin area, m^2	A	0.28	[0.275,0.285]	LN(0.18,0.017), max=0.24	posmeanstddev(0.18,0.017), max=0.24	posmeanstddev(0.18,0.017), max=0.24
Relative dermal absorption	f_{du}	0.14	[0.135,0.145]	0.14	0.14	[0.135,0.145]
Exposure time, day	t_{du}	80	[75,85]	80	80	[75,85]
<u>Inhalation uptake</u>						
Concentration of respirable dust indoors, mg/m^3	$C_{d,in}$	0.052	[0.0515,0.0525]	triangular(0.037,0.069, 0.1)	minmaxmode(0.037,0.1,0.069)	minmaxmode(0.037,0.1,0.069)
Fraction of dust indoors from contaminated area	$f_{d,in}$	0.8	[0.75,0.85]	triangular(0.5,0.65, 0.8)	minmaxmode(0.5,0.65,0.8)	minmaxmode(0.5,0.65,0.8)
Fraction of time spent indoors	$f_{t,in}$	0.88	[0.875,0.885]	uniform(0.75,1)		
Concentration of respirable dust outdoors, mg/m^3	$C_{d,out}$	0.07	[0.065,0.075]	triangular(0.05,0.075, 0.1)	minmaxmode(0.05,0.075,0.1)	minmaxmode(0.05,0.075,0.1)
Fraction of dust outdoors from contaminated area	$f_{d,out}$	0.5	[0.45,0.55]	0.5	minmax(0.75,1)	minmax(0.75,1)
Fraction of time spent outdoors	$f_{t,out}$	$1- f_{t,in}$	$1- f_{t,in}$	$1- f_{t,in}$	$1- f_{t,in}$	$1- f_{t,in}$
Breathing rate, m^3/day	BR	7.6	[7.55,7.65]	7.6	7.6	[7.55,7.65]
Lung retention	LR	0.75	[0.745,0.755]	0.75	0.75	[0.745,0.755]
Exposure time, day	t_{id}	365	365	365	365	365
<u>Intake from vegetables</u>						
Daily consumption of vegetables, kg/day	R_{ig}	0.15	[0.145,0.155]	N(0.13,0.04), min=0	symmeanstddev(0.13,0.04), min=0	symmeanstddev(0.13,0.04), min=0
Fraction of consumed vegetables grown on site	f_h	0.3	[0.25,0.35]	triangular(0,0.13, 0.3)	minmaxmode(0,0.3,0.13)	minmaxmode(0,0.3,0.13)
Exposure time, day	t_{ig}	365	365	365	365	365
<u>Intake with drinking water</u>						
Daily water consumption, dm^3/day	WC	1	[0.5,1.5]	N(0.87,0.49), min=0.1, max=3	symmeanstddev(0.87,0.47), min=0.1, max=3	symmeanstddev(0.87,0.47), min=0.1, max=3
Exposure time, day	t_{iw}	365	365	365	365	365

* Best possible bounds estimated separately from expressions with repeated parameters.

Figure captions

Fig. 1. Transport and exposure pathways considered in this study.

Fig. 2. An example normal distribution of body weight (solid curve) circumscribed by a p-box (dashed lines).

Fig. 3. Estimated soil intake by children as a lognormal distribution (solid curve) and a p-box (dashed lines).

Fig. 4. Cumulative probability distribution for the intake of cadmium (logarithmic scale) with TDI, 5th and 95th percentiles shown.

Fig. 5. Probability bounds for the intake of cadmium (logarithmic scale) with TDI, 5th and 95th percentiles shown.

Fig. 6. Probability bounds with rounding errors for the intake of cadmium (logarithmic scale) with TDI, 5th and 95th percentiles shown.

Fig. 7. Estimated intake of cadmium (logarithmic scale) using different approaches: deterministic (det), Monte Carlo (MC), or probability bounds analysis (PBA), with or without rounding errors (err). The error bars show the difference between high and low estimates (deterministic) or 5th and 95th percentiles (MC and PBA). The 50th percentile is shown as a horizontal line (MC) or as a box (PBA), representing the high and low bounds.

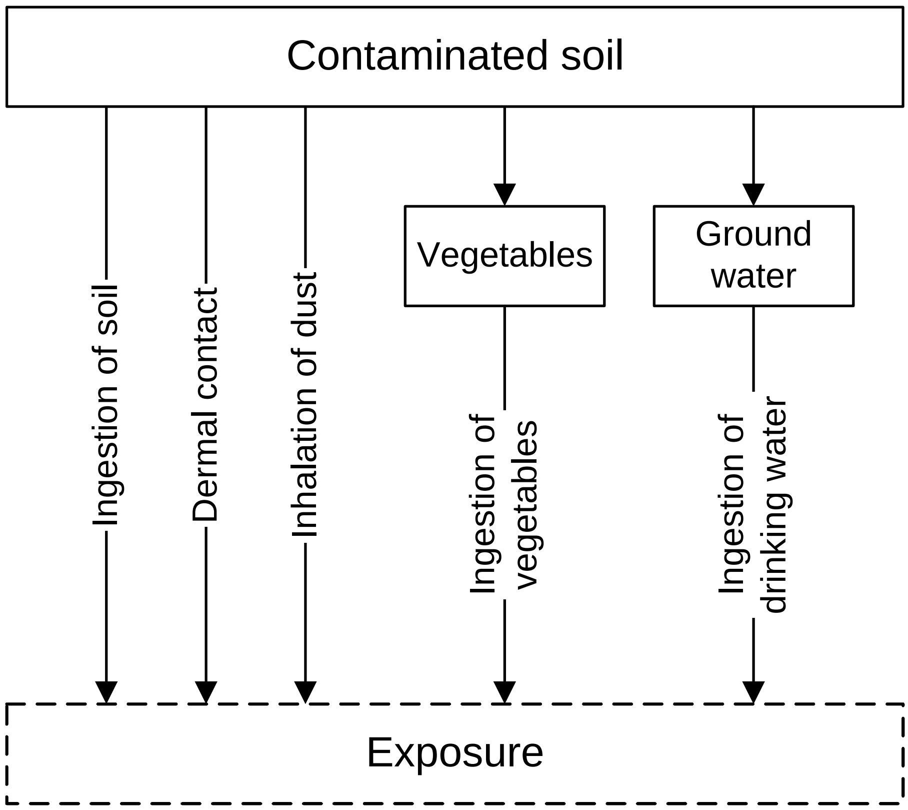
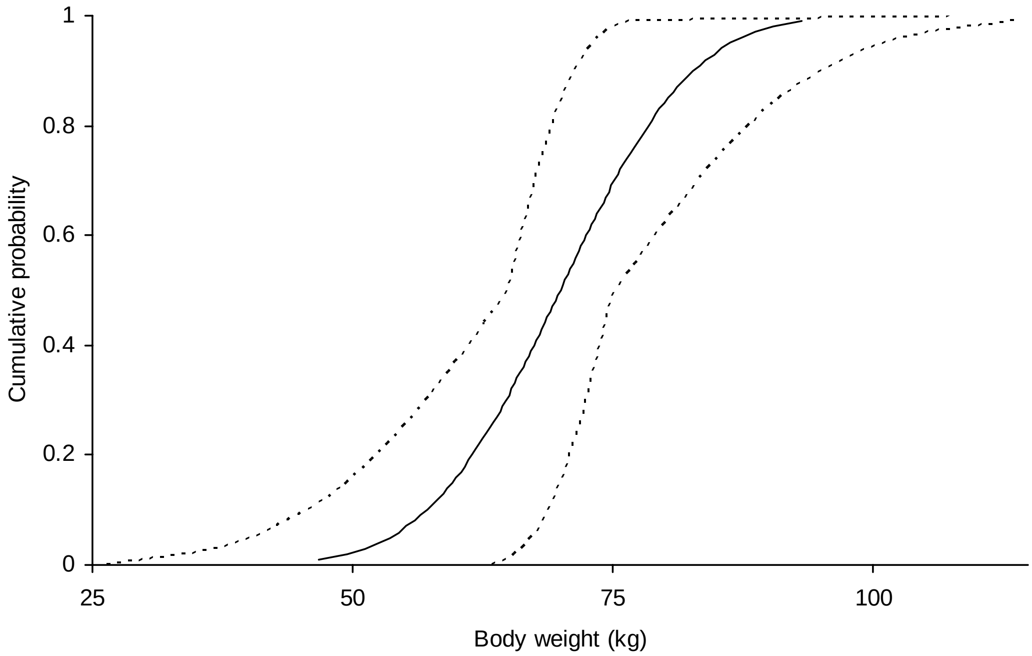

Contaminated soil
Vegetables
Ground water
Ingestion of soil
Dermal contact
Inhalation of dust
Ingestion of vegetables
Ingestion of drinking water
Exposure

Fig. 1



1
0.8
0.6
0.4
0.2
0
Cumulative probability
25
50
75
100
Body weight (kg)

Fig. 2

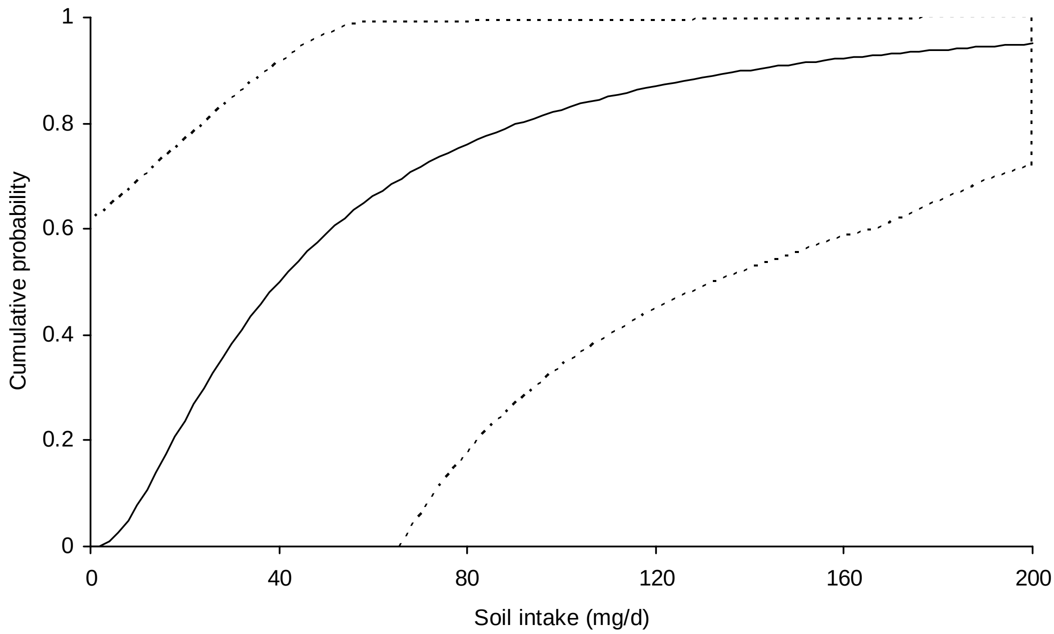

Cumulative probability
1
0.8
0.6
0.4
0.2
0
0
40
80
120
160
200
Soil intake (mg/d)

Fig. 3

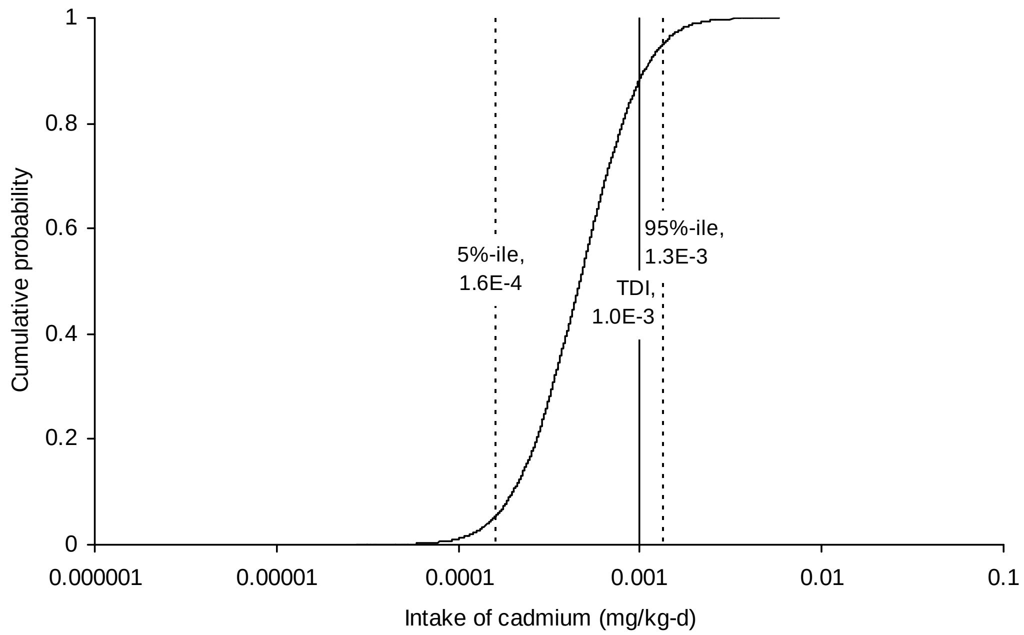

1
0.8
0.6
0.4
0.2
0
Cumulative probability
5%-ile,
1.6E-4
95%-ile,
1.3E-3
TDI,
1.0E-3
0.000001
0.00001
0.0001
0.001
0.01
0.1
Intake of cadmium (mg/kg-d)

Fig. 4

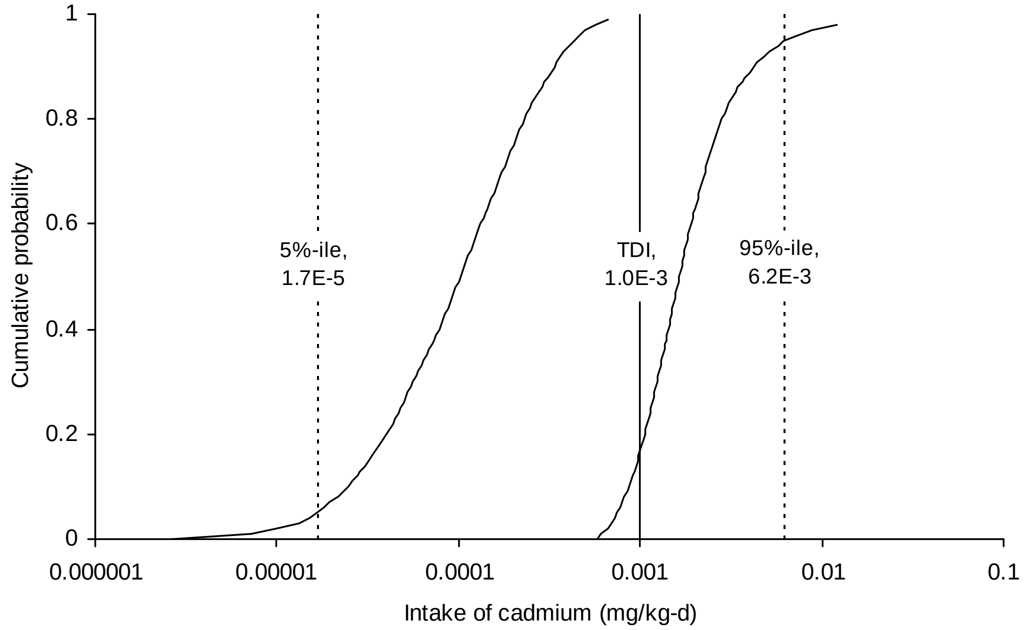
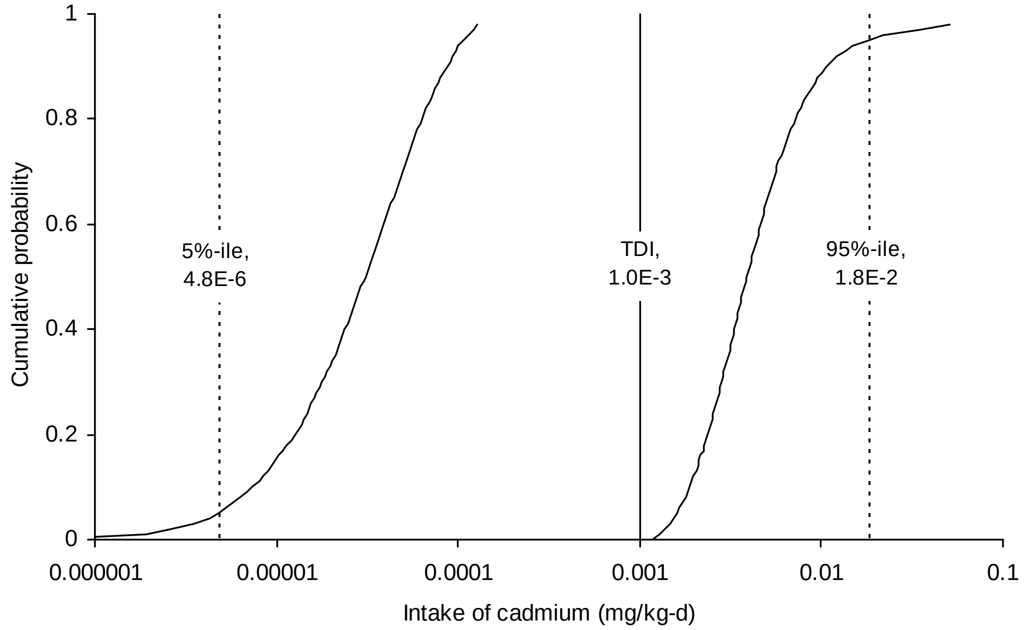
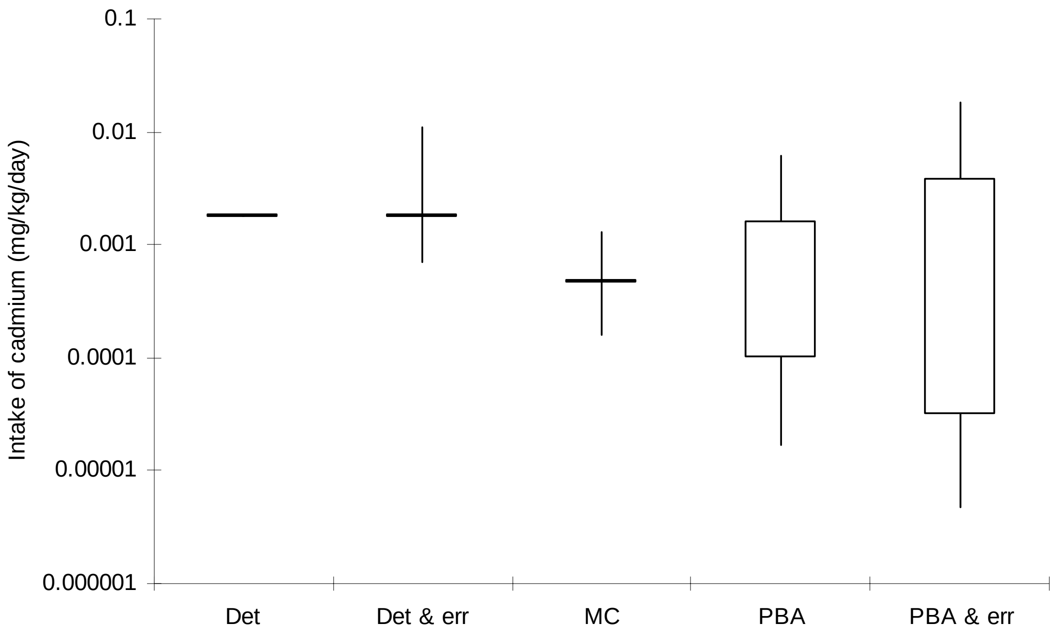

1
0.8
0.6
0.4
0.2
0
Cumulative probability
5%-ile,
1.7E-5
TDI,
1.0E-3
95%-ile,
6.2E-3
0.000001
0.00001
0.0001
0.001
0.01
0.1
Intake of cadmium (mg/kg-d)

Fig. 5



1
0.8
0.6
0.4
0.2
0
Cumulative probability
5%-ile,
4.8E-6
TDI,
1.0E-3
95%-ile,
1.8E-2
0.000001
0.00001
0.0001
0.001
0.01
0.1
Intake of cadmium (mg/kg-d)

Fig. 6



0.1
0.01
0.001
0.0001
0.00001
0.000001
Intake of cadmium (mg/kg/day)
Det
Det & err
MC
PBA
PBA & err

Fig. 7