Case Studies

Comparing Deterministic and Probabilistic Risk Assessments

A case study at a closed steel mill in southern Sweden

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Abstract

Background, Aims and Scope. Contaminated land is a high priority environmental problem in most of Europe and North-America. Sweden is no exception and generic guideline values have been developed for the initial assessment, but site-specific assessments are also needed. The generic guideline values are not applicable when the exposure conditions are different from the typical Swedish conditions or when the site contains a particularly sensitive ecosystem. The Swedish guideline values have, like in many other countries, been set by using deterministic point estimates for all variables and constants in the used multimedia model. The same approach is common also for site-specific assessments, and a limitation is that it fails to quantify variability and uncertainty. Probabilistic risk assessment provided a method to deal with this problem. Variability and uncertainty in the input parameters (variables or constants) are described by probability distributions, and likewise the output (risk or exposure) is presented as a probability distribution. A substantial number of probabilistic risk assessments for contaminated land at sites in North America, Europe and Asia have been published. However, an extensive review of the literature did not identify any study where probabilistic risk assessment was applied to a site contaminated by an iron or steel industry. Here we will describe such a case, where we have compared a deterministic point estimate with a probabilistic risk assessment for six elements and benzo[a]pyrene.

Methods. The site had different metallurgical plants in operation for more than 100 years. Most parts of the steel mill were closed by the mid 1980s, and today the site is used by small-sized enterprises. The soil is contaminated with metals from the previous industrial operations. The present owner plans to develop the site and has therefore initiated extensive investigations of soil contamination. Sixty-two soil samples collected between 1997 and 2000 provided a good coverage of the whole site, and were analyzed for the content of different elements and polycyclic aromatic hydrocarbons (PAH). The exposure assessments were focused on six elements with high concentrations compared to the generic guideline values; arsenic (As), lead (Pb), cadmium (Cd), chromium (Cr), copper (Cu) and zinc (Zn). In addition, benzo[a]pyrene was included due to the high toxicity and comparatively high concentrations. Variability and uncertainty were characterized in a Monte Carlo simulation of exposures (10,000 iterations), and the exposures were evaluated with two land use scenarios; less sensitive use and sensitive use.

Results and Discussion. The deterministic point estimates and the probabilistic estimates of the 95th percentile are in approximately the same ranges in the scenario of less sensitive land use. It is only the exposure for arsenic that is slightly above the toxicological reference value (TRV) in the deterministic assessment. In the probabilistic assessment, the exposure for all elements is below the TRV. The results for sensitive land use are applicable to a scenario where the site is developed for general housing. The deterministic point estimates and the probabilistic estimates of the 95th percentile are also here in approximately the same ranges, but the exposure exceeds the TRV for arsenic, cadmium and lead. Drinking water, vegetables grown on site and soil ingestion are the major exposure pathways for this scenario. In this assessment, the estimated intake distributions are applicable to a randomly selected individual. The probability distributions used here to characterize the different soil parameters are typically representing both variability and uncertainty, and the same is true the majority of the exposure variables. We therefore decided not to attempt to separate variability and uncertainty at this stage, but with additional data from a more in-depth site investigation it might be possible to achieve this.

Conclusions and Outlook. To the best of our knowledge, this study is the first report on a probabilistic risk assessment on a former iron and steel works site. The materials handled by this industry were less toxic than for many other metallurgical operations, but contaminants may still severely limit the options for future land use. This case study shows that probabilistic exposure estimates for a set of soil contaminants can be quite similar to deterministic point estimates. The main difference is instead to be found in the additional information obtained with the probabilistic assessment. The sensitivity analyses show pathways and input variables that contribute most to variations in the total intake of each contaminant, e.g. dermal contact and ingestion of soil, vegetables and drinking water. This information can be used both in the planning of future land use and for active measures to reduce current exposure. The probabilistic assessment also provides information on the magnitude of exposure and the margin of safety. This information may facilitate risk communication between decision-makers and stakeholders. The presentation of results from probabilistic risk assessments is only briefly discussed in the literature and here we see a need for research and opportunities for enhancement. The choice of data analytical tools may then be of importance, since more complex multimedia models are rather difficult to decipher when implemented within traditional spreadsheet software. Some of the research needs are identified here and in a previous review article in this journal.

Keywords: Arsenic; contaminated soils; drinking water; exposure assessments; Monte Carlo simulation; multimedia models; probabilistic risk assessments; sensitivity analysis; steel mills; uncertainties

Introduction

Contaminated land is a high priority environmental problem in most of Europe and North-America [1,2]. Sweden is no exception and it is estimated that about 50,000 contaminated sites exist. These sites are prioritized after a preliminary assessment and those with the highest ranking are investigated further. Generic guideline values have been developed for the initial assessment, to indicate the degree of contamination, and to develop clean-up goals. These generic guideline values are not always applicable, and they can be substituted with a site-specific assessment when appropriate. A site-specific assessment is needed when the exposure conditions are different from the typical Swedish conditions or when the site contains a particularly sensitive ecosystem.

The generic guideline values have been developed for three types of land use [3]: Sensitive use, less sensitive use with groundwater extraction, and less sensitive use without groundwater extraction. A main difference between these land use scenarios is the number of human exposure pathways considered (**Fig. 1**). Soil ingestion, dermal contact and inhalation of dust and vapours are included in all three exposure scenarios. Ingestion of drinking water is included in both the scenarios of sensitive use and less sensitive use with groundwater extraction. Ingestion of vegetables and fish is only considered in the scenario of sensitive land use.

The methodology used to develop the Swedish guideline values is similar to that employed in other countries, e.g. the Netherlands, the Unites States and Canada. A simple exposure model has been defined and expressed mathematically for each pathway considered. The exposure from each of these pathways is then added and compared to specified toxicological and ecotoxicological criteria. Assumptions are made about constant concentration of contaminants and equilibrium partitioning between different media.

The guideline values are derived by rearrangement of the mathematical model expressions, insertion of the toxicological reference values and subsequent 'back-calculation' to get a reference concentration for that media. As an example, the intake from vegetables grown on the site may be expressed as:

$$Intake = C_s \cdot R_{ig} \cdot f_b \cdot K_{pl}$$

where C_s is the soil concentration of the contaminant, R_{ig} is the average daily consumption, f_b is the fraction of vegetables grown on the site, and K_{pl} is the plant-soil concentration ratio.

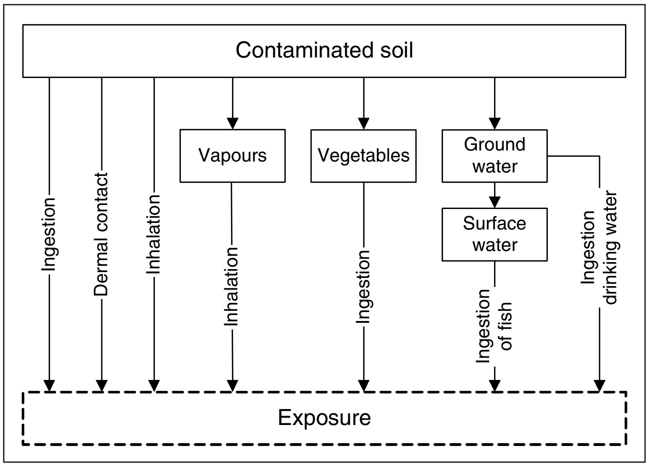

Fig. 1: Transport and exposure pathways considered for the Swedish generic guideline values

The soil reference concentration for this pathway (C_{ig}) is then calculated by substituting the intake with the toxicological reference value (*TRV*) and rearranging the expression to:

$$C_{ig} = TRV / (R_{ig} \cdot f_b \cdot K_{pl})$$

The *TRV* represent a tolerable daily intake or a lifetime excess cancer risk of 1E-5. Subsequently, the inverse of the sum of the inverted reference soil concentrations for all exposure pathways considered is taken as the integrated human health value (C_{unadj}). These integrated health values are, after some minor adjustments, adopted as generic guideline values:

$$C_{unadj} = 1 / \Sigma (1 / C_i)$$

The Swedish guideline values have, like in many other countries, been set by using deterministic point estimates for all variables and constants in the used multimedia model. The limitation with this approach is that it fails to quantify variability and uncertainty [4]. The approach adopted to deal with uncertainty is instead to use conservative assumptions and data in the model, but this does not provide any information on the margin of safety or the magnitude of the risks for the exposed populations.

The problems with the deterministic method have been extensively discussed, and by the early 1990s it became apparent that there was a need of further development and improvement [5]. The unrealistic risk estimates emanating from applying the traditional deterministic method had already attracted attention [6]. It was also noticed that no guidance was available to decision makers on whether to conduct additional investigations or select from available options to mitigate risks [7]. Probabilistic risk assessment provided a method to deal with these problems. Variability and uncertainty in the input parameters (variables or constants) are described by probability distributions, and the output (risk or exposure) is likewise presented as a probability distribution [8].

The probabilistic method involves a characterization of uncertainty (lack of knowledge) and variability (natural variation) to obtain a better basis for risk management decisions. Parameter uncertainty is used here to denote the uncertainty in the estimates of variables used in the final exposure model. Partition constants and bioconcentration factors are two examples of model parameters that contribute significantly to the uncertainty in health and environmental risk assessments [9–11].

Interindividual variability (natural variation between individuals) is of major importance in all types of risk assessments. The differences between children and adults is the perhaps most noticeable factor to consider. Different lifestyles, food consumption, physiological characteristics, gender, diseases and occupation are some of the other factors that will have an influence on most health and environmental risks [7]. Spatial variability (variations in space) is another important aspect in risk assessments of contaminated land. The spatial distribution of soil pollutants is an obvious factor to evaluate, but soil properties may also vary [12].

A substantial number of probabilistic risk assessments for contaminated land at sites in North America, Europe and Asia have been published [13–24]. The experiences have in general been favourable and the probabilistic methodology has increased the understanding of uncertainty and variability, and thereby improved the risk management decision process [17,25]. It has been shown that the traditional deterministic risk estimates are sometimes too conservative and exaggerate the risks involved, but examples are available when the opposite is true and the probabilistic risk assessment supports more stringent cleanup goals [13,16–18].

An extensive review of the literature did not identify any study where probabilistic risk assessment was applied to a site contaminated by an iron or steel industry [4]. Here we will describe such a case, where we have compared a deterministic point estimate with a probabilistic risk assessment for six elements and benzo[a]pyrene. The purpose is to highlight the differences and evaluate what information the probabilistic method may add.

1 Materials and Methods

The site investigated is situated in Kallinge, a suburb to Ronneby, in the south-eastern corner of Sweden. Here, different metallurgical plants were in operation between 1849 and 1991. The first rolling mill for iron and sheet steel was built in 1854 and most parts of the steel mill were closed by the mid 1980s. The site has an area of approximately 25 hectare (250,000 m^2). Today the site is used by small-sized enterprises.

The soil is contaminated with metals from these previous industrial operations. Slag was extensively used as a filling material. Particulates and sludges from flue gas cleaning systems may also have contributed to this contamination. The present owner plans to develop the site and has therefore initiated extensive investigations of soil contamination. These investigations were carried out by the Karlskrona office of the consultants AB Jacobson & Widmark (now WSP Sweden AB). Data from these investigations were used by us as input in the comparative study of risk assessment methods.

Sixty-two soil samples collected between 1997 and 2000 provided a good coverage of the whole site, but some bias may have been introduced by more intensive sampling of areas assumed to be heavily contaminated. The analyses were carried out by laboratories accredited according to recognized European standards. SGAB Analytica (now Analytica AB, Stockholm, Sweden) analyzed the content of different elements, using inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and mass spectrometry (ICP-MS). Omegam Laboratoria (Amsterdam, the Netherlands) performed the analyses of polycyclic aromatic hydrocarbons (PAH). Site specific soil water distribution coefficients, hydraulic conductivity and the flow of groundwater were determined by the Swedish Geotechnical Institute (Linköping, Sweden).

The Swedish EPA has derived generic guideline values using a multimedia exposure model similar to the Dutch CSOIL model [3]. The same multimedia exposure model was used here as a basis for the comparative exposure assessments with the deterministic and probabilistic approaches. The exposure assessments were focused on six elements with high concentrations compared to the generic guideline values; arsenic (As), lead (Pb), cadmium (Cd), chromium (Cr), copper (Cu) and zinc (Zn). In addition, benzo[a]pyrene was included due to the high toxicity and comparatively high concentrations.

The 95% upper confidence limit (UCLM) of the arithmetic mean for each pollutant was estimated by bootstrapping, resampling with replacement, using the MS Excel add-in Resampling Stats for Excel (Resampling Stats Inc., Arlington, Virginia) [26]. This UCLM estimate was used in the deterministic assessment. In the probabilistic assessment, the uncertainty of the mean was described with lognormal distributions derived from the 5% lower confidence limit (LCLM) and the UCLM of the resampling distributions. Different bootstrap estimates were calculated for the depth of 0–1, 1–2 and >2 m.

Variability and uncertainty were propagated together in a Monte Carlo simulation of exposures (10,000 iterations) and the Spearman rank correlation coefficient was used for sensitivity analyses (correlation between the input variables and the outcome). The software used for the simulations was the MS Excel add-in CrystalBall (Decisioneering Inc., Denver, Colorado). Settings and distributions for the other input variables were chosen from the documentation of the Swedish model, the US EPA Exposure Factors Handbook [27], the Exposure Factors Sourcebook for European Populations [28], the revised CSOIL parameter set [29], and from statistics provided by the SCB Statistics Sweden and the Swedish National Food Administration.

The exposures were evaluated with two land use scenarios; less sensitive use and sensitive use. The first scenario encompasses use for offices, industry, roads, etc. Adults are assumed to be in the area during working hours, but children only temporarily. The second scenario, sensitive use, encompasses all type of land use, e.g. residential areas, kindergarten, agriculture and ground water extraction. The difference between these two scenarios thus rests mainly in the exposure pathways being considered.

2 Results

Exposure calculations with a deterministic and probabilistic approach were compared to the toxicological reference values used by the Swedish EPA [3]. It should be noted that in a Monte Carlo simulation it is generally not possible to directly back-calculate site specific guideline values, due to the dependency between the contaminant concentration in the soil and the estimated exposure [30].

2.1 Less sensitive land use

The results for less sensitive land use correspond to the present situation at the site. The deterministic point estimates and the probabilistic estimates of the 95th percentile are in approximately the same ranges (**Table 1**).

It is only the exposure for arsenic that is slightly above the toxicological reference value (TRV) in the deterministic assessment. In the probabilistic assessment, exposure for all elements are below the TRV. The cumulative probability distribution for the intake of arsenic is shown in **Fig. 2**.

It is mainly dermal contact and oral intake of soil that contributes to the exposure for arsenic and the other elements. The sensitivity to changes in the input variables may be estimated by the rank correlation coefficient, which is a distribution free approach. This sensitivity analysis also shows that the dermal intake by adults is of major importance for the total intake of arsenic (**Table 2**). However, soil ingestion by children temporarily at the site contributes substantially as well.

Table 2: Spearman's rank regression coefficients for the most important input variables describing the total intake of arsenic in the scenario of less sensitive land use

Input variable	Exposure pathway	Coefficient
Time of exposure, adult	Dermal contact	0.49
Exposed skin area, adult	Dermal contact	0.39
Soil ingestion, child	Soil ingestion	0.23
Dermal soil exposure, adult	Dermal contact	0.18
Soil concentration	Soil ingestion	0.16

2.2 Sensitive land use

The results for sensitive land use are applicable to a scenario where the site is developed for general housing. The deterministic point estimates and the probabilistic estimates of the 95th percentile are also here in approximately the same ranges (**Table 3**).

The exposure exceeds the TRV for arsenic, cadmium and lead in both the deterministic and probabilistic assessments of this land use scenario. The estimated intakes of arsenic

Table 1: Toxicological reference values (TRV) and the estimated total intake of six elements and benzo[a]pyrene (mg/kg-d) in the scenario of less sensitive land use

	As	Cd	Cr	Cu	Pb	Zn	B[a]P
TRV (oral)	6.0E-6	1.0E-3	1.0E+0	5.0E-1	3.5E-3	1.0E+0	2.3E-5
Deterministic	6.8E-6	1.2E-5	1.5E-4	1.8E-4	7.2E-4	2.9E-3	8.0E-8
Probabilistic*	3.8E-6	3.6E-4	5.1E-6	7.8E-5	1.2E-4	1.1E-3	1.2E-7

* 95th percentile

Table 3: The estimated total intake of six elements and benzo[a]pyrene (mg/kg-d) and percentages of the toxicological reference values (TRV) in the scenario of sensitive land use

	As	Cd	Cr	Cu	Pb	Zn	B[a]P
Deterministic	9.2E-4	1.9E-3	2.8E-3	4.8E-2	4.9E-2	3.6E-1	1.3E-5
% of TRV	15,000	190	0.28	10	1,400	36	56
Probabilistic*	4.3E-4	1.2E-3	3.7E-3	5.8E-2	2.9E-2	2.3E-1	8.7E-6
% of TRV	7,100	120	0.37	12	820	23	38

* 95th percentile

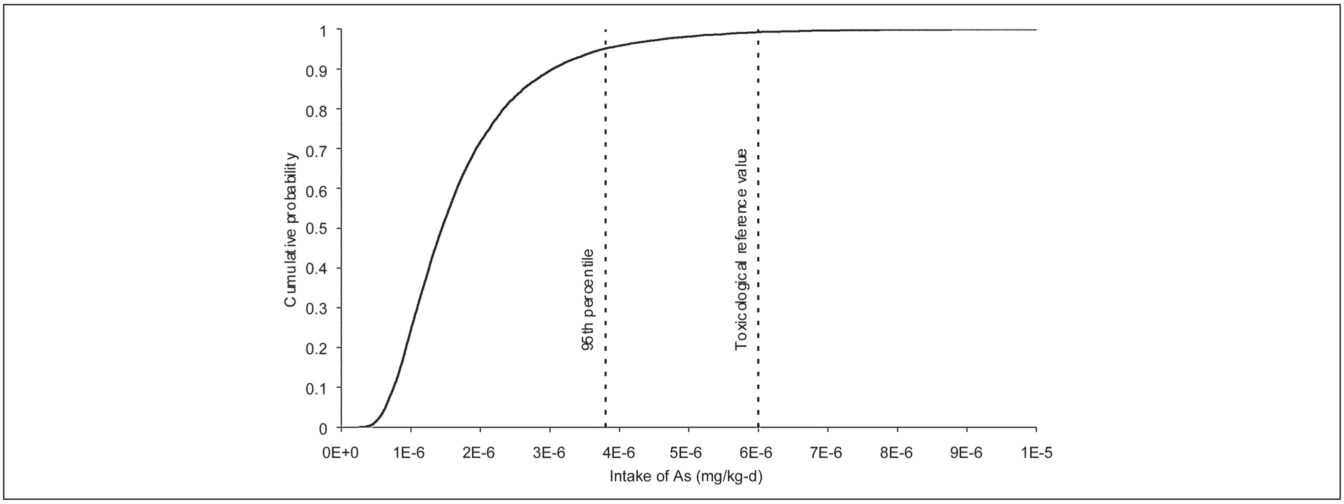

Fig. 2: Cumulative probability distribution for the intake of arsenic with UCLM and TRV denoted (scenario of less sensitive land use)

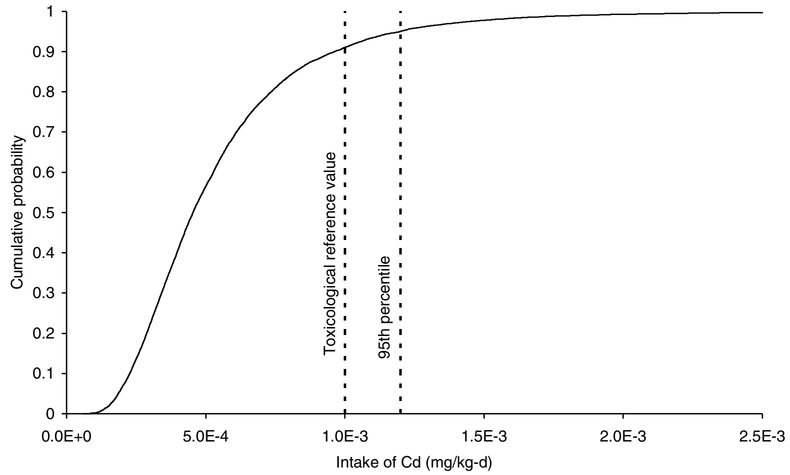

Fig. 3: Cumulative probability distribution for the intake of cadmium with TRV and UCLM denoted (scenario of sensitive land use)

and lead are substantially higher than the recommended health based TRV, while the intake of cadmium is only moderately above this value. The cumulative probability distribution for the intake of cadmium is shown in **Fig. 3**.

The exposure pathways included in this scenario and their relative contributions to the total intake of As, Cd and Pb are given in **Table 4**. The relative contributions in the probabilistic exposure assessment are specified at the 95th percentile.

Drinking water, ingestion of vegetables grown on site and soil ingestion are the major exposure pathways for this scenario. In the probabilistic assessment dermal contact is also important and in particular for arsenic. A sensitivity analysis for this element is given in **Table 5**.

2.3 Ecological effects

Onsite effects were evaluated by comparing the 95% upper confidence limit (UCLM) of the arithmetic mean for each pollutant, estimated by bootstrapping, with the Swedish guideline values (derived from the Dutch intervention values, **Table 6**). The ecotoxicological values for less sensitive land use are assumed to protect 50% of the soil organism species, but this level of protection was considered insuffi-

Table 5: Spearman's rank regression coefficients for the most important input variables describing the total intake of arsenic in the scenario of sensitive land use

Input variable	Exposure pathway	Coefficient
Time of exposure, adult	Drinking water	0.37
Time of exposure, adult	Dermal contact	0.35
Water consumption, children	Drinking water	0.32
Soil concentration	Drinking water	0.26
Soil exposure, adult	Dermal contact	0.25
Bioconcentration, roots	Ingestion of vegetables	0.20
Water consumption, adult	Drinking water	0.19
Exposed skin area, adult	Dermal contact	0.17

Table 6: The 95% UCLM for six elements and benzo[a]pyrene (mg/kg d.w.) together with the Swedish ecotoxicological values for less sensitive and sensitive land use

	As	Cd	Cr	Cu	Pb	Zn	B[a]P
UCLM	37	17	120	400	2,200	12,000	0.32
Less sensitive	40	12	250	200	300	700	40
Sensitive	20	6	120	100	150	350	20

Table 4: Relative contribution of each exposure pathway to the total intake of As, Cd and Pb (%) in the scenario of sensitive land use

Exposure pathway	Deterministic			Probabilistic		
	As (%)	Cd (%)	Pb (%)	As (%)	Cd (%)	Pb (%)
Soil ingestion	7.6	2.8	30	3.0	1.3	15
Dermal contact	0.5	1.0	0.4	36	7.9	3.9
Inhalation of dust	0.05	0.00	0.04	0.03	0.00	0.05
Inhalation of vapours	0.00	0.00	0.00	0.00	0.00	0.00
Drinking water	62	34	44	44	41	63
Ingestion of vegetables	30	62	26	17	50	18

cient for sensitive land use [3]. To protect the majority of ecosystems, the guideline values for sensitive land use are set to half the previous levels.

The guideline values for less sensitive land use are exceeded for Cd, Cu, Pb and Zn. The guideline values for sensitive land use are exceeded for all elements except chromium.

3 Discussion

The part of the exposure assessment presented here does not consider current exposure barriers in the form of asphalt pavement, approximately 50% of the site, or exposure off-site due to background concentrations. Such data are available, but does not change the results much. However, the exposure for arsenic would be below the guideline value for less sensitive land use if the whole site was covered with pavement.

It seems to be a general experience that deterministic point estimates are too conservative and often overestimate risks compared to the probabilistic risk assessments. This pattern is seen here as well, but the difference is marginal and the same contaminants exceed the TRV using either method. The two estimates thus seem to corroborate each other, but the uncertainty that is associated with the model structure is not described.

The contribution of the different exposure pathways in the total intake is not always the same with both methods. This is particularly noticeable for arsenic in the scenario of sensitive land use where dermal contact is more important than for the deterministic point estimate. This difference is mainly due to the specification of the input probability distribution for time of exposure in the dermal contact pathway.

The importance of the drinking water pathway for the scenario with sensitive land use could be put into question. Private wells are not required since the municipality provides drinking water to all houses within their area of duty. The quality of the ground water has also been investigated and the metal concentrations were generally low, except for lead in one monitoring well.

In this assessment, the estimated intake distributions are applicable to a randomly selected individual. It is often recommended that variability and uncertainty should be characterized separately in order to facilitate the interpretation [7,8]. However, a two-dimensional Monte Carlo simulation is more complex and time-consuming, and sometimes it is also difficult to separate the sources of uncertainty and variability. The probability distributions used to characterize the different soil parameters in this assessment are typically representing both variability and uncertainty, and the same is true for the majority of the exposure variables. We therefore decided not to attempt to separate variability and uncertainty at this stage, but with additional data from a more in-depth site investigation it might be possible to achieve this.

4 Conclusions and Outlook

This case study illustrates how a multimedia exposure model – previously used for deterministic point estimates – can be adopted for a probabilistic risk assessment. All calculations can be implemented with a spreadsheet version of the model and a suitable add-in to execute the Monte Carlo simulation. The additional information needed is data to specify probability distributions for the input variables.

To the best of our knowledge, this study is the first report on a probabilistic risk assessment on a former iron and steel works site. The materials handled by this industry were less toxic than for many other metallurgical operations, such as copper and lead smelters, but contaminants may still severely limit the options for future land use.

The total intake of arsenic from work-time exposure at this site may exceed the toxicological reference value. The risk of exceeding the reference values also for other elements increase substantially if the site is used for housing, kindergartens, etc. However, a large portion of the increased exposure is due to consumption of drinking water from private wells which is less likely to occur.

Data was not available to separate variability and uncertainty in this assessment. It is therefore preferable if such data was collected in a follow-up study to provide the basis for a two-dimensional Monte Carlo simulation. Sampling according to a statistical plan would help remove any bias introduced in the previous investigations [31,32].

This case study shows that probabilistic exposure estimates for a set of soil contaminants can be quite similar to deterministic point estimates. The main difference is instead to be found in the additional information obtained with the probabilistic assessment. The sensitivity analyses show which pathways and input variable that contribute most to variations in the total intake of each contaminant, e.g. dermal contact and ingestion of soil, vegetables and drinking water. This information can be used both in the planning of future land use and for active measures to reduce current exposure.

The probabilistic assessment also provides information on the magnitude of exposure and the margin of safety. This information may facilitate risk communication between decision-makers and stakeholders. The presentation of results from probabilistic risk assessments is only briefly discussed in the literature and here we see a need for research and opportunities for enhancement. The choice of data analytical tools may then be of importance, since more complex multimedia models are rather difficult to decipher when implemented within traditional spreadsheet software.

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