

# Manual reproduction of $K_d$ and CR parameter values in SR-PSU

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# 1 Introduction

One option for reviewing and quality assure the K<sub>d</sub>/CR data selection process and the resulting selection of parameter values is to manually reproduce selected parameter cases. This option makes it possible to reassure that the correct results are obtained in the automatic data selection procedures in the two Access databases without needing to investigate the technical details. The implementation of the procedure in the two databases are to be seen as tools for handling the vast number of parameters, and it is not necessary to understand the details of the databases in order to review and quality assure the results.

In this document instructions are given on how to manually reproduce and review the parameter values based on the original data files and additional information on data selections. Examples are given in order to illustrate the steps. The procedure can be divided into two main steps; i) if available, the calculation of site-specific K<sub>d</sub> and CR values and ii) the final data evaluation and selection based on all available data sources including literature data.

The files listed below are referred to in this document and they are needed for the manual reproduction of the K<sub>d</sub> and CR values:

- **SKB\_Chemistry\_SR\_PSU.xlsx**
- **Matched\_SNO.xlsx**
- **Excluded\_samples.xlsx**
- **Kd\_CR.xlsx**
- **ConversionFactors.xlsx**

## 2 Calculation of site-specific K<sub>d</sub> and CR

The site-specific parameter values used in the SR-PSU safety assessment could be manually reproduced from original concentration data in combination with information of the specific samples selected per parameter and the general principles described in Tröjbom et al. (2013). The site-specific concentration data could be derived from the Excel-file “**SKB\_Chemistry\_SR\_PSU.xlsx**” that is based on traceable data from the SKB SICADA database. This file has been quality assured and is used as the original chemistry data file within the SR-PSU project. Concentration data from this file has been selected for calculation of K<sub>d</sub> and CR values.

Information of which concentration samples that are selected and combined for each parameter is listed in the file “**Matched\_SNO.xlsx**”. This file is an excerpt from the Access database (cf. Section 2.3.2 in Appendix A of the document “*Guide to implementation of the SR-PSU K<sub>d</sub> and CR parameterisation process in two Access databases*” (Grolander and Tröjbom 2016). The samples are defined by their unique SKB sample numbers (SNO), for which concentration data could be found in the original data file “**SKB\_Chemistry\_SR\_PSU.xlsx**”. The principles used for calculating K<sub>d</sub> and CR parameter values are described in Section 4.2.1 in Tröjbom et al. (2013). These principles are summarised in the list below:

1. K<sub>d</sub> and CR ratios are calculated by taking the concentration of the sample in the column denoted “Sample number numerator” in the “**Matched\_SNO.xlsx**” file and dividing it with the concentration of the sample in column denoted “Sample number denominator”.
  - a. K<sub>d</sub> parameters are calculated by using true sample pairs, where samples from each IDCODE (location) and SECUP (soil depth) are combined. The population statistics are based on these pairs, either per site or both sites in combination.
  - b. For CR parameters all biota samples per site are combined to all soil or water samples from the same site (Forsmark and Laxemar, respectively). The population statistics, which are based on all possible permutations per site, are calculated for Forsmark and Laxemar separately, and for all permutations from each site in combination.
2. All samples for which the concentrations are reported as under reporting limits are excluded prior to the combination into concentration pairs (these samples are marked as negative values in the original data file where the number represents the reporting limit).
3. The geometric mean (GM) and the geometric standard deviation (GSD) are calculated for the population of ratios from the combined samples. This is made both per site (Forsmark and Laxemar, respectively), and for all data from Forsmark and Laxemar in combination.
4. The sample number for each parameter (N) is defined by the lowest number of unique samples from either the numerator or denominator of the selected samples.

Some of the samples in the original data file were excluded by various reasons, for example laboratory duplicates. These are listed in the file “**Excluded\_samples.xlsx**” and in Table E-1 in Appendix E in Tröjbom et al. (2013), where the motivations for exclusion of each sample are given in Swedish.

### 2.1 Example K<sub>d</sub> for deep till (kD\_regoLow)

The sample numbers selected for kD\_regoLow are found in **Matched\_SNO.xlsx**. K<sub>d</sub> for till is based on seven paired samples (Table 2-1). None of these samples were excluded from the

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calculation, which can be checked by using the file Excluded\_sampels.xlsx, where none of the sample numbers are listed.

*Table 2-1. Sample numbers used for the parameter kD\_regoLow.*

Parameter	Sample number, denominator	Sample number, numerator
kD_regoLow	23537	23475
kD_regoLow	23538	23477
kD_regoLow	23539	23478
kD_regoLow	23540	23479
kD_regoLow	23541	23480
kD_regoLow	23542	23481
kD_regoLow	23543	23483

### 2.1.1 kD\_regoLow for Nickel (Ni)

Using these sample numbers the data for the element of interest can be found in the file **SKB\_Chemistry\_SR\_PSU.xlsx**. The concentration of Ni in soil and pore water are listed in Table 2-2. The ratios are calculated per unique location (IDCODE) and depth (SECUP) combination and they represent true sample pairs. The resulting ratio per concentration pair is listed in the rightmost column of the table. Using these ratios ( $K_d$  values), statistics for the parameter are calculated as GM, GSD, min, max. The number of samples for the parameter is in this case defined as 7 since there are seven true concentration pairs available (minimum value of 7 in both the numerator and denominator).

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*Table 2-2. Ni concentrations in soil and pore water for seven sampling locations (IDCODE) and depths (SECUP). The ratios ( $K_d$  value) calculated per location and depth are listed in the rightmost column. Statistics derived from the seven ratios are reported below the table.*

IDCODE	SECUP	Soil concentration Ni (ppm)	Pore water concentration Ni (ppm)	Ratio ( $m^3/kgdw$ )
PFM007690	1.8	3.26	5.26	0.620
PFM007691	3.5	3.08	4.9	0.629
PFM007692	0.5	4.98	5.03	0.991
PFM007692	1	4.16	2.55	1.63
PFM007693	0.3	5.01	8.09	0.619
PFM007693	1	2.90	4.16	0.697
PFM007694	2.5	3.76	5.21	0.722

GM	0.79 $m^3/kgdw$
GSD	1.4
N	7
minimum	0.62 $m^3/kgdw$
maximum	1.6 $m^3/kgdw$

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### 2.1.2 kD\_regoLow for Iodine (I)

Using the sample numbers in Table 2-1 the concentration of I in soil and pore water are derived from the file SKB\_Chemistry.xls and listed in Table 2-3. The resulting  $K_d$  values for each sample are listed in the rightmost column and the resulting statistics are listed below.

*Table 2-3. I concentrations in soil and pore water for seven sampling locations (IDCODE) and depths (SECUP). The ratios ( $K_d$ ) calculated per location and depth are listed in the rightmost column. Statistics derived from the seven ratios are reported below the table.*

IDCODE	SECUP	Soil concentration (ppm)	Pore water concentration (ppm)	Ratio ( $m^3/kgdw$ )
PFM007690	1.8	0.336	7.8	0.043
PFM007691	3.5	0.077	7.6	0.010
PFM007692	0.5	0.436	11.8	0.037
PFM007692	1	0.088	5	0.018
PFM007693	0.3	0.566	83.9	0.0068
PFM007693	1	0.159	16.8	0.0095
PFM007694	2.5	0.041	6.7	0.0061

GM	0.014	$m^3/kgdw$
GSD	2.2	
N	7	
minimum	0.0061	$m^3/kgdw$
maximum	0.043	$m^3/kgdw$

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### 2.1.3 kD\_regoLow for Calcium (Ca)

The concentrations of Ca in soil and pore water are listed in Table 2-4. The resulting  $K_d$  values for each sample are listed in the rightmost column and the statistics are listed below.

*Table 2-4. Ca concentrations in soil and pore water for seven sampling locations (IDCODE) and depths (SECUP). The ratios ( $K_d$ ) calculated per location and depth are listed in the rightmost column. Statistics derived from the seven ratios are reported below the table.*

IDCODE	SECUP	Soil concentration (ppm)	Pore water concentration (ppm)	Ratio ( $m^3/kgdw$ )
PFM007690	1.8	44200	172000	0.257
PFM007691	3.5	41200	165500	0.249
PFM007692	0.5	45000	99400	0.453
PFM007692	1	47900	90100	0.532
PFM007693	0.3	54900	175600	0.313
PFM007693	1	34200	238700	0.143
PFM007694	2.5	49900	197500	0.253

GM	0.29	$m^3/kgdw$
GSD	1.5	
N	7	
minimum	0.14	$m^3/kgdw$
maximum	0.53	$m^3/kgdw$

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#### 2.1.4 kD\_regoLow for Molybdenum (Mo)

The concentrations of Mo in soil and pore water are listed in Table 2-5. The resulting  $K_d$  values for each sample are listed in the rightmost column and the statistics are listed below.

*Table 2-5. Mo concentrations in soil and pore water for seven sampling locations (IDCODE) and depths (SECUP). The ratios ( $K_d$  value) calculated per location and depth are listed in the rightmost column. Statistics derived from the seven ratios are reported below the table.*

IDCODE	SECUP	Soil concentration (ppm)	Pore water concentration (ppm)	Ratio ( $m^3/kgdw$ )
PFM007690	1.8	0.163	9.3	0.0175
PFM007691	3.5	0.64	16.7	0.0383
PFM007692	0.5	0.214	3.2	0.0669
PFM007692	1	0.132	8.1	0.0163
PFM007693	0.3	0.162	5.5	0.0295
PFM007693	1	0.106	3.7	0.0286
PFM007694	2.5	0.224	85.9	0.00261

GM	0.021	$m^3/kgdw$
GSD	2.8	
N	7	
minimum	0.0026	$m^3/kgdw$
maximum	0.067	$m^3/kgdw$



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## 2.1.5 kD\_regoLow for Uranium (U)

The concentrations of U in soil and pore water are listed in Table 2-6. The resulting  $K_d$  values for each sample are listed in the rightmost column and the statistics are listed below.

*Table 2-6. U concentrations in soil and pore water for seven sampling locations (IDCODE) and depths (SECUP). The ratios ( $K_d$ ) calculated per location and depth are listed in the rightmost column. Statistics derived from the seven ratios are reported below the table.*

IDCODE	SECUP	Soil	Pore water		Ratio (m <sup>3</sup> /kgdw)
		concentration (ppm)	concentration (ppm)		
PFM007690	1.8	1.26	69.9		0.0181
PFM007691	3.5	1.30	75		0.0174
PFM007692	0.5	1.96	15.2		0.129
PFM007692	1	1.72	49.5		0.0349
PFM007693	0.3	2.50	72.6		0.0344
PFM007693	1	1.77	116		0.0152
PFM007694	2.5	3.70	1260		0.00295

GM	0.022	m3/kgdw
GSD	3.1	
N	7	
minimum	0.0029	m3/kgdw
maximum	0.13	m3/kgdw

## 2.2 Example CR for limnic fish (cR\_Lake\_fish)

CR for fish is calculated from the available water and fish concentration measurements. The sample numbers used are found in **Matched\_SNO.xlsx** and are also listed in Table 2-7. Each lake water sample from Forsmark are combined with all fish samples from the Forsmark and all lake water samples from Laxemar are combined with all fish samples from Laxemar. For this parameter this means that the three lake water samples from Forsmark are combined with the 16 fish samples from Forsmark and the three lake water samples from Laxemar are combined with the 6 fish samples from Laxemar (according to the Table 2-7). Using these sample numbers the concentration data for any element of interest can be found in the file **SKB\_Chemistry\_SR\_PSU.xlsx**. Below data for Ni, I, Ca, Mo and U are presented as examples.

None of these samples were excluded from the calculation, which can be checked by using the file **Excluded\_sampels.xlsx**. None of the samples are listed in this file.

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*Table 2-7. Sample numbers used for the parameter cR\_Lake\_fish.*

<b>Parameter</b>	<b>Site</b>	<b>Sample number, denominator</b>	<b>Sample number, numerator</b>
cR_Lake_Fish	FORSMARK	23117	23601
cR_Lake_Fish	FORSMARK	23117	23602
cR_Lake_Fish	FORSMARK	23117	23604
cR_Lake_Fish	FORSMARK	23117	23606
cR_Lake_Fish	FORSMARK	23117	23608
cR_Lake_Fish	FORSMARK	23117	23635
cR_Lake_Fish	FORSMARK	23117	23637
cR_Lake_Fish	FORSMARK	23117	23668
cR_Lake_Fish	FORSMARK	23117	23669
cR_Lake_Fish	FORSMARK	23117	23670
cR_Lake_Fish	FORSMARK	23117	23671
cR_Lake_Fish	FORSMARK	23117	23672
cR_Lake_Fish	FORSMARK	23117	23673
cR_Lake_Fish	FORSMARK	23117	23674
cR_Lake_Fish	FORSMARK	23117	23675
cR_Lake_Fish	FORSMARK	23117	23678
cR_Lake_Fish	FORSMARK	23118	23601
cR_Lake_Fish	FORSMARK	23118	23602
cR_Lake_Fish	FORSMARK	23118	23604
cR_Lake_Fish	FORSMARK	23118	23606
cR_Lake_Fish	FORSMARK	23118	23608
cR_Lake_Fish	FORSMARK	23118	23635
cR_Lake_Fish	FORSMARK	23118	23637
cR_Lake_Fish	FORSMARK	23118	23668
cR_Lake_Fish	FORSMARK	23118	23669
cR_Lake_Fish	FORSMARK	23118	23670
cR_Lake_Fish	FORSMARK	23118	23671
cR_Lake_Fish	FORSMARK	23118	23672
cR_Lake_Fish	FORSMARK	23118	23673
cR_Lake_Fish	FORSMARK	23118	23674
cR_Lake_Fish	FORSMARK	23118	23675
cR_Lake_Fish	FORSMARK	23118	23678
cR_Lake_Fish	FORSMARK	23120	23601
cR_Lake_Fish	FORSMARK	23120	23602
cR_Lake_Fish	FORSMARK	23120	23604
cR_Lake_Fish	FORSMARK	23120	23606
cR_Lake_Fish	FORSMARK	23120	23608
cR_Lake_Fish	FORSMARK	23120	23635
cR_Lake_Fish	FORSMARK	23120	23637
cR_Lake_Fish	FORSMARK	23120	23668
cR_Lake_Fish	FORSMARK	23120	23669

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cR_Lake_Fish	FORSMARK	23120	23670
cR_Lake_Fish	FORSMARK	23120	23671
cR_Lake_Fish	FORSMARK	23120	23672
cR_Lake_Fish	FORSMARK	23120	23673
cR_Lake_Fish	FORSMARK	23120	23674
cR_Lake_Fish	FORSMARK	23120	23675
cR_Lake_Fish	FORSMARK	23120	23678
cR_Lake_Fish	LAXEMAR	23262	23822
cR_Lake_Fish	LAXEMAR	23262	23826
cR_Lake_Fish	LAXEMAR	23262	23832
cR_Lake_Fish	LAXEMAR	23262	23897
cR_Lake_Fish	LAXEMAR	23262	23899
cR_Lake_Fish	LAXEMAR	23262	23901
cR_Lake_Fish	LAXEMAR	23263	23822
cR_Lake_Fish	LAXEMAR	23263	23826
cR_Lake_Fish	LAXEMAR	23263	23832
cR_Lake_Fish	LAXEMAR	23263	23897
cR_Lake_Fish	LAXEMAR	23263	23899
cR_Lake_Fish	LAXEMAR	23263	23901
cR_Lake_Fish	LAXEMAR	23265	23822
cR_Lake_Fish	LAXEMAR	23265	23826
cR_Lake_Fish	LAXEMAR	23265	23832
cR_Lake_Fish	LAXEMAR	23265	23897
cR_Lake_Fish	LAXEMAR	23265	23899
cR_Lake_Fish	LAXEMAR	23265	23901

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### 2.2.1 cR\_lake\_fish for Nickel (Ni)

In Table 2-8 and Table 2-9 the concentrations used for Ni are listed. The concentration in fish is converted into carbon units by using the carbon content of each specific sample. This information can be found in the **SKB\_Chemistry\_SR\_PSU.xlsx** file. For many of the samples the concentrations were below reporting limits, and according to the selection principles these samples were excluded.

The ratios (CR) are calculated by dividing each fish concentration by all available water samples per site (data from Forsmark and Laxemar are not mixed). The resulting ratios are listed in Table 2-10. The statistics (GM, GSD, min, max) are calculated based on the ratios for both sites separately and also for all ratios from both sites combined (Table 2-11).

The sample number (N) is defined as the lowest number of samples found in either numerator or denominator. For Ni only one fish sample from Laxemar had concentrations above reporting limits, and no samples from Forsmark. Therefore statistics are only presented for Laxemar based on three ratios.

*Table 2-8. Ni concentrations in lake water from Laxemar and Forsmark sites.*

Sample number	Site	Lake water concentration (ppm)
23117	FORSMARK	0.5
23118	FORSMARK	0.51
23120	FORSMARK	0.62
23262	LAXEMAR	1
23263	LAXEMAR	1.2
23265	LAXEMAR	2.2

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*Table 2-9. Ni concentrations in limnic fishes from Laxemar and Forsmark sites are listed in the table. The carbon content of each sample is also listed and the concentrations are converted into carbon units. The negative numbers indicate samples under reporting limits that were excluded from the CR calculations (marked in red below).*

SITE	Sample number	Fish muscle concentration (mg/kgdw)	Carbon content (kgC/kgdw)	Fish muscle concentration (mg/kgC)
FORSMARK	23601	-0.02	0.43	-0.0465
FORSMARK	23602	-0.02	0.43	-0.0465
FORSMARK	23604	-0.02	0.45	-0.0444
FORSMARK	23606	-0.02	0.42	-0.0476
FORSMARK	23608	-0.1	0.45	-0.222
FORSMARK	23635	-0.2	0.44	-0.455
FORSMARK	23637	-0.1	0.44	-0.227
FORSMARK	23668	-0.02	0.43	-0.0465
FORSMARK	23669	-0.02	0.44	-0.0455
FORSMARK	23670	-0.02	0.45	-0.0444
FORSMARK	23671	-0.02	0.43	-0.0465
FORSMARK	23672	-0.02	0.43	-0.0465
FORSMARK	23673	-0.02	0.45	-0.0444
FORSMARK	23674	-0.02	0.43	-0.0465
FORSMARK	23675	-0.02	0.46	-0.0435
FORSMARK	23678	-0.02	0.45	-0.0444
LAXEMAR	23822	-0.03	0.42	-0.0722
LAXEMAR	23826	-0.03	0.43	-0.0700
LAXEMAR	23832	-0.03	0.42	-0.0709
LAXEMAR	23897	0.038	0.42	0.0903
LAXEMAR	23899	-0.03	0.43	-0.0697
LAXEMAR	23901	-0.03	0.43	-0.0705

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Table 2-10. The resulting ratios are presented for the Forsmark and Laxemar site ( $m^3/kg$ ).

Forsmark			
Sample number	23117	23118	23120
23601			
23602			
23604			
23606			
23608			
23635			
23637			
23668			
23669			
23670			
23671			
23672			
23673			
23674			
23675			
23678			

Laxemar			
Sample number	23262	23263	23265
23822			
23826			
23832			
23897	0.0903	0.0753	0.0411
23899			
23901			

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*Table 2-11. The calculated statistics for Forsmark, Laxemar and a combined Forsmark and Laxemar data set. No data above reporting limits are available from Forsmark, and therefore the statistics for the combination of Forsmark and Laxemar data are identical to the Laxemar data.*

<b>Forsmark</b>	<b>m<sup>3</sup>/kg<sub>C</sub></b>
GM	
GSD	
minimum	
maximum	
N	
N numerator	
N denominator	
<b>Laxemar</b>	<b>m<sup>3</sup>/kg<sub>C</sub></b>
GM	0.0654
GSD	1.5
minimum	0.0411
maximum	0.0903
N	1
N numerator	3
N denominator	1
<b>Forsmark and Laxemar</b>	<b>m<sup>3</sup>/kg<sub>C</sub></b>
GM	0.0654
GSD	1.5
minimum	0.0411
maximum	0.0903
N	1
N numerator	3
N denominator	1

### 2.2.2 cR\_lake\_fish Iodine (I)

In Table 2-12 and

Table 2-13 the concentrations used for I are listed. The concentration in fish is converted to carbon units by using the carbon content of each specific sample. This information can also be found in **SKB\_Chemistry\_SR\_PSU.xlsx**, which is also listed in Table 2-12. For many of the samples the concentrations were below reporting limits, and these samples were excluded according to the selection principles.

The ratios (CR) were calculated by dividing each fish concentration by all available water samples per site (data from Forsmark and Laxemar are not mixed). The resulting ratios are listed in Table 2-14. The statistics (GM, GSD, min, max) are calculated based on the ratios, for both sites separately and also for all ratios from both sites combined (Table 2-15). The sample number (N) is defined as the lowest number of samples found in either numerator or denominator. For I only one fish sample from Forsmark had measured concentrations above reporting limits. N for Forsmark is therefore defined as 1. For Laxemar six fish samples and 3 water samples were available. N for Laxemar is therefore defined as 3.

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*Table 2-12. I concentrations in lake water from Laxemar and Forsmark sites.*

Sample number	Site	Lake water concentration (ppm)
23117	FORSMARK	4
23118	FORSMARK	4
23120	FORSMARK	3
23262	LAXEMAR	4
23263	LAXEMAR	17
23265	LAXEMAR	25

*Table 2-13. I concentrations in limnic fish from Laxemar and Forsmark sites. The carbon content of each sample is also listed and the concentrations are converted into carbon units in the rightmost column. The negative numbers indicate samples under reporting limits that were excluded from the CR calculations.*

SITE	Sample number	Fish muscle concentration (mg/kgdw)	Carbon content (kgC/kgdw)	Fish muscle concentration (mg/kgC)
FORSMARK	23601	-0.4	0.43	-0.930
FORSMARK	23602	-0.4	0.43	-0.930
FORSMARK	23604	-0.4	0.45	-0.889
FORSMARK	23606	1	0.42	2.4
FORSMARK	23608	-0.5	0.45	-1.11
FORSMARK	23635	-0.6	0.44	-1.36
FORSMARK	23637	-0.5	0.44	-1.13
FORSMARK	23668	-0.4	0.43	-0.930
FORSMARK	23669	-0.4	0.44	-0.909
FORSMARK	23670	-0.4	0.45	-0.889
FORSMARK	23671	-0.4	0.43	-0.930
FORSMARK	23672	-0.4	0.43	-0.930
FORSMARK	23673	-0.4	0.45	-0.889
FORSMARK	23674	-0.4	0.43	-0.930
FORSMARK	23675	-0.4	0.46	-0.870
FORSMARK	23678	-0.4	0.45	-0.889
LAXEMAR	23822	4.38	0.42	10.5
LAXEMAR	23826	2.91	0.43	6.79
LAXEMAR	23832	3.35	0.42	7.92
LAXEMAR	23897	1.23	0.42	2.92
LAXEMAR	23899	1.63	0.43	3.79
LAXEMAR	23901	1.34	0.43	3.15



Manual reproduction of Kd and CR parameter values in SR-PSU

Table 2-14. The resulting ratios are presented for the Forsmark and Laxemar site ( $m^3/kg$ ).

<b>Forsmark</b>			
<b>Sample number</b>	23117	23118	23120
23601			
23602			
23604			
23606	0.595	0.595	0.794
23608			
23635			
23637			
23668			
23669			
23670			
23671			
23672			
23673			
23674			
23675			
23678			

<b>Laxemar</b>			
<b>Sample number</b>	23262	23263	23265
23822	2.636	0.620	0.422
23826	1.697	0.399	0.272
23832	1.980	0.466	0.317
23897	0.731	0.172	0.117
23899	0.947	0.223	0.152
23901	0.787	0.185	0.126

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-15. The calculated statistics for Forsmark, Laxemar and a combined Forsmark and Laxemar data set.*

<b>Forsmark</b>	<b>m<sup>3</sup>/kg<sub>c</sub></b>
GM	0.655
GSD	1.8
minimum	0.595
maximum	0.794
N	1
N numerator	1
N denominator	3

<b>Laxemar</b>	<b>m<sup>3</sup>/kgC</b>
GM	0.436
GSD	2.6
minimum	0.117
maximum	2.64
N	1
N numerator	3
N denominator	1

<b>Forsmark and Laxemar</b>	<b>m<sup>3</sup>/kgC</b>
GM	0.436
GSD	2.4
minimum	0.117
maximum	2.64
N	1
N numerator	6
N denominator	7

Manual reproduction of Kd and CR parameter values in SR-PSU

### 2.2.3 cR\_lake\_fish Calcium (Ca)

In Table 2-16 and Table 2-17 the concentrations used for Ca are listed. The concentration in fish is converted into carbon units by using the carbon content of each specific sample. This information can be found in **SKB\_Chemistry\_SR\_PSU.xlsx** and is also listed in Table 2-17. The ratios (CR) are calculated by dividing each fish concentration by all available water samples per site (data from Forsmark and Laxemar are not mixed). The resulting ratios are listed in Table 2-18. The statistics (GM, GSD, min, max) are calculated based on the ratios for both sites separately and also for all ratios from both sites combined (Table 2-19). The sample number (N) is defined as the lowest number of samples found in either the numerator or denominator.

*Table 2-16. Ca concentrations in lake water from Laxemar and Forsmark sites are listed in the table.*

Sample number	Site	Lake water concentration (ppm)
23117	FORSMARK	47000
23118	FORSMARK	49000
23120	FORSMARK	57000
23262	LAXEMAR	8000
23263	LAXEMAR	10000
23265	LAXEMAR	7800

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-17. Ca concentrations in limnic fish from Laxemar and Forsmark sites. The carbon content of each sample is also listed and the concentrations are converted into carbon units in the rightmost column.*

<b>SITE</b>	<b>Sample number</b>	<b>Fish muscle concentration (mg/kgdw)</b>	<b>Carbon content (kgC/kgdw)</b>	<b>Fish muscle concentration (mg/kgC)</b>
FORSMARK	23601	3430	0.43	7980
FORSMARK	23602	5290	0.43	12300
FORSMARK	23604	7230	0.45	16100
FORSMARK	23606	2860	0.42	6810
FORSMARK	23608	1200	0.45	2670
FORSMARK	23635	5400	0.44	12300
FORSMARK	23637	2560	0.44	5820
FORSMARK	23668	801	0.43	1860
FORSMARK	23669	982	0.44	2230
FORSMARK	23670	1990	0.45	4420
FORSMARK	23671	776	0.43	1800
FORSMARK	23672	759	0.43	1770
FORSMARK	23673	3840	0.45	8530
FORSMARK	23674	3010	0.43	7000
FORSMARK	23675	669	0.46	1450
FORSMARK	23678	4490	0.45	9980
LAXEMAR	23822	575	0.42	1380
LAXEMAR	23826	3450	0.43	8050
LAXEMAR	23832	1660	0.42	3930
LAXEMAR	23897	2720	0.42	6470
LAXEMAR	23899	2730	0.43	6350
LAXEMAR	23901	2540	0.43	5970

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 2-18. The resulting ratios are presented for the Forsmark and Laxemar site ( $m^3/kg$ ).

<b>Forsmark</b>			
<b>Sample number</b>	<b>23117</b>	<b>23118</b>	<b>23120</b>
23601	0.1697	0.1628	0.1399
23602	0.2618	0.2511	0.2158
23604	0.3418	0.3279	0.2819
23606	0.1449	0.1390	0.1195
23608	0.0567	0.0544	0.0468
23635	0.2611	0.2505	0.2153
23637	0.1238	0.1187	0.1021
23668	0.0396	0.0380	0.0327
23669	0.0475	0.0455	0.0392
23670	0.0941	0.0902	0.0776
23671	0.0384	0.0368	0.0317
23672	0.0376	0.0360	0.0310
23673	0.1816	0.1741	0.1497
23674	0.1489	0.1429	0.1228
23675	0.0309	0.0297	0.0255
23678	0.2123	0.2036	0.1750

<b>Laxemar</b>			
<b>Sample number</b>	<b>23262</b>	<b>23263</b>	<b>23265</b>
23822	0.173	0.138	0.177
23826	1.006	0.805	1.032
23832	0.491	0.393	0.503
23897	0.808	0.647	0.829
23899	0.793	0.635	0.814
23901	0.746	0.597	0.765

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-19. The calculated statistics for Forsmark, Laxemar and a combined Forsmark and Laxemar data set.*

<b>Forsmark</b>	<b>m<sup>3</sup>/kg<sub>c</sub></b>
GM	0.096
GSD	2.2
minimum	0.026
maximum	0.34
N	3
N numerator	16
N denominator	3

<b>Laxemar</b>	<b>m<sup>3</sup>/kgC</b>
GM	0.549
GSD	1.8
minimum	0.138
maximum	1.032
N	3
N numerator	6
N denominator	3

<b>Forsmark and Laxemar</b>	<b>m<sup>3</sup>/kgC</b>
GM	0.155
GSD	2.9
minimum	0.026
maximum	1.032
N	6
N numerator	22
N denominator	6

Manual reproduction of Kd and CR parameter values in SR-PSU

#### 2.2.4 cR\_lake\_fish Molybdenium (Mo)

In Table 2-20 and Table 2-21 the concentrations used for Mo are listed. The concentration in fish is converted into carbon units by using the carbon content of each specific sample. This information can be found in **SKB\_Chemistry\_SR\_PSU.xlsx** and is also listed in Table 2-21. The ratios (CR) are calculated by dividing each fish concentration by all available water samples per site (data from Forsmark and Laxemar are not mixed). The resulting ratios are listed in Table 2-22. The statistics (GM, GSD, min, max) are calculated based on the ratios for both sites separately and also for all ratios from both sites combined (Table 2-23). The sample number (N) is defined as the lowest number of samples found in either the numerator or the denominator.

*Table 2-20. Mo concentrations in lake water from Laxemar and Forsmark sites.*

Sample number	Site	Lake water concentration (ppm)
23117	FORSMARK	0.25
23118	FORSMARK	0.62
23120	FORSMARK	0.65
23262	LAXEMAR	0.11
23263	LAXEMAR	0.5
23265	LAXEMAR	0.92

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-21. Mo concentrations in limnic fish from Laxemar and Forsmark sites. The carbon content of each sample is also listed and the concentrations are converted into carbon unit in the rightmost column. The negative numbers indicate samples below reporting limits that were excluded from the CR calculations.*

SITE	Sample number	Fish muscle concentration (mg/kgdw)	Carbon content (kgC/kgdw)	Fish muscle concentration (mg/kgC)
FORSMARK	23601	0.01	0.43	0.0233
FORSMARK	23602	0.01	0.43	0.0233
FORSMARK	23604		0.45	
FORSMARK	23606	0.01	0.42	0.0238
FORSMARK	23608	-0.01	0.45	-0.0222
FORSMARK	23635	0.05	0.44	0.114
FORSMARK	23637	0.02	0.44	0.0455
FORSMARK	23668	0.03	0.43	0.0698
FORSMARK	23669	0.02	0.44	0.0455
FORSMARK	23670	0.02	0.45	0.0444
FORSMARK	23671	0.02	0.43	0.0465
FORSMARK	23672	0.02	0.43	0.0465
FORSMARK	23673	0.02	0.45	0.0444
FORSMARK	23674	0.03	0.43	0.0698
FORSMARK	23675	0.02	0.46	0.0435
FORSMARK	23678	0.02	0.45	0.0444
LAXEMAR	23822	0.01	0.42	0.0241
LAXEMAR	23826	0.01	0.43	0.0233
LAXEMAR	23832	0.01	0.42	0.0236
LAXEMAR	23897	0.02	0.42	0.0475
LAXEMAR	23899	0.01	0.43	0.0232
LAXEMAR	23901	0.01	0.43	0.0235



Manual reproduction of Kd and CR parameter values in SR-PSU

Table 2-22. The resulting ratios are presented for the Forsmark and Laxemar site ( $m^3/kg$ ).

Sample number	23117	23118	23120
23601	0.0930	0.0375	0.0358
23602	0.0930	0.0375	0.0358
23604			
23606	0.0952	0.0384	0.0366
23608			
23635	0.4545	0.1833	0.1748
23637	0.1818	0.0733	0.0699
23668	0.2791	0.1125	0.1073
23669	0.1818	0.0733	0.0699
23670	0.1778	0.0717	0.0684
23671	0.1860	0.0750	0.0716
23672	0.1860	0.0750	0.0716
23673	0.1778	0.0717	0.0684
23674	0.2791	0.1125	0.1073
23675	0.1739	0.0701	0.0669
23678	0.1778	0.0717	0.0684

#### Laxemar

Sample number	23262	23263	23265
23822	0.2188	0.0481	0.0262
23826	0.2121	0.0467	0.0254
23832	0.2150	0.0473	0.0257
23897	0.4322	0.0951	0.0517
23899	0.2113	0.0465	0.0253
23901	0.2136	0.0470	0.0255

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-23. The calculated statistics for Forsmark, Laxemar and a combined Forsmark and Laxemar data set.*

<b>Forsmark</b>	<b>m<sup>3</sup>/kg<sub>c</sub></b>
GM	0.096
GSD	1.9
minimum	0.036
maximum	0.46
N	3
N numerator	14
N denominator	3
<b>Laxemar</b>	<b>m<sup>3</sup>/kgC</b>
GM	0.072
GSD	2.6
minimum	0.025
maximum	0.43
N	3
N numerator	6
N denominator	3
<b>Forsmark and Laxemar</b>	<b>m<sup>3</sup>/kgC</b>
GM	0.088
GSD	2.1
minimum	0.025
maximum	0.46
N	6
N numerator	20
N denominator	6

Manual reproduction of Kd and CR parameter values in SR-PSU

## 2.2.5 cR\_lake\_fish for Uranium (U)

In Table 2-24 and Table 2-25 the concentrations used for U are listed. The concentration in fish is converted into carbon units by using the carbon content of each specific sample. This information can also be found in **SKB\_Chemistry\_SR\_PSU.xlsx** and is also listed in Table 2-25. For some of the samples the concentrations were below reporting limits. These samples were excluded according to the selection principles.

The ratios (CR) were calculated by dividing each fish concentration by all available water samples per site (data from Forsmark and Laxemar are not mixed). The resulting ratios are listed in Table 2-26. The statistics (GM, GSD, min, max) are calculated based on the ratios for both sites separately and also for all ratios from both sites combined (Table 2-27). The sample number (N) is defined as the lowest number of samples found in either the numerator or the denominator.

*Table 2-24. U concentrations in lake water from Laxemar and Forsmark sites.*

Sample number	Site	Lake water concentration (ppm)
23117	FORSMARK	1.4
23118	FORSMARK	3.7
23120	FORSMARK	2.8
23262	LAXEMAR	0.25
23263	LAXEMAR	0.38
23265	LAXEMAR	0.37

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-25. U concentrations in limnic fish from Laxemar and Forsmark sites. The carbon content of each sample is also listed and the concentrations are converted into carbon units in the rightmost column. The negative numbers indicate samples below reporting limits that were excluded from the CR calculations.*

SITE	Sample number	Fish muscle concentration (mg/kgdw)	Carbon content (kgC/kgdw)	Fish muscle concentration (mg/kgC)
FORSMARK	23601	0.0001	0.43	0.000233
FORSMARK	23602	0.0004	0.43	0.000930
FORSMARK	23604	0.0004	0.45	0.000889
FORSMARK	23606	0.0007	0.42	0.00167
FORSMARK	23608	-0.0006	0.45	-0.00133
FORSMARK	23635	0.003	0.44	0.00682
FORSMARK	23637	-0.0006	0.44	-0.00136
FORSMARK	23668	0.0005	0.43	0.00116
FORSMARK	23669	0.0006	0.44	0.00136
FORSMARK	23670	0.0013	0.45	0.00289
FORSMARK	23671	0.0003	0.43	0.000698
FORSMARK	23672	0.0004	0.43	0.000930
FORSMARK	23673	0.0051	0.45	0.0113
FORSMARK	23674	0.0018	0.43	0.00419
FORSMARK	23675	0.0001	0.46	0.000217
FORSMARK	23678	0.002	0.45	0.00444
LAXEMAR	23822	-0.0001	0.42	-0.000241
LAXEMAR	23826	0.0002	0.43	0.000467
LAXEMAR	23832	-0.0002	0.42	-0.000473
LAXEMAR	23897	0.0017	0.42	0.00404
LAXEMAR	23899	0.0031	0.43	0.00721
LAXEMAR	23901	0.002	0.43	0.00467

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 2-26. The resulting ratios are presented for the Forsmark and Laxemar site ( $m^3/kg$ ).

**Forsmark**

Sample number	23117	23118	23120
23601	0.00017	0.00006	0.00008
23602	0.00066	0.00025	0.00033
23604	0.00064	0.00024	0.00032
23606	0.00119	0.00045	0.00060
23608			
23635	0.00487	0.00184	0.00244
23637			
23668	0.00083	0.00031	0.00042
23669	0.00097	0.00037	0.00049
23670	0.00206	0.00078	0.00103
23671	0.00050	0.00019	0.00025
23672	0.00066	0.00025	0.00033
23673	0.00810	0.00306	0.00405
23674	0.00299	0.00113	0.00150
23675	0.00016	0.00006	0.00008
23678	0.00317	0.00120	0.00159

**Laxemar**

Sample number	23262	23263	23265
23822			
23826	0.00187	0.00123	0.00126
23832			
23897	0.01620	0.01060	0.01090
23899	0.02880	0.01900	0.01950
23901	0.01880	0.01240	0.01270

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 2-27. The calculated statistics for Forsmark, Laxemar and a combined Forsmark and Laxemar data set ( $m^3/kgC$ ).*

<b>Forsmark</b>	<b><math>m^3/kg_c</math></b>
GM	0.0006
GSD	3.4
minimum	0.000059
maximum	0.008
N	3
N numerator	14
N denominator	3
<b>Laxemar</b>	<b><math>m^3/kgC</math></b>
GM	0.0086
GSD	3.1
minimum	0.0012
maximum	0.029
N	3
N numerator	4
N denominator	3
<b>Forsmark and Laxemar</b>	<b><math>m^3/kgC</math></b>
GM	0.001
GSD	5.0
minimum	0.000059
maximum	0.029
N	6
N numerator	18
N denominator	6

## 3 Evaluation of data and selection among data sources

Data for each parameter are selected from a number of data sources. Both site-specific data (calculated in the previous step) and literature data. The literature data is compiled together with the site-specific data in the Excel-file **K<sub>d</sub>\_CR.xlsx**. This file is identical to the main K<sub>d</sub>/CR table in the database (cf. Section 3.1.1 in Appendix A of Grolander and Tröjbom 2016). In order to reproduce the selection of parameter values for a specific element/parameter case the information presented in Tröjbom et al. (2013) should be used in combination with information from the file **K<sub>d</sub>\_CR.xlsx**. The selection process could be divided into three major steps: In the first step representative data is associated to each parameter. The principles for this step are described in Section 4.4.1 in Tröjbom et al. (2013), and the considerations for each parameter are described in detail in Chapter 5 to 8.

In the second step, when one or several data sources are associated to each parameter, the automatic selection of data is done according to the criteria described in Section 4.4.2 in Tröjbom et al. (2013).

In the third step, the selected data (including the statistic measures) are compared to the other available data sources by a number of so called “sense checks” (cf. Section 4.5 and Table 5-1 in Tröjbom et al. 2013). The information gained from the sense checks is used in the final manual evaluation and selection step where if needed data from other sources or analogues could be assigned to replace the initial selected data.

In the following sections examples of selected parameter cases are given.

### 3.1 Example K<sub>d</sub> for deep till (kD\_regoLow)

As described in Section 5.1 in Tröjbom et al. (2013), site-specific K<sub>d</sub> values for deep till are available and selected as representative for this parameter. Literature data for “mineral soils”, “sand” and “all soils” reported by IAEA (2010) were also selected as representative for the parameter, and categorised as L1, L2 and L3, respectively. The data can be found in the Excel-file **K<sub>d</sub>\_CR.xlsx** and the literature data can also be found in the original reference IAEA (2010). As stated in the selection criteria (cf. Section 4.4 in Tröjbom et al. 2013), site data is prioritised in the automatic selection process.

#### 3.1.1 kD\_regoLow for Nickel (Ni)

*The data available for Ni are listed in*

Table 3-1. Site data were available from Forsmark and for the combination of data from Forsmark and Laxemar. No data are available from Laxemar so the site data sources are identical in this case. IAEA (2010) reported data for the category “all soils”, but no data for “mineral soils” or “sand” were available for Ni. Data on “sand+loam” and “clay+organic” are available for Ni in IAEA (2010) but these were not selected as representative categories for this parameter that represent deep till.

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSD<sub>min</sub> = 2, GSD<sub>mean</sub> = 3 and GSD<sub>max</sub> = 6.

The sense checks of these data are done by comparing the ranges of the available data. In this case the reported IAEA data for “all soils” show a large range and the Forsmark data fall within this range of literature data (marked as S1 the column SC FM for Ni in Table 5-2 of Tröjbom et al. 2013). No other sense check could be done since no other data sources are available. The

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sense checks indicated that there are no contradictions between the data sources and site data is therefore assessed suitable for the parameterisation.

Table 3-1. Representative data selected for the parameter  $kD\_regoLow$  for Ni ( $m^3/kgdw$ ).

Reference	Media Type	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
IAEA (2010)	All soils	64	0.28	7	0.003	7.2	0.011	6.88
Forsmark&Laxemar	n	7 <sup>1</sup>	0.79	1.43	0.62	1.63	0.44	1.43
Forsmark	n	7 <sup>1</sup>	0.79	1.43	0.62	1.63	0.44	1.43

1) N for denominator and numerator is 7.

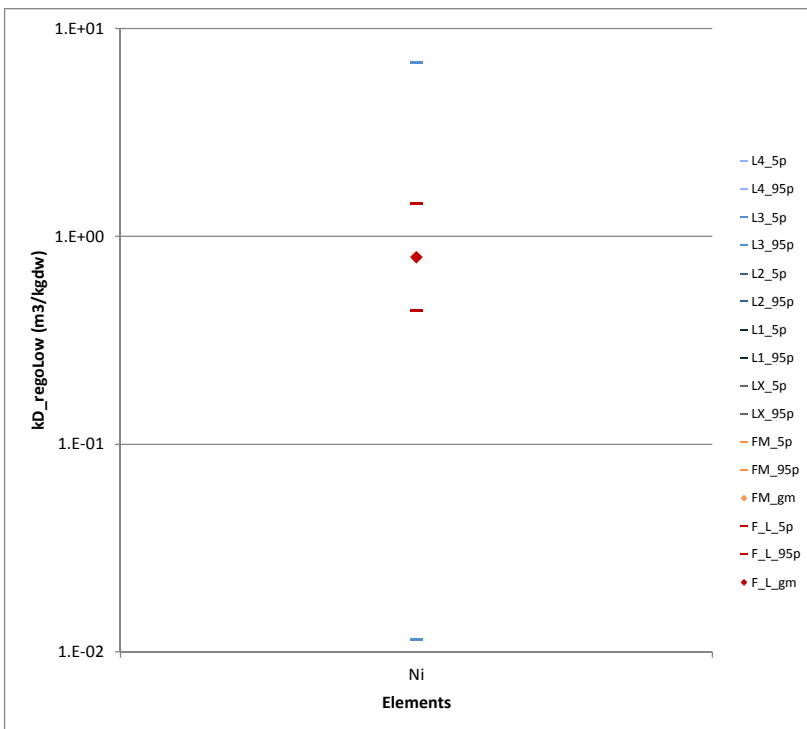


Figure 3-1. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for  $kD\_regoLow$  for Ni. Geometric mean of Forsmark are within the large range of L1 data.

The selections made are described below and the selected data are presented in Table 3-2. According to the selection criteria, where site data are prioritised the site data, is be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.79).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria. In this case it is the same as the GM of the Forsmark data since no Laxemar data exists (0.79).

**Geometric standard deviation (GSD)** - Since the number of samples are 7 (N=7) the GSD of Forsmark data are compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (1.4) it is replaced by the GSDmean limit. In this case the GSD is selected to be 3.

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=3) according to



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the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.62, the calculated 5<sup>th</sup> percentile is 0.13 (based on GM=0.79, GSD=3) and therefore 0.13 is selected. **Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95th percentile calculated using the selected GM and GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 1.63, the calculated 95<sup>th</sup> percentile is 4.82 (based on GM=0.79, GSD=3) and therefore 4.82 is selected.

Table 3-2. Selected data for *kD\_regoLow* for Ni.

Reference	N	GM	GSD	Minimum	Maximum	Distribution
Forsmark	7	0.79	3	0.13	4.82	lognormal

### 3.1.2 kD\_regoLow for Iodine (I)

The data available for I are listed in Table 3-3. Data were available from Forsmark and the combined data from both Forsmark and Laxemar. In this case no data are available from Laxemar so both site data sources are identical. Literature data were available in IAEA (2010) for the category “all soils” and “mineral”, but no data on “sand” were available for I. The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSDmin = 2, GSDmean = 3 and GSDmax = 6.

The sense check of these data is performed by comparing the ranges of the data. In this case the reported IAEA data for “all soils” and “mineral soils” show large ranges, and the Forsmark falls within this range of data. The ranges of data for the two categories “all soils” and “mineral soils” are almost identical. No other sense check could be done since no other data sources are available. The results of the sense check are given in Table 5-1 in Tröjbom et al. (2013) and in Figure 3-2. The sense checks indicated that the data are reasonable and can be used for parameterisation.

Table 3-3. Representative data selected for the parameter *kD\_regoLow* for I ( $m^3/kgdw$ ).

Reference	MediaType	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	7 <sup>1</sup>	0.0141	2.2	0.00612	0.0431	0.00385	0.051615
Forsmark & Laxemar	n	7 <sup>1</sup>	0.0141	2.2	0.00612	0.0431	0.00385	0.051615
IAEA (2010)	Mineral	196	0.007	5.2	0.00001	0.54	0.00046	0.105
IAEA (2010)	All soils	250	0.007	5.4	0.00001	0.58	0.00043	0.111

1) N for denominator and numerator is 7.

Manual reproduction of Kd and CR parameter values in SR-PSU

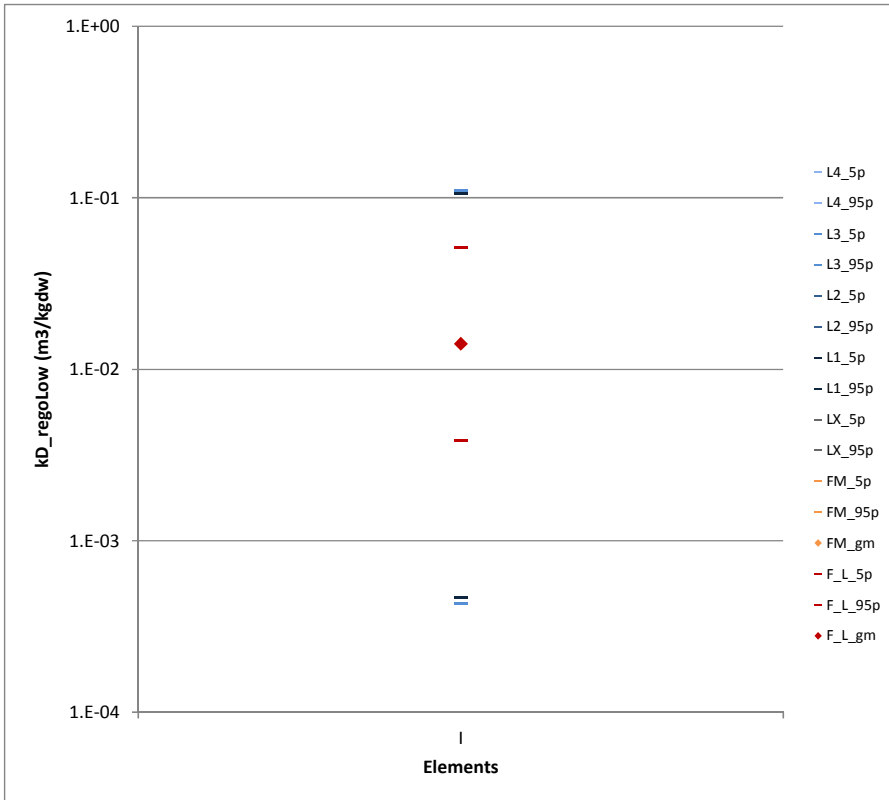


Figure 3-2. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for *kD\_regoLow* for I. The range of site data are within the range of literature data.

The selections made are described below and the selected data are presented in Table 3-4. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.014).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case it is the same as the GM of the Forsmark data since no Laxemar data exists (0.014).

**Geometric standard deviation (GSD)** - Since the number of samples are 7 (N=7) the GSD of Forsmark data are compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (2.2) it is replaced by the GSDmean limit. In this case the GSD is selected to be 3.

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.0061, the calculated 5<sup>th</sup> percentile is 0.0023 (based on GM=0.014, GSD=3) and therefore 0.0023 is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.043, the calculated 95<sup>th</sup> percentile is 0.086 (based on GM=0.014, GSD=3) and therefore 0.086 is selected.

Table 3-4. Selected data for *kD\_regoLow* for I.

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark	7	0.014	0.014	3.00	0.0023	0.086

Manual reproduction of Kd and CR parameter values in SR-PSU

### 3.1.3 kD\_regoLow for Calcium (Ca)

The data available for Ca are listed in Table 3-5. Data were available from Forsmark and the combined data from both Forsmark and Laxemar. No data are available from Laxemar so both site data sources are identical in this case. IAEA (2010) reported data for the category “all soils” and “mineral” soils, but data for “sand” were not available for Ca.

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSDmin = 2, GSDmean = 3 and GSDmax = 6.

The sense checks of these data are done by comparing the ranges of the data. In this case the reported IAEA data show a large ranges and the Forsmark data falls within this range. The ranges of data for the two categories “all soils” and “mineral soils” also overlap each other. The results of the sense checks are listed in Table 5-1 in Tröjbom et al. (2013) and the data are plotted in Figure 3-3. No other sense checks could be done since no other data sources are available. The sense checks indicated that the site data are reasonable and can be used for parameterisation.

Table 3-5. Representative data selected for the parameter kD\_regoLow for Ca (m<sup>3</sup>/kgdw).

Reference	MediaType	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	7 <sup>1</sup>	0.290352	1.5	0.14313	0.531678	0.142	0.592
Forsmark&Laxemar	n	7 <sup>1</sup>	0.290352	1.5	0.14313	0.531678	0.142	0.592
IAEA (2010)	All soils	34	0.008	3.4	0.0007	0.11	0.00107	0.0599
IAEA (2010)	Mineral	33	0.007	3.2	0.0007	0.089	0.00103	0.0474

1) N for denominator and numerator is 7.

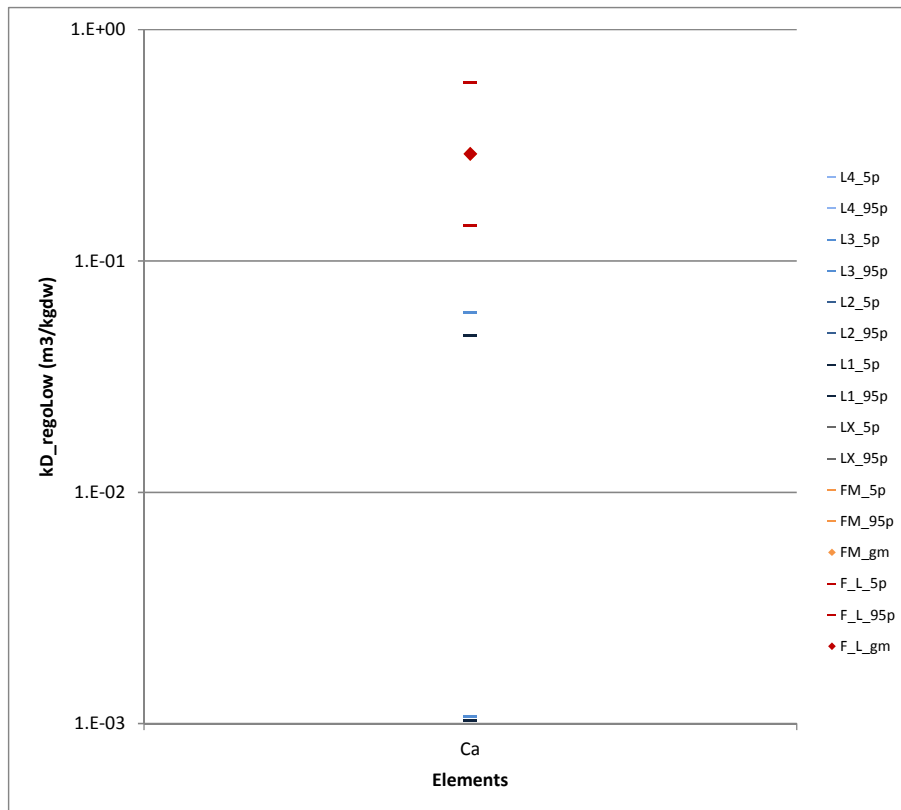


Figure 3-3. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for kD\_regoLow for Ca. The range of site data are within the range of literature data.

Manual reproduction of Kd and CR parameter values in SR-PSU

The selections of data are described below and the selected data are presented in Table 3-6. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.29).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case it is the same as the GM of the Forsmark data since no Laxemar data exists (0.29).

**Geometric standard deviation (GSD)** - Since the number of samples are 7 (N=7) the GSD of Forsmark data are compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (1.5) it is replaced by the GSDmean limit. In this case the GSD is selected to be 3.

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.14, the calculated 5<sup>th</sup> percentile is 0.048 (based on GM=0.29, GSD=3) and therefore 0.048 is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.53, the calculated 95<sup>th</sup> percentile is 1.8 (based on GM=0.29, GSD=3) and therefore 1.8 is selected.

Table 3-6. Selected data for *kD\_regoLow* for Ca.

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark	7	0.29	0.29	3.00	0.048	1.8

### 3.1.4 *kD\_regoLow* for Molybdenium (Mo)

The data available for Mo are listed in Table 3-7. Data were available from Forsmark and the combined data from both Forsmark and Laxemar. No data are available from Laxemar so these site data sources are identical in this case. IAEA (2010) reported data for the category “all soils”, but no data for “mineral soils” or “sand” were available for Mo.

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSDmin = 2, GSDmean = 3 and GSDmax = 6.

The sense checks of these data are done by comparing the ranges of the data. In this case the reported IAEA data for “all soils” partly overlaps the Forsmark data. The result of the comparison is presented as S2 L80% in the Table 5-1 in Tröjbom et al. (2013). This means that the overlap is 80 % of the range of Forsmark data and the Forsmark data are lower (L) than the IAEA data. No other sense check could be done since no other data sources are available. Even though the overlap is not 100% between the data sources, the overlap is large and it is assumed that the data are reasonable and can be used for parameterisation.

Table 3-7. Representative data selected for the parameter *kD\_regoLow* for Mo ( $m^3/kgdw$ ).

Reference	MediaType	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	7 <sup>1</sup>	0.02067	2.8	0.00261	0.06688	0.00380	0.112
Forsmark&Laxemar	n	7 <sup>1</sup>	0.02067	2.8	0.00261	0.06688	0.00380	0.112
IAEA (2010)	All soils	9	0.04	2.8	0.007	0.13	0.00735	0.218

1) N for denominator and numerator is 7.

Manual reproduction of Kd and CR parameter values in SR-PSU

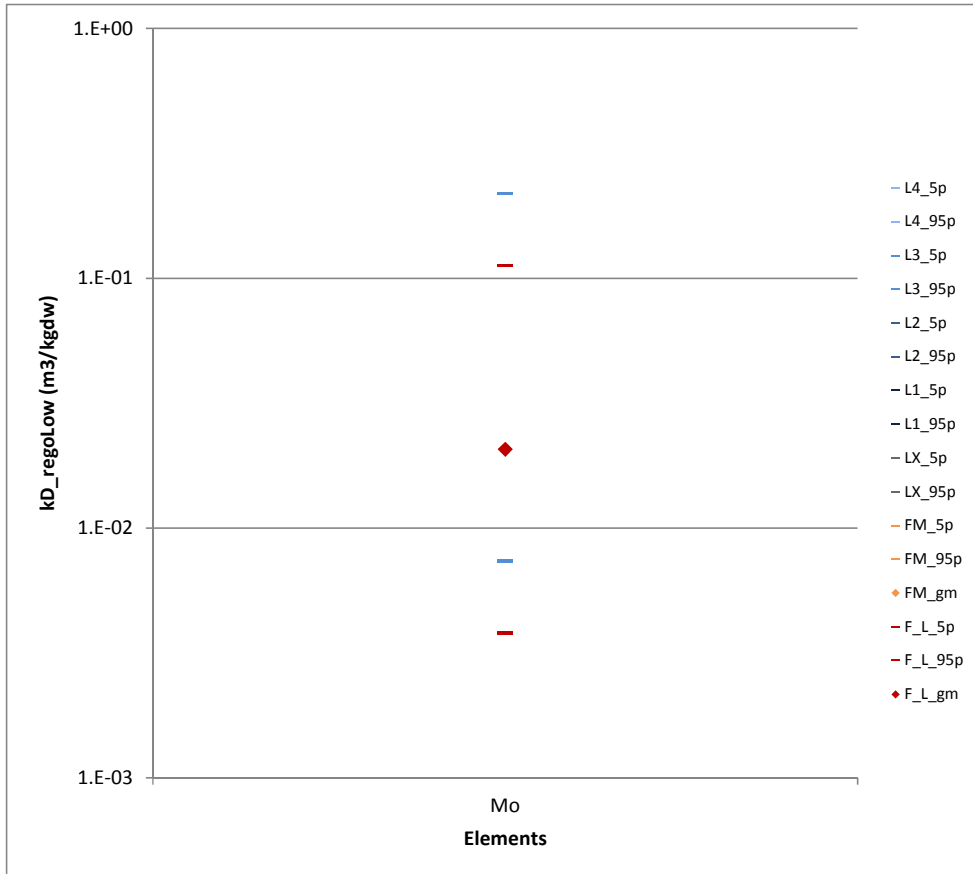


Figure 3-4. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for  $kD_{regolow}$  for Mo. The range of site data partly overlap the range of literature data. The Forsmark data range is lower than the literature data.

The selections of data are described below and the selected data are presented in

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-8. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.021).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case it is the same as the GM of the Forsmark data since no Laxemar data exists (0.021).

**Geometric standard deviation (GSD)** - Since the number of samples are 7 ( $N=7$ ) the GSD of Forsmark data are compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (2.8) it is replaced by the GSDmean limit. In this case the GSD is selected to be 3.

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case  $GSD=3$  according to the criteria in Section 4.4.2 in Tröjbom et al. (2013)). The reported minimum is 0.0026 is lower than the calculated 5<sup>th</sup> percentile (based on  $GM=0.021$ ,  $GSD=3$ ) and therefore 0.0026 is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case  $GSD=3$ ) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.067 the calculated 95<sup>th</sup> percentile is 0.13 (based on  $GM=0.021$ ,  $GSD=3$ ) and therefore 0.13 is selected.

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 3-8. Selected data for  $kD_{regoLow}$  for Mo.*

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark	7	0.021	0.021	3.00	0.0026	0.13

### 3.1.5 $kD_{regoLow}$ for uranium (U)

The data available for U are listed in Table 3-9. Data were available from Forsmark and the combined data from both Forsmark and Laxemar are presented, but in this case no data are available from Laxemar so this data are identical to the Forsmark data. IAEA (2010) reported data for the category “mineral soils” and “all soils”, but no data for “sand” were available for U. The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows:  $GSD_{min} = 2$ ,  $GSD_{mean} = 3$  and  $GSD_{max} = 6$ .

The sense checks of these data are done by comparing the ranges of the data, in this case the reported IAEA data show a large ranges, the Forsmark fall within this range of data. The ranges of data for the two categories “all soils” and “mineral soils” are almost identical, probably the data for “all soils” only consist of data from the category “mineral soils”. No other sense check could be done since no other data sources are available. The sense checks indicated that the data are reasonable and can be used for parameterisation.

*Table 3-9. Representative data selected for the parameter  $kD_{regoLow}$  for U ( $m^3/kgdw$ ).*

Reference	MediaType	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	7 <sup>1</sup>	0.0216	3.1	0.0029	0.1291	0.00331	0.141
Forsmark&Laxemar	n	7 <sup>1</sup>	0.0216	3.1	0.0029	0.1291	0.00331	0.141
IAEA (2010)	All soils	178	0.2	12	0.0007	67	0.00336	11.9
IAEA (2010)	Mineral	146	0.18	13	0.0007	67	0.00265	12.2

1) N for denominator and numerator is 7.

Manual reproduction of Kd and CR parameter values in SR-PSU

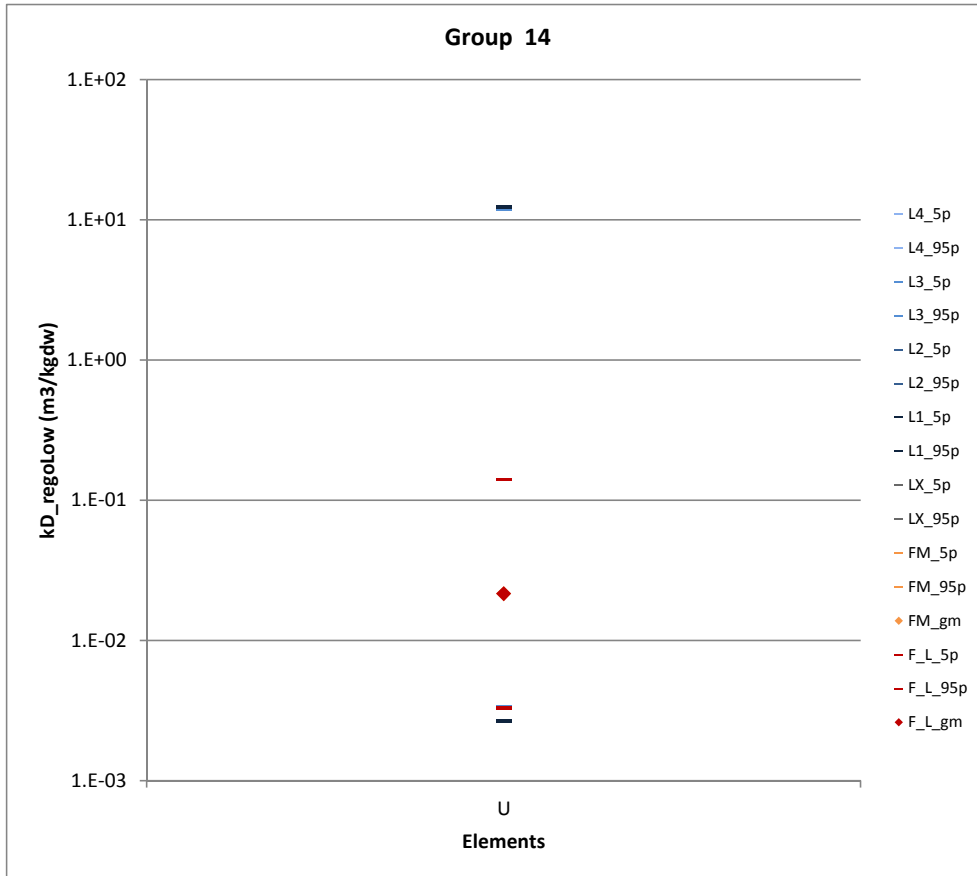


Figure 3-5. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for kD\_regoLow for U. The range of literature data overlaps the site data.

The selections of data are described below and the selected data are presented in



Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-10. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.022).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case it is the same as the GM of the Forsmark data since no Laxemar data exists (0.022).

**Geometric standard deviation (GSD)** - Since the number of samples are 7 ( $N=7$ ) the GSD of Forsmark data are compared to the GSDmean limit, which in this case is 3. Since the reported GSD is higher (3.1) the reported GSD (3.1) is used.

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case  $GSD=3.1$ ) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.0029 which is lower than the calculated 5<sup>th</sup> percentile (based on  $GM=0.79$ ,  $GSD=3$ ) and therefore 0.0029 is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case  $GSD=3$ ) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.13, the calculated 95<sup>th</sup> percentile is 0.14 (based on  $GM=0.0022$ ,  $GSD=3.1$ ) and therefore 0.14 is selected.

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 3-10. Selected data for  $kD_{regoLow}$  for U.*

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark	7	0.022	0.022	3.1	0.0029	0.14

### 3.2 Example for limnic fish (cR\_Lake\_fish)

For limnic fish site-specific data are available from both Forsmark and Laxemar. In addition literature data are available from IAEA (2010) on fish “muscle tissues” and “whole body” samples. Since only the edible part of the fish are of interest when calculating dose to human the muscle tissue data are assumed to be more representative than the “whole body” data. The data sources ERICA (Hosseini et al. 2008) and ICRP (2011) reports data on limnic fish for “whole body”. The IAEA (2010) data on “muscle tissues” are selected as L1 data, IAEA (2010) data for “whole body” as L2 data and ERICA as L3 data (see Section 7.9 in Tröjbom et al. 2013).

The literature data reported by IAEA and ERICA (Hosseini et al. 2008) are given in the unit of L/kgfw. These data were converted into  $m^3/kgC$  by multiplying the data with the factor 0.00856 based on conversion factors given in "**Conversionfactors.xlsx**" (the conversion factors in this table is based on dry matter and carbon content data reported by IAEA (2010). The converted data are given in the examples below in order to facilitate comparisons among the data sources (cf. Appendix A for further information on unit conversions).

#### 3.2.1 cR\_lake\_fish for Nickel (Ni)

The data available for Ni are listed in

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-11. Data were available from Laxemar and the combined data from both Forsmark and Laxemar. No data are available from Forsmark so both site data sources are identical in this case. IAEA (2010) reported data for the category “muscle tissue” and “whole body” and ERICA (Hosseini et al. 2008) reported data for “benthic fish” and “pelagic fish” (the data for these categories were identical).

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows:  $GSD_{min} = 2$ ,  $GSD_{mean} = 3$  and  $GSD_{max} = 5$ .

The sense checks of these data are done by comparing the ranges of the data. The results are given in Table 7-19 in Tröjbom et al. (2013) and the data are plotted in Figure 3-6.

When site-specific data are compared to the range of the literature data it is evident that the site data are lower than the literature data but partly fall within the data range of IAEA (2010) “muscle tissue” (53% of the site data range are within the literature data range, see Table 7-19 in Tröjbom et al. 2013). For the three literature data sources the data on “muscle tissues” from IAEA (2010) are lower than the data reported for “whole body” samples by IAEA (2010) and ERICA (Hosseini et al. 2008) data fall within the range of “whole body” data from IAEA (2010). The sense checks indicated that there is a difference between “muscle tissue” data and “whole body” data. Muscle tissue data are regarded as more representative for this parameter and since this range overlaps the site data range, site data are assumed to be reasonable and can be used for parameterisation.

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-11. Representative data selected for the parameter CR\_lake\_fish for Ni (m<sup>3</sup>/kgC).

Reference	BiotaType	N	GM	GSD	Min	Max	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Laxemar	n	1 <sup>2</sup>	0.0654	1.5	0.0411	0.0903	0.0331	0.129
Forsmark&Laxemar	n	1 <sup>2</sup>	0.0654	1.5	0.0411	0.0903	0.0331	0.129
IAEA (2010)	Fish, Muscle tissue	5	0.180	1.9	0.094	0.377	0.0626	0.517
IAEA (2010)	Fish, Whole body	24	0.608	2.1	0.163	5.653	0.179	2.06
ERICA	Benthic fish	3	0.857 <sup>1)</sup>					

- 1) ERICA data are reported as normal distributed data as arithmetic mean.
- 2) N for denominator is 3 and numerator 1.

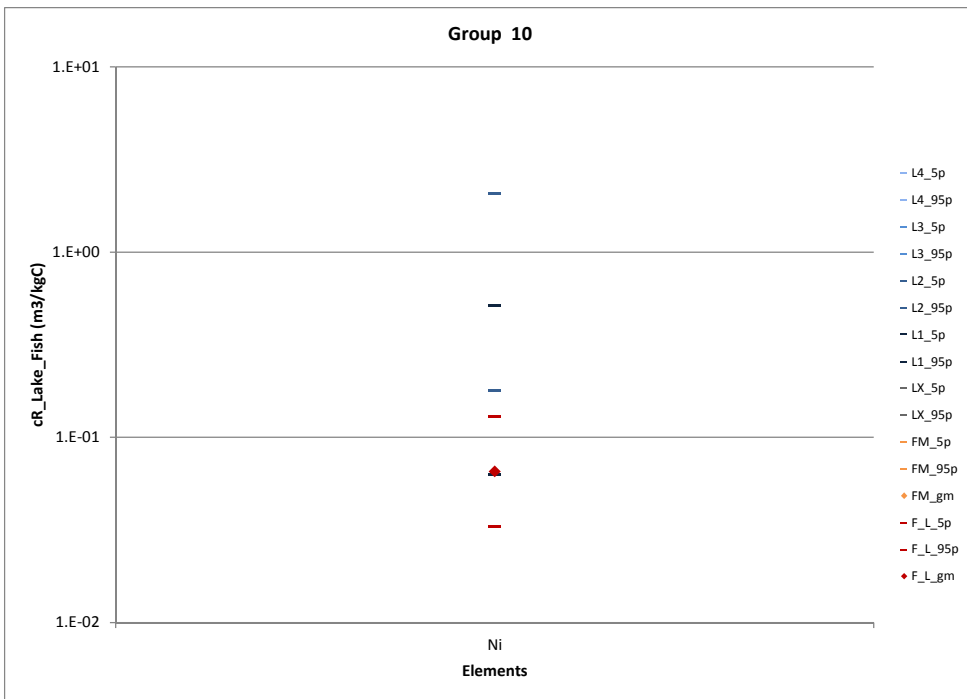


Figure 3-6. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for cR\_lakeFish for Ni. The range of literature data overlaps the site data partly. The data for muscle tissue and whole body differ.

The selections of data are described below and the selected data are presented in Table 3-12. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Laxemar data is selected (0.0654).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria. In this case it is the same as the GM of the Laxemar data since no Forsmark data exists (0.0654).

**Geometric standard deviation (GSD)** - Since the number of samples are only 1 (N=1) the GSD is compared to the GSDmax limit, which in this case is 5. Since the reported GSD is lower (1.5) it is replaced by the GSDmax limit (5).

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=5 according to

Manual reproduction of Kd and CR parameter values in SR-PSU

the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.0411 and the calculated 5<sup>th</sup> percentile (based on GM=0.0654, GSD=5) is 0.0046 and therefore is the 5<sup>th</sup> percentile is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95th percentile calculated using the selected GM and GSD (in this case GSD=5) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.0903 the calculated 95<sup>th</sup> percentile is 0.9227 (based on GM=0.065, GSD=5) and therefore 0.9227 is selected.

*Table 3-12. Selected data for cR\_lake\_fish for Ni (m3/kgC).*

Reference	N	BE	GM	GSD	Minimum	Maximum
Laxemar	1	0.065	0.065	5	0.0046	0.92

### 3.2.2 cR\_lake\_fish for Iodine (I)

The data available for I are listed in Table 3-13. Data were available from Forsmark, Laxemar and the combined data from both Forsmark and Laxemar. IAEA (2010) reported data for the category “muscle tissue” and “whole body” and ERICA (Hosseini et al. 2008) reported for “benthic fish” and “pelagic fish” (the data for these categories were identical). ERICA data are reported as arithmetic mean and arithmetic standard deviation.

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSDmin = 2, GSDmean = 3 and GSDmax = 5.

The sense checks of these data are done by comparing the ranges of the data. When site-specific data is compared to the range of the literature data it is evident that the site data falls within the literature data range. For the three literature data sources the data on “whole body” from IAEA (2010) are higher than data on “muscle tissue”.

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-13. Representative data selected for the parameter CR\_lake\_fish for I (m<sup>3</sup>/kgC).

Reference	BiotaType	N	GM	GSD	Minimum	Maximum	Distribution
Forsmark	n	1 <sup>2</sup>	0.655	1.2	0.595	0.794	lognormal
Laxemar	n	3 <sup>3</sup>	0.436	2.6	0.117	2.636	lognormal
Forsmark&Laxemar	n	6 <sup>4</sup>	0.462	2.4	0.117	2.636	lognormal
IAEA (2010)	Fish, Muscle tissue	50	0.257	2.5	0.094	3.426	lognormal
IAEA (2010)	Fish, Whole body	94	5.567	2.1	0.857	385	lognormal
ERICA	Benthic fish	10	1.542 <sup>1)</sup>	3.0 <sup>1)</sup>	0.069	6.852	normal

- 1) ERICA data are reported as normal distributed data as arithmetic mean and standard deviation.
- 2) N for denominator is 3 and numerator 1.
- 3) N for denominator is 3 and numerator 6.
- 4) N for denominator is 6 and N for numerator 7.

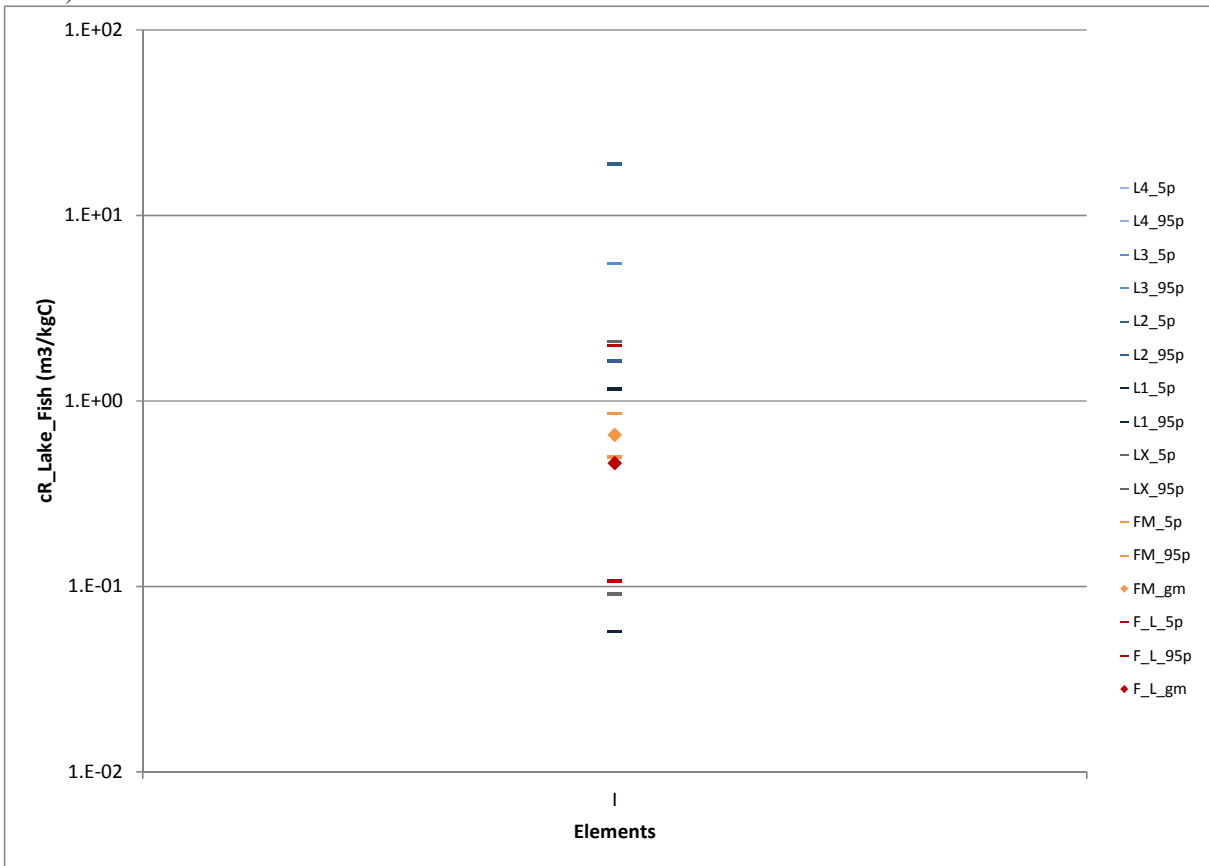


Figure 3-7. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for cR\_lakeFish for I. The range of literature data overlaps the site data.

The selections of data are described below and the selected data are presented in Table 3-14. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.655).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data are selected according to the criteria, in this case it is 0.462.

**Geometric standard deviation (GSD)** - Since the number of samples are 6 (N =6) the reported GSD is compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (2.4) it is replaced by the GSDmean limit (3).

Manual reproduction of Kd and CR parameter values in SR-PSU

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.117 and the calculated 5<sup>th</sup> percentile (based on GM=0.655, GSD=3) is 0.076 and therefore is the 5<sup>th</sup> percentile is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95th percentile calculated using the selected GM and GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 2.636 the calculated 95<sup>th</sup> percentile is 2.81 (based on GM=0.655, GSD=3) and therefore 2.81 is selected.

*Table 3-14. Selected data for cR\_lake\_fish for I (m3/kgC).*

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark&Laxemar	6	0.655	0.462	3	0.076	2.81

### 3.2.3 cR\_lake\_fish for Calcium (Ca)

The data available for Ca are listed in Table 3-15 and

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-11. Data were available from Forsmark, Laxemar and the combined data from both Forsmark and Laxemar. IAEA (2010) reported data for the category “muscle tissue” and “whole body”.

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows:  $GSD_{min} = 2$ ,  $GSD_{mean} = 3$  and  $GSD_{max} = 5$ .

The sense checks of these data are done by comparing the ranges of the data by using the 5<sup>th</sup> and 95<sup>th</sup> percentile of all available data and comparing the area of overlap. The ranges are plotted in Figure 3-8. The result of the sense checks are also presented in Table 7-19 of Tröjbom et al (2013). Forsmark and Laxemar data show a partial overlap, where the range of Laxemar data are higher. When Forsmark and Laxemar data are compared to the range of the literature data it is evident that the site data fall within the literature data range (see Table 7-19 in Tröjbom et al. 2013). For the two literature data sources the data on “muscle tissues” from IAEA (2010) are lower than the data reported for “whole body” samples by IAEA (2010). This is to be expected since bones, which are included in the whole body samples, contain high concentrations of Ca.



Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-15. Representative data selected for the parameter CR\_lake\_fish for Ca (m<sup>3</sup>/kgC).

Reference	BiotaType	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	3 <sup>1</sup>	0.096	2.2	0.026	0.342	0.0258	0.357
Laxemar	n	3 <sup>2</sup>	0.549	1.8	0.138	1.032	0.200	1.51
Forsmark&Laxemar	n	6 <sup>3</sup>	0.155	2.9	0.026	1.032	0.0265	0.902
IAEA (2010)	Fish, Muscle tissue	104	0.103	2.5	0.0171	0.831	0.0228	0.464
IAEA (2010)	Fish, Whole body	119	8.57	3.4	0.805	48.0	1.14	64.1

- 1) N for denominator is 3 and N for numerator is 16.
- 2) N for denominator is 3 and N for numerator is 6.
- 3) N for denominator is 6 and N for numerator is 22.

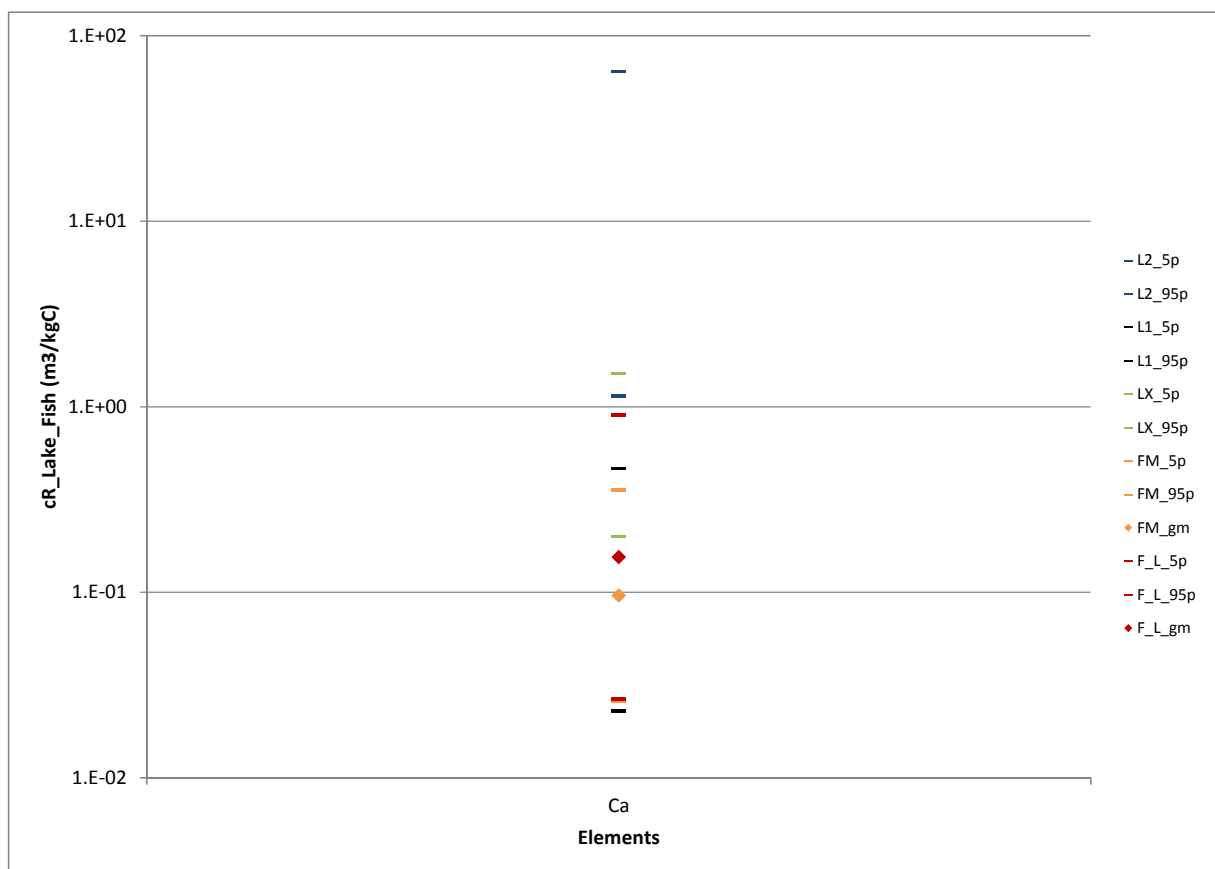


Figure 3-8. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for limnic fish for Ca. Site data fall within the literature data range. The literature data for muscle tissue are lower than the literature data for whole body.

The selections of data are described below and the selected data are presented in Table 3-16. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark is selected (0.096).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case 0.155.

**Geometric standard deviation (GSD)** - Since the number of samples are 6 (N =6) the GSD is compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (2.9) it is replaced by the GSDmean limit (3).

Manual reproduction of Kd and CR parameter values in SR-PSU

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.026 and the calculated 5<sup>th</sup> percentile (based on GM=0.155, GSD=3) is 0.025 and therefore is the 5<sup>th</sup> percentile is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case GSD=3) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 1.032 which is higher than the calculated 95<sup>th</sup> percentile (based on GM=0.065, GSD=5) and therefore 1.032 is selected.

Table 3-16. Selected data for cR\_lake\_fish for Ca (m<sup>3</sup>/kgC).

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark&Laxemar	6	0.096	0.155	3	0.025	1.032

### 3.2.4 cR\_lake\_fish for Molybdenium (Mo)

The data available for Mo are listed in Table 3-17. Data were available from Forsmark, Laxemar and the combined data from both Forsmark and Laxemar. IAEA (2010) reported data for the category “muscle tissue” and “whole body”.

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSDmin = 2, GSDmean = 3 and GSDmax = 5.

The sense checks of these data are done by comparing the ranges of the data. Forsmark and Laxemar data are within the same range. When the site-specific data are compared to the range of the literature data it is evident that the site data are within the total literature data range (see Table 7-19 in Tröjbom et al. 2013). For the literature data, the two categories do not overlap. The data on “muscle tissues” from IAEA (2010) is lower than the data reported for “whole body” samples by IAEA (2010). The site data fall partly within the range of the “muscle tissue” data, and is higher in comparison to this data category. The sense checks indicated that there is a difference between muscle tissue data and “whole body” data and that the site data are in between these two literature data sets.

Table 3-17. Representative data selected for the parameter CR\_lake\_fish for Mo (m<sup>3</sup>/kgC).

Reference	Biota Type	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	3 <sup>1</sup>	0.096	1.9	0.036	0.455	0.0346	0.265
Laxemar	n	3 <sup>2</sup>	0.072	2.6	0.025	0.432	0.0148	0.346
Forsmark&Laxemar	n	6 <sup>3</sup>	0.088	2.1	0.025	0.455	0.0257	0.299
IAEA (2010)	Fish, Muscle tissue	64	0.016	2.1	0.000034	0.171	0.00480	0.0552
IAEA (2010)	Fish, Whole body	91	0.231	1.9	0.0180	1.627	0.0805	0.665

1) N for denominator is 3 and N for numerator is 14.

2) N for denominator is 3 and N for numerator is 6.

3) N for denominator is 6 and N for numerator is 20.

Manual reproduction of Kd and CR parameter values in SR-PSU

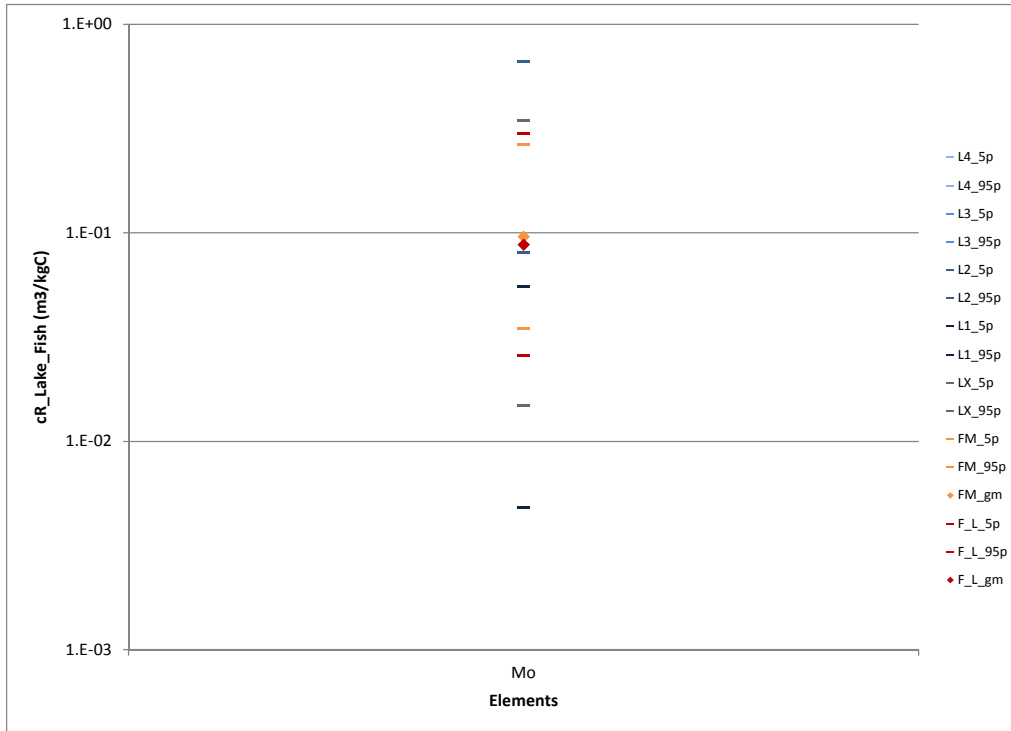


Figure 3-9. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for limnic fish for Ca. Site data fall within the literature data range. The literature data for muscle tissue are lower than the literature data for whole body.

The selections of data are described below and the selected data are presented in

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-18. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.096).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case it is 0.088.

**Geometric standard deviation (GSD)** - Since the number of samples are 6 ( $N=6$ ) the GSD is compared to the GSDmean limit, which in this case is 3. Since the reported GSD is lower (2.1) it is replaced by the GSDmean limit (3).

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case  $GSD=3$ ) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.025 and the calculated 5<sup>th</sup> percentile (based on  $GM=0.088$ ,  $GSD=3$ ) is 0.014 and therefore is the 5<sup>th</sup> percentile is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case  $GSD=3$ ) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.455 the calculated 95<sup>th</sup> percentile is 0.535 (based on  $GM=0.088$ ,  $GSD=3$ ) and therefore 0.535 is selected.

Manual reproduction of Kd and CR parameter values in SR-PSU

*Table 3-18. Selected data for cR\_lake\_fish for Mo (m3/kgC).*

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark&Laxemar	6	0.096	0.088	3	0.014	0.535

### 3.2.5 cR\_lake\_fish for Uranium (U)

The data available for U are listed in Table 3-19. Data were available from Forsmark, Laxemar and the combined data from both Forsmark and Laxemar. IAEA (2010) reported data for the category “muscle tissue” and “whole body” and ERICA (Hosseini et al. 2008) reported data for “benthic fish” and “pelagic fish” (the data for these categories were identical).

The GSD limits for this parameter are according to Table 4-3 in Tröjbom et al. (2013) as follows: GSDmin = 2, GSDmean = 3 and GSDmax = 5.

The sense checks of these data sources are done by comparing the ranges of the data. The ranges are listed in Table 3-19 and plotted in Figure 3-10. Forsmark and Laxemar data partly overlap each other, and the Laxemar data is lower than the Forsmark data. The reason for this deviation is not known. The ranges of site data are almost enclosed by the large range of IAEA (2010) data for “muscle tissue”. The range of ERICA data is narrower and higher than the site data (cf. Table 7-19 in Tröjbom et al. 2013).

Manual reproduction of Kd and CR parameter values in SR-PSU

Table 3-19. Representative data selected for the parameter CR\_lake\_fish for U (m<sup>3</sup>/kgC).

Reference	BiotaType	N	GM	GSD	Minimum	Maximum	5 <sup>th</sup> percentile	95 <sup>th</sup> percentile
Forsmark	n	3 <sup>1</sup>	0.00062	3.4	5.88E-05	0.00810	8.42E-05	0.00450
Laxemar	n	3 <sup>2</sup>	0.00863	3.1	0.00123	0.0288	0.00135	0.0551
Forsmark&Laxemar	n	6 <sup>3</sup>	0.00111	5.0	5.88E-05	0.0288	7.8E-05	0.0157
IAEA (2010)	Fish, Muscle tissue	9	0.00822	12	0.00017	0.00822	0.000138	0.490
IAEA (2010)	Fish, Whole body	2	0.02056	-	0.0126	0.0283	-	-
ERICA	Benthic fish	11	0.2570	0.51	0.00257	1.71	0.0143	0.926

- 1) N for denominator is 3 and N for numerator is 14.
- 2) N for denominator is 3 and N for numerator is 4.
- 3) N for denominator is 6 and N for numerator is 18.

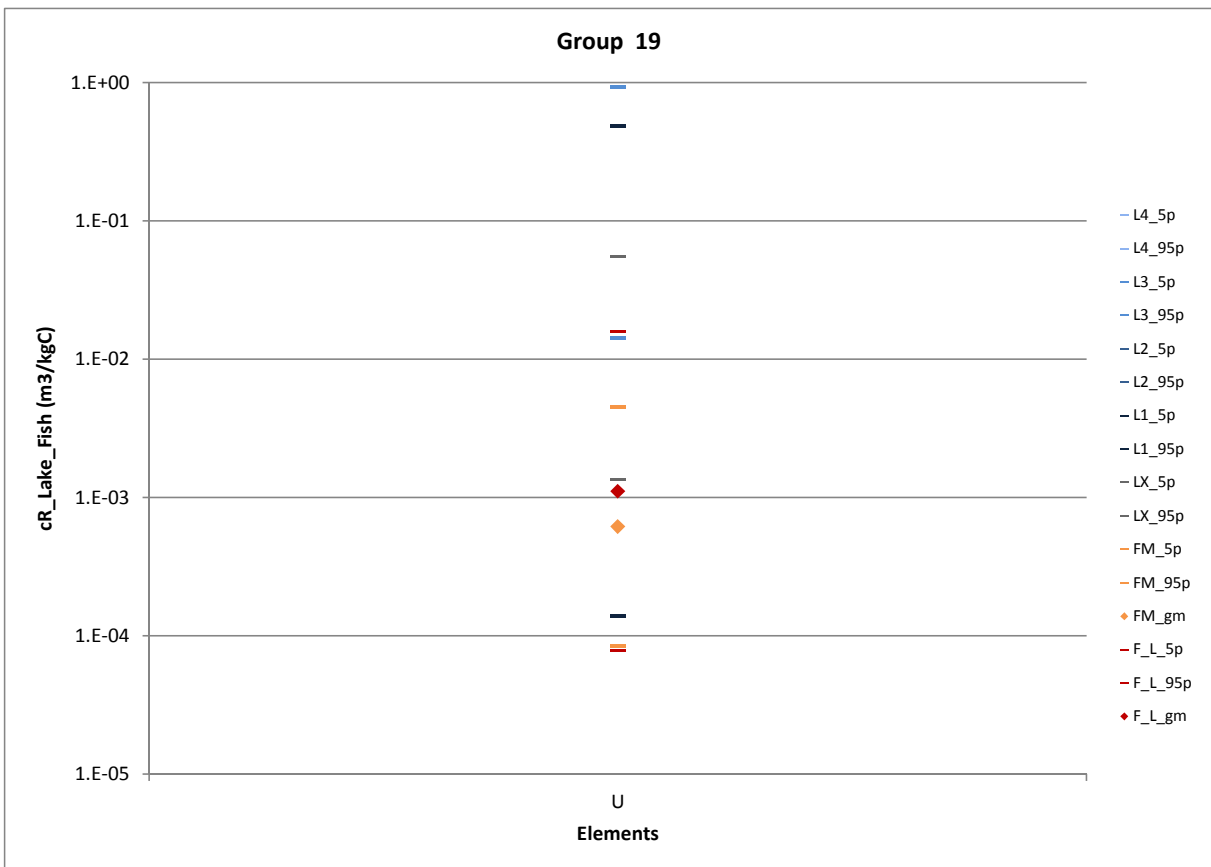


Figure 3-10. Ranges (5<sup>th</sup> and 95<sup>th</sup> percentiles) of data available for limnic fish for U. Site data fall within the large literature data range of muscle tissue data from IAEA (2010). The literature data for ERICA /whole body samples are higher than the literature data for muscle tissue (IAEA 2010).

The selections of data are described below and the selected data are presented in Table 3-20. According to the selection criteria where site data are prioritised the site data would be selected as the most representative data.

**Best estimate (BE)** - According to the selection criteria the GM of the Forsmark data is selected (0.00062).

**Geometric mean (GM)** - The GM of the combined Forsmark and Laxemar data should be selected according to the criteria, in this case it is 0.00111).

Manual reproduction of Kd and CR parameter values in SR-PSU

**Geometric standard deviation (GSD)** - Since the number of samples are 6 (N =6) the GSD is compared to the GSDmean limit, which in this case is 3. Since the reported GSD is higher (5) the reported GSD is used.

**Minimum value (min)** - The minimum value should be the lowest of the reported minimum value or the 5<sup>th</sup> percentile calculated using the selected GSD (in this case GSD=5) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported minimum is 0.000058 is lower than the calculated 5<sup>th</sup> percentile (based on GM=0.00111, GSD=5) and therefore the reported minimum value is selected.

**Maximum value (max)** - The maximum value should be the highest of the reported maximum value or the 95<sup>th</sup> percentile calculated using the selected GM and GSD (in this case GSD=5) according to the criteria in Section 4.4.2 in Tröjbom et al. (2013). The reported maximum is 0.0288 is higher the calculated 95<sup>th</sup> (based on GM=0.0011, GSD=5) and therefore it is selected.

*Table 3-20. Selected data for cR\_lake\_fish for U (m<sup>3</sup>/kgC).*

Reference	N	BE	GM	GSD	Minimum	Maximum
Forsmark&Laxemar	6	6.16E-04	1.11E-03	5.0	5.88E-05	2.88E-02

## 4 References

**Grolander S, Tröjbom M, 2016.** Guide to implementation of the SR-PSU K<sub>d</sub> and CR parameterisation process in two Access databases. Detailed descriptions based on three examples. SKBdoc 1555970 ver 1.0, Svensk Kärnbränslehantering AB.

**Hosseini A, Thørring H, Brown J E, Saxén R, Ilus E, 2008.** Transfer of radionuclides in aquatic ecosystems – Default concentration ratios for aquatic biota in the Erica Tool. Journal of Environmental Radioactivity 99, 1408–1429.

**IAEA, 2010.** Handbook of parameter values for the prediction of radionuclide transfer in terrestrial and freshwater environments. Vienna: International Atomic Energy Agency. (Technical Report Series 472)

**ICRP, 2011.** Wildlife Transfer Parameter Database. International Commission on Radiological Protection. Available at: <http://www.wildlifetransferdatabase.org> [Februari 2011].

**Tröjbom M, Grolander S, Rensfeldt V, Nordén S, 2013.** K<sub>d</sub> and CR used for transport calculation in the biosphere in SR-PSU. SKB R-13-01, Svensk Kärnbränslehantering AB.



## Appendix A - Unit conversions

The literature data used are imported into the database in the original units given in the literature source. Since these units can be different from the units used in this study unit conversions are needed. Conversion factors are calculated based on dry matter and carbon content data from IAEA (2010), which are listed in the file DMC & CC database.xlsx where also detailed references to the original tables in the IAEA (2010) are given. The equations for the conversion factors used for unit conversions between fresh weight, dry weight, carbon content and L and m<sup>3</sup> are listed in Table 4-1 in Tröjbom et al. (2013). The resulting conversion factors for each data category and each unit is presented in the file **ConversionFactors.xlsx**. These factors are used in the parameterisation process to convert data from literature sources into common units.

Two typing have been detected in Table 4-1 in the printed report (Tröjbom et al. 2013), which have been corrected in Table A-1 below. The implementations of these functions in the database were, however, correct and the parameterisations was hence not affected.

*Table A-1. Equations for the conversion factors used to convert between units of literature data.*

	$\text{kg}_{\text{dw}}/\text{kg}_{\text{fw}}$	$\text{kg}_{\text{dw}}/\text{kg}_{\text{C}}$	$\text{kg}_{\text{dw}}/\text{kg}_{\text{dw}}$		
$\text{kg}_{\text{dw}}/\text{kg}_{\text{fw}}$	1	$1/(\text{CC}*\text{DMC})$	$1/\text{DMC}$		
$\text{kg}_{\text{dw}}/\text{kg}_{\text{C}}$	$\text{CC}*\text{DMC}$	1	CC		
$\text{kg}_{\text{dw}}/\text{kg}_{\text{dw}}$	DMC	$1/\text{CC}$	1		
	$\text{L}/\text{kg}_{\text{dw}}$	$\text{m}^3/\text{kg}_{\text{C}}$	$\text{m}^3/\text{kg}_{\text{dw}}$	$\text{m}^3/\text{kg}_{\text{fw}}$	$\text{L}/\text{kg}_{\text{fw}}$
$\text{L}/\text{kg}_{\text{dw}}$	1	$1/(1000*\text{CC})$	$1/1000$	$\text{DMC}/1000$	DMC
$\text{m}^3/\text{kg}_{\text{C}}$	$1000*\text{CC}$	1	CC	$\text{CC}*\text{DMC}$	$1000*\text{CC}*\text{DMC}$
$\text{m}^3/\text{kg}_{\text{dw}}$	1000	$1/\text{CC}$	1	DMC	$1000*\text{DMC}$
$\text{m}^3/\text{kg}_{\text{fw}}$	$1000/\text{DMC}$	$1/(\text{CC}*\text{DMC})$	$1/\text{DMC}$	1	1000
$\text{L}/\text{kg}_{\text{fw}}$	$1/\text{DMC}$	$1/(\text{CC}*\text{DMC}*1000)$	$1/(\text{DMC}*1000)$	$1/1000$	1