

## Draft Reports from Brainstorm group discussions

There was some overlap in discussions. Where these occurred, the relevant text has been moved to the most appropriate topic area.

### Database Working Group

The working group has discussed about the possibility of constructing a common  $K_d$  database based on regrouping  $K_d$  compilations of different environmental compartments, such as soils, freshwater and marine environments. This common database could permit combined analyses and comparisons between these media. Although this objective is relevant for modelers, it seems difficult to be reached rapidly because there is not yet a database for marine environments (although it could be built up from already existing data) and the existing  $K_d$  compilations for soils and freshwater use different approaches in terms of criteria for data acceptance, compiled parameters, and preliminary statistical treatments. This is illustrated by:

- The treatment of replicates. The soil  $K_d$  compilation considers only the average value for a given replicate set. Conversely, the compilation for freshwater  $K_d$  conserves all the replicates to take into account the variability associated to a replicate set.
- The parameters and variables included in the compilations. The compilation for soil  $K_d$  is mainly structured around soil properties (pH, organic matter content, texture, soil solution composition...), whereas the freshwater compilation is much more based on the experimental approaches and variables (contact time, mass/volume ratios, aging time...).

For a single database to be built, these differences would require checking the raw data again to try to harmonize the compilations, requiring work that is not compatible with the time dedicated to this project. Besides, the added value of an integrated database is not clear. Consequently, it is proposed to transform the existing compilations (currently in the form of Excel files) into three independent databases (soil, freshwater, and marine), but sharing the same software, and with common structure, criteria for data acceptance and relevant parameters.

The establishment of similar data acceptance criteria allows a better comparison of the  $K_d$  of the different media and, eventually, to better introduce the analogue approach to fill data gaps. The main data acceptance criteria are listed as follows:

- Experimental method must be identified to clearly identify the type of approach followed to derive the  $K_d$  values. The accepted approaches are: batch sorption; *in situ* desorption; batch desorption; *in situ* desorption with natural/stable isotopes (indigenous (stable isotope) data).
- In case of several replicates for the same location and/or conditions and the same reference (e.g., soil type, pH, background aqueous salt concentrations) only average values are to be recorded and not the results of each individual analytical replicate. A  $K_d$  value is often given with its standard deviation - we should also take into account this information and think about how to use it during statistical analysis. Authors rarely provide replicate results, making it difficult to consistently input such data.
- Samples with a specific treatment (e.g. pH or salt concentration) or origin (e.g. locations at a study site), could be individually entered into the database. This may be appropriate when several soil samples are collected from a study site which is variable, or where the samples have been treated differently. This will capture how individual  $K_d$  values vary in relation to the treatment or soil properties at that field site. This means we identify two

types of data sets: 1) replicates of the same experiment (previous section) and 2) several different samples of the same campaign.

- No data from either diffusion experiments or from parametric equations/models should be accepted.
- In principle, no data from pure mineral phases should be accepted. This criterion could be revised in the future to permit filling data gaps. Our intent is to prioritize data gathered from natural complex systems, and then use such pure phase data to fill in data gaps, such data would be clearly identified as of a “lower/different status.”
- Regarding sorption isotherms, a single value representative for the linear  $C_s$  vs.  $C_{eq}$  range could be entered.
- Data not representative of environmental conditions could be accepted, to better evaluate the role of cofactors (e.g.,  $K_d$  obtained at extreme values of pH,  $E_h$ , ionic strength...). This notion supports one of the overall objectives of this DB of not only providing users with  $K_d$  values for their unique applications, but also to help understand the underlying cofactors responsible for  $K_d$  variability.

Once the data acceptance criteria are agreed, the data already entered in the respective databases should be adapted to these criteria. In a second stage, the common structure for the databases could be discussed and the existing compilations could be transferred to a database-friendly software, such as Access. In a further stage, it will be necessary to decide a common approach for statistical treatments. Outstanding issues associated with this work are summarized as follows:

- **Construction of an “intelligent” (Access-based) database.** Sustainability (+ quality control); how to report values?; hierarchic and combined use of cofactors; flexibility to access/create output data: the end user may be interested in calculating their own (best estimate)  $K_d$  value, or a correlation, or a distribution function...
- **Guidance/help document:** Identify the objectives of the database and its intended applications. Also identify incorrect applications (beyond the original intent) of the database, terms and approach definitions (e.g., “stable isotope data”, “sorption batch data”); data acceptance criteria should be clearly documented and explained; how the data was derived from the source (e.g., from a table or a figure; calculated from raw data...).
- **Accessibility.** Decisions on the level of accessibility to the databases for the scientific community.

### Statistical Working Group

The challenge is to deal with those cases where there is a limited, or no, data for the  $K_d$ . In a particular situation, there may be missing values which are not important with respect to dose.

It is important to initially consider data available for the magnitude of the source term, the potential hazard due to exposure to the radioisotope and the probability of release before making a judgment on whether it is necessary to input a  $K_d$  value from data rather than using a conservative derived value. It is evident that there are different ways in which data can be considered to be limited including (i) insufficient numbers of different  $K_d$  values, (ii) lack of data about cofactors.

Statistical methods cannot replace experimental data, but the need for more data will depend on a number of factors such as:

- situations where the expected variability of a  $K_d$  is relatively high (e.g. more data is needed for freshwater than for the ocean.)
- the need for sufficient data to allow for environmental variability for modeling purposes

Sensitivity analyses may help establish the acceptable uncertainty for modeling. When there is no, or limited,  $K_d$  data available, risk assessment procedures should inform the decision on the quantity / quality of the  $K_d$  data needed to robustly carry out an assessment at that tier. Thus, the need for data will vary for a screening assessment compared with a site specific assessment. The use of safety factors at tier 1 will ensure a conservative value. For further tiers more data will be needed (and guidance should be provided). There ought to be a big difference how cases are treated where there is no  $K_d$  data vs. where there are not enough data. Test should address this distinction. For more detailed assessment at Tier 3, if possible,  $K_d$  values would vary as a function of cofactors.

There is much discussion on the need for more  $K_d$  data. Guidelines should be set for future experimental studies (related, for instance to cofactors if they have been identified) to ensure the quality and applicability of data on  $K_d$  for the modeling community. Expert judgment can be used for transferring data from one site to another, taking into account the potential impact of cofactors. Knowledge of the effect of cofactors on  $K_d$  can also be used qualitatively to assess the data relevance for a screening or initial assessment. However, quantitative relationships between  $K_d$  and cofactors should be defined if statistically possible for radioisotopes of concern.

We need to identify these different gaps in the data compilations. In many cases there may be no  $K_d$  value. It may be possible to use the mean GSD (calculated from other elements) or the relationship between GMs and GSDs if such a relation exists. For many radionuclides, there are small data sets which give an idea of what the  $K_d$  may be and can be used as the basis for other approaches such as Bayesian derivation.

### **Filling gaps working group**

What is a data gap – the term can have different meanings under different circumstances. For example, there may be a need for time-dependent  $K_d$ , since modeling is conducted for both short or long timescales (especially for geological disposal). If the introduction of BET was pursued then there would be a need for relevant data for many radionuclides. Alternatively, there may be a lack of confidence in available  $K_d$  data, even if it is relatively numerous, if the available  $K_d$  values are considered to be unrepresentative of the particular situation being assessed. We therefore need to define different types of  $K_d$  and use them appropriately.

#### **Key questions include:**

Do we really need to fill gaps?

Are derived (or extrapolated)  $K_d$  values acceptable or can it be argued that they cannot replace definitively appropriately derived experimental data?

#### Extrapolating $K_d$ values from Soils to sediments

The derivation of  $K_d$  data varies, from batch experiments are often subdivided into different types of solid phase: namely soil/sediment (FW and SW) and/or ‘mineral’ phases. Since soil erosion produces sediment in aquatic systems, it can be argued that the use of soil data (mainly clay soil) for sediment may provide an appropriate analogy. If it is shown that there is no distinction between the two types of solid phase, then the data can be pooled for analyses. However, the use of a clay soil/sediment extrapolation needs to be carefully investigated as the sediment composition needs to be similar to that of clay. For instance, gyttja, a freshwater

deposit, has a high OM content and is very different to clay. Nevertheless, there is some merit in considering whether we can categorize sediments as soils, or at least having common criteria to classify and distinguish between them when necessary. The possible inclusion of marine  $K_d$  data (at least from estuary areas) should also be considered.

To test these ideas, there is a need for a new analysis of the complete  $K_d$  dataset comparing similar data, and (i) devising criteria and rules to homogenise the data, (ii) exploring the relationship between all soils/all sediments. It would be useful if a single ratio can be derived, but is probably better to focus on a number of categories (cf. previous comments above).

#### Freshwater $K_d$ values

Bottom sediment is considered separately from suspended sediment. Moreover, for bottom sediment, the distinction should be made between the surficial/active layer and the deeper layers. The surficial sediment is the biologically active layer which is oxygenated. The deeper sediment layers are deoxygenated and, as such, are of interest with respect to waste repositories. For aquatic modeling, the sedimentation rate is an important parameter (for the active layer) which is often not reported.

#### Use of stable isotope

$K_d$  data for stable isotope are being added to the database as they are relevant for long term assessment where there is an equilibrium situation. However, for other situations, it needs to be kept in mind that there is an exchange between stable and radioactive isotopes (moving towards equilibrium?). Geochemical modeling can theoretically be used to explore relationships between stable isotope and radioactive  $K_d$  values but this is constrained by a lack of data. If there is a gap in terms of  $K_d$  values, it is more than probable that the required environmental factors (such as a physico-chemical description) necessary to be able to run geochemical models will also be missing.

For a given element if we are able to establish a kind of relationship, regardless its nature (e.g. qualitative or quantitative), between the soil/sediment categories and the value of stable isotope  $K_d$ , we could theoretically apply it to the relevant radioactive  $K_d$ . For example, if there is a decreasing trend of the stable isotope  $K_d$  value with increasing grain size of the solid phase, the same trend should apply to the radioactive  $K_d$ . But this means that at least one radioactive  $K_d$  value should be available for one of the categories. Any characteristic allowing definition of solid phase categories could be used in this way, from a qualitative or quantitative point of view.

If it is possible to define a correction factor for a given element between stable isotope and radioactive  $K_d$  values, there is no justification to apply this factor to another element as the correction factor will be specific to the element

Ultimately, the use of stable isotope data is a user choice and depends on the context. For long term assessments it is justified to use stable isotope  $K_d$  values as there is an equilibrated situation. However, for « short » term assessment there is no equilibrium, and no justification to directly use stable isotope  $K_d$  values.

#### Correlation between CR and $K_d$ values

Soil  $K_d$  values should theoretically be correlated to soil/plant CRs, as root uptake is from the amount of the radionuclide in the soil solution which is influenced by  $K_d$ . Indeed, this has been previously reported where  $\ln(K_d) = a + b \times \ln(CR)$ <sup>1</sup>. The correlation should be taken into account for the assessment itself - you cannot independently use a  $K_d$  and a root uptake CR as

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<sup>1</sup> Baes CF (1982). Prediction of radionuclides  $K_d$  values from soil-to-plants concentrations ratios. Trans. American Nuclear Society, 41: 53-54.

they are linked. The choice of a value for the CR should guide/impact/influence that of  $K_d$ , and vice versa. The correlation was used in TRS 364 (extrapolation to fill gaps) and could be explored further to derive new values of  $K_d$  values and identify outliers. Such an approach was not used in TRS 472. CR vary with many plant properties, such as age and species/variety and with rainfall conditions. Importantly, such correlations may make it difficult to take into account ancillary information about the influence of soil co-factors on  $K_d$ .

It would be useful to test the hypothesis that there is a single relationship for all elements between root transfer CR and  $K_d$  values, which might be tested for the different soil categories?

The concept may be transferrable to aquatic systems, with respect to phytoplankton CRs.

To explore this approach, it would be important that the  $K_d$  database structure should be consistent with that used for the soil-plant CR values.

### Analogues

The use of analogues is often applied, but rarely rigorously tested. When selecting suitable analogues many different characteristics might be evaluated including whether the analogue has a similar atomic radii, valence, biological role, complexation behavior, and abundance.

We have identified some ways to go forward, but initially we need to build the database, incorporate homogeneous data already available from soil and aquatic compilations and add new data.

### Geochemical models

Alternatively, geochemical models can be used to produce virtual  $K_d$  dataset, where it is calculated from the model based on the composition of a soil, sediment or water as long as there is confidence in the known chemistry of the element considered. This requires a full knowledge of relevant cofactors and a complete characterization of the liquid and solid phases. Experimental studies should concentrate on those elements of concern, for which few data exist.