Translating natural concentrations and fluxes into safety indicators for radioactive waste repositories

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Abstract. Natural deposits of radioactive elements can provide important and very useful information for safety evaluation of radioactive waste repositories. The information is especially helpful for public communication. However, a simple comparison between the calculated fluxes and concentrations in a proposed repository and those natural ones can be ambiguous. This ambiguity arises from high complexity, imprecise knowledge, different data formats and units. This work suggests the use of a methodology, based on fuzzy logic tools, to handle this ambiguous information. A case study is presented as an example.

Introduction

There are many sources of uncertainties in the traditional dose and risk calculations used in Performance Assessment (PA). A main source of uncertainties is the need for making assumptions regarding human future habits, and the repository performance during its useful life. (IAEA1999; Kozak 1997)

In an attempt to improve confidence and public acceptance of the results of the performance assessment calculations, the use of complementary safety indicators has been suggested. (Miller et al. 2000) One of these complementary methodologies would be to compare predictions of repository releases with natural fluxes and concentrations of chemical species. This methodology would have an additional advantage which is the use of a natural context for safety demonstration making it easier for the public to understand.

However, the use of natural fluxes and concentrations requires the use of a huge amount of data that may not be readily available. The lack of data together with spatial variations, are important sources of uncertainties and ambiguousness in data analysis.

Some solutions to this problem, such as a global average flux value (for example, the global average activity flux due to groundwater discharge) masks considerable variation in the fluxes which occur at different sites, and in different geological and climatic environments.

This shows that the use of these complementary safety indicators will not reduce uncertainties, rather they have the advantage of placing the calculations in a framework that can be compared to natural processes. While these safety indicators do enhance confidence, there still exist ambiguousness in the results due to the uncertainties.

It is within this context that this work suggests the use of a methodology, based on fuzzy logic tools, which is designed to handle ambiguous data and allows the use of natural language terms for the comparisons between repository system and natural environments.

Fuzzy relations

Fuzzy relations are calculated through logic compositions. The mapping of elements of one universe Y to other universe X is made through a cartesian product of the two universes. The strength of the relation is measured with a membership function. Methods to accomplish this are described in (Ross 1995). One of these methods is the max-min. It can be imagined as the links of a chain. The strength of a chain is equal to the strength of the weakest link. In case of two parallel chains, the strongest one will determine the strength of the two of them. This can be shown by the equations:

$T=R \cdot S$, where : R is a fuzzy relation on the cartesian space X × Y and S is a fuzzy relation on the cartesian Y × Z space, and T is a fuzzy relation on the X × Z space. Then:

$$\chi_{\boldsymbol{T}}(\boldsymbol{x},\boldsymbol{z}) = \bigvee_{\boldsymbol{y} \in \boldsymbol{Y}} (\chi_{\boldsymbol{R}}(\boldsymbol{x},\boldsymbol{y}) \wedge \chi_{\boldsymbol{S}}(\boldsymbol{y},\boldsymbol{z})) \qquad (1)$$

Where χT is the characteristic function of T in the interval [0,1]. This function measures the strength of the relation, i.e., a value of 1means full relation and 0 no relation.(Ross 1995)

$\wedge$ is minimum and, $\vee$ is a maximum value.

Fuzzy pattern recognition

Site parameters can be defined as fuzzy sets. In fuzzy sets, the known patterns typically are represented as class structures, where each class structure is described by a number of features. A typical problem in pattern recognition is to collect data from a physical process and classify them into known patterns or rank them according to a pre-determined criteria.

Suppose we have patterns represented as fuzzy sets A_i on X(i=1,2....m) and a new piece of data, perhaps consisting of a group of observations, is represented by a fuzzy set B on X. The task now is to find which A_i the sample B most closely matches.

According to (Ross 1995) if we define two fuzzy vectors, say **A** and **B**, then if the vectors are identical (same length and same elements) their inner product $\boldsymbol{A \bullet B^T}$ reaches a maximum value as their outer product, $\boldsymbol{A \oplus B^T}$ reaches a minimum value. These two norms can be used simultaneously in pattern recognition studies because they measure closeness or similarity.

$$(\boldsymbol{A},\boldsymbol{B})_1 = (\boldsymbol{A \bullet B}) \wedge \left(\overline{\boldsymbol{A \oplus B}}\right) \tag{2}$$

$$(\boldsymbol{A},\boldsymbol{B})_2 = \frac{1}{2}\left[(\boldsymbol{A \bullet B}) + \left(\overline{\boldsymbol{A \oplus B}}\right)\right] \tag{3}$$

In particular, when either of the values of (A,B) above approaches 1, then the two fuzzy sets **A** and **B** are more closely similar. When either of the values are close to zero they are more far apart or dissimilar. As some of the features may be more important than others, weights can be introduced, ω_j, where:

$$\sum_{j=1}^{m} \omega_j = 1 \tag{4}$$

Therefore, equations 2 and 3 are then modified for each known pattern (i=1,2.......c):

$$(\boldsymbol{B}, \boldsymbol{A_i}) = \sum_{j=1}^{m} \omega_j (\boldsymbol{B_j}, \boldsymbol{A_{ij}}) \tag{5}$$

Sample **B** is closest to pattern $\mathbf{A}_j$ when,

$$(\boldsymbol{B}, \boldsymbol{A_j}) = \max_{1 \le i \le c} \{(\boldsymbol{B}, \boldsymbol{A_i})\} \tag{6}$$

Where **B** is a collection of fuzzy sets, $\mathbf{B}=\{\mathbf{B}_1, \mathbf{B}_2, ...\mathbf{B}_n\}$, and when **B** is a collection of crisp singletons, i.e., $\mathbf{B}=\{x_1, x_2,. ...x_n\}$ then equation (3) reduces to

$$\mu_{Ai}(x) = \sum_{j=1}^{m} \omega_j \cdot \mu_{Aij}(x_j) \tag{7}$$

in the maximum approach degree, sample x is closest to pattern A_j when equation (5) reduces to

$$\mu_A(x) = \max_{1 \le i \le c} \{\mu_{Ai}(x)\} \tag{8}$$

The use of elemental flux as a natural safety indicator

Calculated fluxes of naturally occurring materials are result of a series of processes (or features) in the surface and subsurface environments (Miller et al. 2000). In order to keep this example simple, a few of the most important features will be considered in the analysis. This list can be changed upon experts agreement.

Typically, it is very difficult to obtain a consistent database of natural geochemical and process rate data, and therefore accurate determinations of average values. A number of assumptions have to be made when quantifying natural concentrations and fluxes to be compared against the repository source term.

Processes driving natural fluxes have considerable variation in their rates. However, these variations are not always due to differences in the inherent properties of the geological materials (such as hydraulic conductivities). They can also be a consequence of external factors such as climate which alters the impact of certain processes (e. g., erosion) and indeed, climate is indicated to be one of the largest causes of erosion of a granitic pluton (Miller et al.2000).

Elemental fluxes may be calculated for specific processes and so a range of mass fluxes corresponding to different processes can be generated for the same element (e.g. flux due to groundwater discharge, erosion, river flow, etc.). In this manner the most significant mass transport mechanism can be readily identified. In terms of providing direct comparisons with repository releases, it is anticipated that fluxes associated with processes which drive the transfer of materials from the groundwater discharge (solute transfer) and erosion (solid transfer) will dominate.

Repository system

The calculated fluxes inside a repository will depend on a number of parameters and processes. For example, intrinsic factors of the waste: the radionuclide's waste stream, waste form, and container control release from the waste (Sullivan, 1993). These factors together with radionuclide specific parameters such as half life, solubility limits, transport parameters (Kd), water flow and moisture contents, initial conditions and boundary conditions will fully describe the problem.

However, due to the large number of different container types and waste forms, it is not always possible to have precise values for all the parameters in order to model the release processes. Rather, analysts professional experience is used to find a model representative of the system.

Let's say containers fall into 3 types, A, B, and C. Type A has an expected lifetime of 1 – 150 years. Type B from 30 – 500 years, and Type C from 300 – 1000 years. A deterministic, conservative (early failure or worst case) model would assign lifetimes of 1, 30 and 300 years to each categories. A probabilistic approach would sample along the ranges and values combined randomly. However, as can been seen, the categories blend in each others intervals, therefore it would not be clear during calculations how a container which expected life time of 100 years would be classified in the category A or B.

A fuzzy set approach would address the problem by using language terms to define the containers conditions such as category A (short life), B (medium) and C (long life). Now a container with life time of 100 years would be placed in both categories A and B, however with different degrees of memberships. The same rationale would be used for determining the release mechanisms in order to describe classes of waste forms.

Upon analysts agreement, it is possible to determine a group of features or parameters (fuzzy sets), to compose vectors for comparison between the repository and the sites features. An example of this approach will be given in the next section.

Example calculations

Suppose one wishes to demonstrate how differently a disposal unit would affect candidate sites' environments. The pattern recognition technique can be used in two ways. First, according to the degree of similarity, the approach can be used to provide a measure of the similarity between each site and the repository. Second, it can determine an ordering of similarity between each site and the repository features. In other words, what site would the repository most closely match.

In a traditional procedure a list of 20 or more sites would be screened for use as a repository site. Simple screening criteria would be evaluated to narrow the list to 5 potential repository sites. These five sites would be presented to decision makers for further consideration. For these sites, it is required to know the effect repository construction and performance would have on each of the near field environment of these sites. Assuming that the sites which are least impacted by the repository should receive further consideration, two sites can be selected.

At the point where there is a list of 5 sites, it would be necessary to conduct a more detailed analysis, with a more detailed data collection and more complex performance analysis. However, making a complete site characterization for 5 sites would be extremely expensive. Even for well studied sites, such as Poços de Caldas in Brazil, the lack of data, force analysts to use natural language (ambiguous) to describe site conditions. (Lemos et al. 2001)

A question remains on how to enhance confidence that one meets the objectives of the site selection, i.e., a list of 5 sites with acceptable degrees of safety and how the repository will affect the selected site.

In this example, a list of 5 candidate sites will be studied and two that have the closest match to the repository will be selected for further characterization, just for demonstration purposes. Then the influence of the repository on the sites will be assessed.

Upon experts agreement the features to be used as comparison factors in this example are:

A- Inventory concentration
B- Redox fronts
C- Sorption

D- Dispersion/diffusion
E- Water flow rate
F- pH
G- Speciation
H- Colloid concentrations

Table I shows a set of features, for each site and repository, after a study of their respective characteristic functions. Some of these features may be typically very different inside the repository and in the environment or between two different sites and this does not necessarily mean that one site has better performance features. How can we then compare the features at both sites? For example, how can one make a comparison between the repository and the site if pH inside the repository is between 9 and 11, and in the environment it is between 6-8 If either range of pH has very little influence on the calculated fluxes for their respective context how should they be compared? Conversely, if pH has a large impact on predicted flux what is the basis for comparison?

An answer would be the characteristic function χ which is defined in the interval [0,1]. This function measures the strength of the link on a relation. In this example, the link is a measure of the impact of a parameter on contaminant flux to the environment. For the first parameter, pH, if Repository pH (between 9-11 due to cementitious materials used to construct the repository) has a very weak link to flux (where $T = pH \cdot Flux$) then χ(pH) will be "low", the same is valid for site pH 6-8. If this range of pH, for any reason, has a weak link to flux it will also generate a "low" characteristic function. Now the characteristic functions can be compared and in this example they would be similarly "low".

This reasoning can be applied to other features such as colloid concentrations, dissolution limits and others. Cs 137, for example, has a high sorption capacity and therefore a high water flow rate may not have a high impact on the calculated flux. However, the transport can be facilitated by the presence of colloids from package corrosion. So, instead of simply comparing water flow rate, it would be more effective to compare between the characteristic function of its link to the flux, depending on each context.

Table I: Example of characteristic functions for each site and repository to be compared

Mode (process)	χ(pH) ω_1=0.05	χ(Redox) ω_2=0.1	χ(Gwt flow rate) ω_3=0.1	χ(Inventory com.) ω_4=0.3	χ(sorption) ω_5=0.05	χ(colloid conc.) ω_6=0.2	χ(dispersion/diff.) ω_7=0.2
Site 1	Medium	Medium	High	Low	High	Medium	High
Site 2	Low	High	Very high	Very low	High	High	Low
Site 3	Medium	Low	Medium	High	Medium	Very high	Low
Site 4	Very low	Low	Medium	Low	Medium	Medium	High
Site 5	Low	Medium	Low	High	High	Low	Medium
Repository	Low	Medium	Medium	Medium	High	Low	Medium

Fig. 1 shows a representation of fuzzy sets low and medium χ(pH)
for repository and site 1 respectively. Applying equation (1) to find the degree of compatibility between site 1 and repository for the comparison factor pH gives :

$\mu($ Repository χ (pH) $\bullet$ site 1 χ (pH)) = max([(0∧1),(0∧0.75), (0.4∧0.4), 0.25∧0.75), (1∧0)]= 0.4

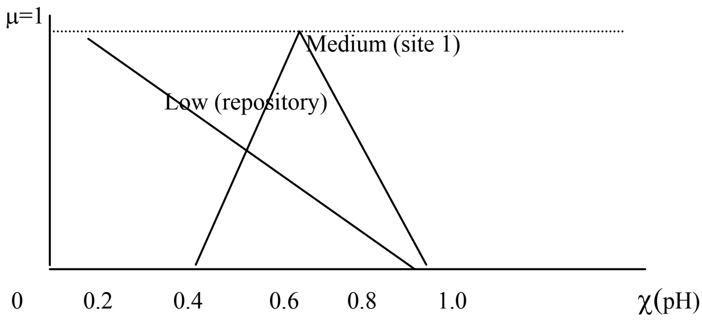

Fig. 1. Example of a comparison between fuzzy sets describing influence of pH on flux, χ(pH), between repository and site 1.

In the above expression, the values for the membership function are evaluated over the domain of the characteristic function at several points. At each point, the degree of compatibility between the two fuzzy sets (pH characteristics in the repository and site 1) is taken as the minimum at each point. The maximum value from this set of minimums is the degree of compatibility, Equation 1.

The final degree of compatibility will be the sum of each of the features degrees of approaching along with respective weights, Equation 6. For site 1 the analysis found the following::

(Repository, site 1) = 0.4·0.05 + 0.3·0.1 + 0.5·0.1 + 0.3·0.3 + 0.8·0.05 + 0.1·0.2 + 0.5·0.2 = 0.02 + 0.03 + 0.05 + 0.09 + 0.24 + 0.02 + 0.1 = 0.55

This same calculation is repeated for all pairs (site, repository), and the following results were obtained, Table II.

Table II: Comparison of compatibility of the repository with each site.

Repository/site	Degree of compatibility or approaching
Site 1	0.55
Site 2	0.50
Site 3	0.3
Site 4	0.6
Site 5	0.2

This analysis indicates that the proposed repository will be more closely similar to sites 4 and 1 regarding the selected features. After a more detailed analysis, the values of 0.6 or 0.55 could also lead to the conclusion that, as it is close to 1, it would not have a strong impact on the site's environment, while a value of 1 would suggest no impact. It is important to recognize that the fuzzy set approach has taken the ambiguous data in Table II and permitted a ranking among the sites. This clearly could not be done by inspection of Table I.

Conclusions

A fuzzy logic based approach has been developed to examine site information which are usually given in ambiguous expressions, so they can be treated in a mathematical basis and yet keep its natural language characteristics.
The major advantages of the approach are :

- a- It translates language expressions into mathematical values, or fuzzy sets.
- b- The use of natural language makes it easier for the public and decision maker to be more familiar with the meaning of the results.

A simple example that examined the compatibility of five hypothetical repository sites with the proposed repository conditions was performed and it was found that the approach successfully met its objective to give support for a site selection decision that would best match natural conditions with those envisaged for the repository.

This calculation has another advantage of being easier to communicate to the public as it uses natural language expressions which are familiar to public and decision makers. In addition, the approach is flexible and readily permits incorporation of new information into the analysis as it becomes available.

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