Development of Next-generation Technology for Integrated Site Characterization of Deep Geological Repositories - 9132

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ABSTRACT

As site investigation proceeds and information obtained on geological environments increases, the characterization plan has to be iteratively reviewed and modified to reflect improved understanding. Such modification would also be needed when changes occur in technical or socio-political boundary conditions. JAEA teams involved in implementation of URL projects have used a geosynthesis data flow diagram to integrate a huge amount of practical experience in order to carry out such management functions. However, much of this experience was gained in the past, when it was possible for staff to learn by taking leading roles in novel, complex and important projects and learn by successes – and mistakes – under boundary conditions that were much more casual than they are at present. It is necessary to transfer such tacit knowledge to implementing and regulatory organizations in a practical manner before it is lost with the retirement of senior staff. An option being examined involves application of advanced technology, termed the Information Synthesis and Interpretation System (ISIS), to capture experience using Knowledge Engineering methods. This is being tested for practical applicability in an exercise involving stepwise “optimization” of a site characterization plan.

INTRODUCTION

Site characterization for geological disposal is a dynamic and complex process that needs close links with repository design and performance assessment (PA). As site investigation proceeds, huge volumes of information are obtained on the site, which have to be integrated to improve the site descriptive model. This, in turn, allows the characterization plan to be reviewed and modified on the basis of improved site understanding. Such modification would also be needed if changes occur in socio-political boundary conditions or, in long-term programs, in response to developments in technology.

A “geosynthesis” methodology has been developed to facilitate integration of site characterization information flow, incorporating feedback from design and PA users. Trial application of this approach is now ongoing within JAEA studies at two generic URL sites (Mizunami and Horonobe) [1]. The methodology of site characterization has evolved from simple geosynthesis data flow diagrams, which traced how measurements during site investigation generated data sets for end-users in a transparent and quality-assured manner. As opposed to recording what has been done in the past, application during an active site investigation is more challenging. In fact, initial data flow diagrams for two generic URL projects have been revised several times so far as a result of such analysis [2].
JAEA (previously PNC, then JNC) was the lead organization for generic R&D to demonstrate the feasibility of HLW disposal in Japan, producing seminal R&D technical reports referred to as H3 [3] and H12 [4-8]. On the basis of the technical background provided by the “H12” suite of technical reports, the Japanese geological disposal program for vitrified high-level radioactive waste (HLW) moved in 2000 from a platonic R&D stage towards implementation. At this time, the law regulating implementation (the “Specified Radioactive Waste Final Disposal Act”) was passed and the implementing entity, the Nuclear Waste Management Organization of Japan (NUMO), was established. In the implementing phase after 2000, JAEA has been assigned the responsibility for R&D to enhance reliability of disposal technology and safety assessment methodology together with associated databases; this should support both the implementer (NUMO) and the relevant regulatory organizations. With such a responsibility, JAEA has initiated development of an advanced knowledge management system (KMS) for the Japanese HLW disposal program [9,10].

A particular feature of JAEA’s activities in this phase involves R&D in two purpose-built URLs (underground research laboratories): one at Mizunami in crystalline rock and the other at Horonobe in sediments. These URLs are generic research facilities and thus distinct from the site-specific underground facilities that will be constructed by NUMO at volunteer sites, during the detailed investigation stage of site characterization.

JAEA teams involved in these URL projects have used a formal approach – termed the geosynthesis data flow diagram – in order to synthesize the huge amount of practical experience and data into a consistent site descriptive model. Here experience is critical, much of which was gained in times when it was possible for new staff to take leading roles in important and challenging multidisciplinary projects and learn by successes – and mistakes – under boundary conditions that were much more casual than they are at present. By its very nature, most of such experience is undocumented and, if no focused action is taken soon, will be permanently lost. A novel approach to transfer the experience and knowledge obtained in these URL projects is thus necessary to support the site characterization and subsequent safety assessment at potential repository sites by NUMO and the formulation of guidelines by regulatory organizations.

A key issue – and the focus of this paper – is development of advanced technology from the field of Knowledge Engineering, termed the Information Synthesis and Interpretation System (ISIS)\(^1\), which incorporates past experience and know-how currently being obtained in complex URL projects within Expert System (ES) modules. ISIS is a component of the comprehensive JAEA KMS [11], focused on supporting safety case development or review on the basis of data and understanding resulting from site characterization. This is intended both to support the site characterization and subsequent safety assessment at potential repository sites by NUMO and the formulation of guidelines by regulatory organizations.

**BASIC CONCEPT OF ISIS**

The approach embodied within ISIS emphasizes the flexibility required to allow stepwise, real-time optimization of the site characterization plan. ISIS has the key function of providing “knowledge” to support a site characterization project manager when assessing the significance of field observations (especially surprises) and making decisions on any needed modification of the characterization plan. This knowledge includes fundamental understanding of relevant geological environments, technical know-how on application of complex investigation techniques, experience gained in past site work, etc. Much of this is “tacit knowledge” [12, 13], undocumented experience accumulated over decades by experts in relevant disciplines and experienced multidisciplinary project coordinators.

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ISIS is being developed by applying advanced electronic information technology and knowledge engineering approaches and will include an extensive knowledge base and expert systems with inference engine and archive for rule-based/case-based reasoning as major constituent elements (Fig. 1). Analysis of results from past R&D activities in JAEA and elicitation of tacit knowledge, in particular from the experience at the two URLs, was initiated to provide the “knowledge” that will be input to such elements. An extensive survey of available technology has led to trial applications of the expert systems that could be eventually incorporated in an operational ISIS.

Fig. 1. Basic concept of ISIS

Analysis of knowledge relevant to site investigation

Site characterization is a very complex, multidisciplinary process that may extend over many years and needs development of an optimized program that balances the diverse – and often contradictory – requirements of the many specialists involved in this work. A vast depth of knowledge is necessary to structure and then optimize planning, implementing and analyzing the output from site investigations, which normally proceed in a stepwise fashion.

Knowledge needed in optimization processes can be divided into task knowledge and domain knowledge, using the terminology of knowledge engineering [14]. Task knowledge defines or explains the problem: procedures in component tasks can be represented using rule-based reasoning (e.g. IF…THEN format) or case-based reasoning (when…happened in the past, the result was…) [15]. Domain knowledge, which describes the fundamental supporting information and knowledge in an application domain, can be represent using knowledge mapping based on a knowledge network model that shows relationships between domain knowledge units.

This process appears fairly academic, so it is important to summarize it as an operational procedure (Fig.
2) and illustrate its application for specific knowledge management problems.

1) Illustrating the detailed task flow diagram resulting from expert elicitation; Figure 3 shows a detailed task flow diagram. The overall task flow for a complete program of interpretation of the results of borehole investigations can be subdivided into topical units – e.g. as shown here, the task flow for estimation of dominant redox reactions in order to support understanding of groundwater evolution processes.

2) Describing task contents; as illustrated in Figure 2, the topical unit task is put in context, received knowledge from preceding tasks and knowledge to be provided for subsequent tasks are identified, along with required resources and domain knowledge needed through expert elicitation.

3) Representing knowledge using methods from the field of knowledge engineering; Figure 4 shows an illustration of a part of rule flow and IF…THEN rules for estimation of relevant chemical species within the task of assessing the dominant redox buffer(s) in a hydrogeological system (illustrating Tasks 2 and 3 in Figure 3(b)). Here, task knowledge can be utilized as a form of inference engine.

Figure 5 shows a knowledge network model for structuring domain knowledge to establish correlations between hydrogeological properties and formation of faults/alteration zones in a pull-apart basin. In this way, domain knowledge can be searched and utilized as background information for the task.

ISIS is intended to be implemented as a user-friendly expert system, with contents and scope expanding in a step by step manner within a five-year program.
Geochemical modeling

Understand the distribution of groundwater chemistry and the evolution process of groundwater

- Estimate the distribution of groundwater chemistry
- Estimate the evolution process of groundwater

Estimation of dominant redox reaction

Task 1: Measure Eh
Task 2: Estimate possible chemical species by plotting data on Eh-pH
Task 3: Estimate possible redox reaction by plotting data on specific Eh-pH diagram
Task 4: Thermodynamic calculation of Eh and comparison of measured Eh/calculated Eh
Task 5: Thermodynamic calculation of saturation index
Task 6: Observe occurrence of redox related rocks/minerals
Task 7: Isotopic analysis of dissolved chemical species and minerals

(a) Task flow focused on making synthesized program of borehole investigations

(b) Task flow for estimation of a dominant redox reaction

Requirements from performance assessment and design

Quality evaluation and interpretation of data obtained in previous investigations

Integration of geological environment model

Selection of investigation methods

Synthesized program of borehole investigations

Rock mechanical modeling

Hydrogeological modeling

Geological modeling

Geomechanical modeling

Geochemical modeling
Fig. 3. Illustration of a detailed task flow diagram for estimation of dominant redox reaction(s)

<table>
<thead>
<tr>
<th>Rule</th>
<th>Measurement Data Can</th>
<th>Then</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rule A1</td>
<td>can be plotted near the redox equilibrium line of iron (within ±10 mV)</td>
<td>use phase diagram regarding iron (go to 2-1)</td>
</tr>
<tr>
<td>Rule A2</td>
<td>can be plotted near the redox equilibrium line of sulfur (within ±10 mV)</td>
<td>use phase diagram regarding sulfur (go to 2-2)</td>
</tr>
<tr>
<td>Rule An</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Rule Ax</td>
<td>can not be plotted near the redox equilibrium line</td>
<td>ease criteria on the comparison between redox equilibrium line and measured data, after reviewing quality of the data (go to 2-x)</td>
</tr>
<tr>
<td>Rule J1</td>
<td>using criteria can be adopted (±50 mV can be adopted because variation of data measured by some different electrodes are within ±50 mV)</td>
<td>select the phase diagrams of the chemical species within easing criteria (within ±50 mV) (go to 2-1 or 2-2) *: In the following analysis, error of ±50 mV should be considered.</td>
</tr>
<tr>
<td>Rule J2</td>
<td>can not be adopted</td>
<td>data should not be used in the following analysis because the data may be influenced by degassing etc.</td>
</tr>
</tbody>
</table>
Fig. 4. Illustration of task flow and IF...THEN rules for estimation of possible redox controls, shown as Tasks 2 and 3 in Figure 3(b)

DESIGN OF ISIS

Some key goals of the development of ISIS are:

- Providing past experience and know-how obtained in the URL and other R&D projects to support planning and implementation of future site characterization
- Aiding user-friendly communication of progress within site characterization among the teams involved and to interested stakeholders
- Providing flexible restructuring of tasks and information flow paths for the case of program changes (either due to surprises, changes in boundary conditions or as a result of reassessment at project milestones)
- Assisting in production of comprehensive and quality assured documentation of site characterization
- Establishing a process for overall program optimization via operational feedback and iterations with the design and safety assessment teams

In consideration of these goals, ISIS includes the following three functions (Fig. 6):

- Expert systems to acquire, preserve and continuously update relevant experience and know-how obtained in URL R&D and other relevant work
- User-friendly interface to aid communication and facilitate acceptance of this toolkit
- Knowledge base which includes an archive of all relevant past data, software and documents, accessible by a smart search engine.

The functionality needed to derive feedback through iteration with the design and safety assessment teams is identified as a priority and will be designed and developed by the JAEA KMS team in the near future.

Although the Japanese knowledge base will need to be complemented by input from international partner
programs with wider practical experience, all indications to date suggest that, although very much pushing the state of the art, development of such an intelligent system is feasible with existing technology.

A CASE STUDY OF EXTERNALIZATION USING AN EXPERT SYSTEM

As noted above, acquiring expert knowledge and incorporating it into ES modules is a key component of ISIS development plans (termed “externalization” in KE). This has thus been a focus for development work and testing via case studies. For example, in site characterization it is important to describe and integrate site models/data sets for use in performance assessment. Therefore, some tasks from the borehole drilling program, focused on geochemical system understanding, have been examined in order to confirm the approach and applicability of methods for developing expert systems (Fig. 7).

Figure 8 shows some output from an ES for specifying water-rock interactions controlling redox, based on the task flow and numbering of Figure 3(b). By using the ES, relevant chemical species and redox reaction formulae can be identified from the equilibrium diagram, derived by thermodynamic calculations in Tasks 2 and 3 (Fig. 8(a) and (b)). In addition, the theoretical values for the redox potential and saturation index of relevant minerals are calculated as Tasks 4 and 5 (Fig. 8(c)). Observed minerals from microscope and electron microscope images can be compared with minerals expected to be saturated as Task 6 (Fig. 8(e) and (f)). Finally, a dominant redox reaction can be identified and its relevance for system understanding assessed.

It is concluded that, in this particular application, the methodology works and can produce relevant output in a user-friendly manner (Fig. 8). Nevertheless, experience gained will feed back to allow improvement of both knowledge acquisition procedures and software tools to be used in the next stage of work.
- Objectives
- Precondition

Overview diagram of borehole drilling program
- ...
- Requirement of tracer for
- ...

Drilling water tracer
- Tracer
- Number of tracer

Watersampling
Chemical analysis of groundwater

Measured data

ES for drawing schematic overview of borehole drilling program
ES for selecting tracer for drilling fluid
ES for quality evaluation of data on groundwater chemistry
ES for estimation of a dominant redox reaction to support understanding of groundwater evolution process

Fig. 7. Case study of externalization using an expert system

(a) Output from Task 2 shown in Figure 3(b) (b) Output from Task 3 shown in Figure 3(b)
The theoretical value of oxidation-reduction potential (ORP) is calculated to be...

The observed value is...

ORP difference between theoretical and observed values has ±25 [mV] error margin.

Selected redox reaction can be considered appropriate.

If the difference is more than ±25 [mV], select another redox reaction.

Refer to the photograph database on rock and mineral at the investigation depth and compare the photographs with a general photographic image. Then, please check for the presence of the above minerals.

Confirm the selected redox reaction?

Fig. 8. Some output from an expert system for assessment of dominant redox reaction(s)

FURTHER STEPS TOWARDS DEVELOPMENT OF AN OPERATIONAL SYSTEM

The activities of focusing site characterization involve the planning of knowledge management during the characterization of potential repository sites – a particularly challenging task due to both the great complexity of the data that need to be assessed and integrated in a synthesis process and the need to make rapid decisions that feed back to refining the site plan on the basis of experience gained, in consideration of the trade-offs with socio-political and economic boundary conditions.

A key challenge is to incorporate functionality, so that this can be used as the basis of a tool to assist in the process of data logging, review / QA, integration and trend analysis. Although, at present, this work is
Currently carried out by teams that have accumulated experience in this area, an intention is to examine the extent to which aspects can be automated, e.g. using expert systems. Although involving considerable effort, this will be justified for the case where several sites may need to be investigated in parallel, when experienced manpower resources may be the main limiting factor. These activities of site characterization are also necessary to establish a process to derive feedback through iterations with the design and safety assessment teams. Initial work has indicated that a “blackboard architecture system” could be applicable here (Fig. 9), with a control shell that identifies when particular decisions have to be made and solicits input from appropriate experts (either real or virtual). This will be taken further by focusing on specific technical areas and utilizing a formal “problem-solving method” in which control knowledge (the inference process that experts use in a particular situation) is incorporated into the expert system shell [15].

Such tasks are currently included in a CommonKADS [14] module, which includes:
- Elicitation of control knowledge from relevant experts
- Analysis and structuring of such knowledge
- Reworking it into a form that can be utilized in a computer toolkit.

For an illustration of use, the specific example of the flow of information during the drilling of a deep borehole is being considered. This is a particular example of an exploration technique where surprises often occur and the process of online synthesis of data can be usefully combined with trend analysis to identify various types of deviation from expectations, which then triggers a set of automatic notification steps, possibly including soliciting of expert interpretations. The results of this polling of input are presented to the decision-makers, along with expert recommendations and the consequences of any response logged (Fig. 9).

There is no doubt that the envisaged system is at (or even beyond) the limits of what is feasible with existing technology. Nevertheless, this is an extremely dynamic and fast-moving field and there seems to be good chances that all defined goals can be met. The work will be very challenging but, as the fundamental requirement for a new, 21st century approach to the management of site characterization becomes more widely accepted, the opportunities to share the load in collaborative projects will expand. Certainly, JAEA will work closely with other relevant organizations in Japan that are producers and/or users of knowledge, but extended cooperation with international partners is also a high priority goal for the near future.
CONCLUSIONS AND A LOOK TO THE FUTURE

The development of this ambitious ISIS is certainly a long-term process; it will evolve gradually and expand in capabilities with increasing experience gained through particular applications. In a five-year program, the basic ISIS, including experience and know-how from surface-based investigations at two URLs (Mizunami, Horonobe) and other projects on coastal site characterization at Horonobe, will be established as a key component of the strategy for R&D to support HLW implementation. It is hoped that, even while it is in a development stage, stepwise implementation of this ISIS to expanded case studies of critical site characterization processes will not only ensure practicality of methods and software/toolkits incorporated into this ISIS, but also directly provide benefits to the implementing entity and the regulators. The goals of ISIS are acknowledged to be very ambitious, but seem to lie within the range of existing technology - or reasonable extrapolations thereof. While not replacing experienced staff, it could greatly help them manage site characterization, an otherwise increasingly intractable problem as technology...
becomes more sophisticated, data production rates increase exponentially and resources of experienced manpower shrink.

REFERENCES