[Form 2 (to be reported to Committee on Countermeasures for Contaminated Water Treatment and to be disclosed to public)

Technology Information	
Area	4, 5 (Select the number from "Areas of Technologies Requested")
Title	CABARET reactive transport software for modelling barrier behaviour for planning barrier implementation and mitigation measures
Submitted by	Quintessa Ltd

1. Overview of Technologies (features, specification, functions, owners, etc.)

TEPCO is considering a number of different methods for managing inflows of groundwater to the Fukushima site itself and, more specifically, to buildings on the site. Considered measures include ground freezing to develop a hydraulic barrier up gradient of the o.p. 10m area, filling water stops from inside the buildings, and implementing soil improvement by putting water glass, silica gel, etc., in gaps between neighbouring buildings. The long-term behaviour of the materials used in these alternative barriers, and their implications for water and contaminant migration, needs to be evaluated when:

  ▲ planning the implementation of optimized barriers;

  ▲ when designing mitigation plans should installed barriers prove ineffective; and

  ▲ planning final site restoration.

These design and planning activities need to take into account many "coupled" processes, including the:

  ▲ different physical and chemical processes by which different materials may degrade, such that they become more permeable over time (e.g. concrete if cracking occurs due to ingress of sulphate-bearing water);

  ▲ different capabilities of barrier materials to retard radionuclides, and hence the degree to which radionuclides become concentrated in different barrier materials;

  ▲ effect of barriers on the chemistry of the surrounding groundwater and the possible consequences for contaminant transport and behaviour of adjacent solid materials (e.g. the localized increase in salinity that may occur in the vicinity of a frozen barrier).

CABARET is a software package developed by for modelling these type of coupled geochemical processes and groundwater flow, in multiple dimensions. CABARET therefore has many features that would be highly beneficial in supporting the design and implementation of engineered barriers to control groundwater and contaminant migration at Fukushima.

CABARET can be used as it stands, or adapted to simulate specific conditions. Presently the software can simulate systems represented by 1D or 2D grid geometries, but can be adapted readily to undertake simulations in 3D. The software has a user-friendly graphical user interface (GUI) that enables users to specify models and to control the outputs from them (Figure1). The software can use a variety of thermodynamic databases, which can be adapted to meet the specific requirements of a problem (ranges of salinity, chemical components in solution, solid phases etc).

Figure 1: CABARET GUI showing part of the input for a simulated reaction between cement, bentonite and porewater and a plot of simulated mineral assmblages across the cement across the cement-bentonite boundary (at the left margin of the plot), produced using graphing software bundled with CABARET.

CABARET is innovative in combining the following features:

▲ capability to model reactive transport processes by *fully coupling* the relevant equations providing better founded, and more detailed, results;

▲ capability of users to specify relationships between parameters (e.g. diffusion coefficients as a function of porosity and temperature);

▲ capability for users to specify kinetic reaction rate laws, which include temperature, mineral saturation, pH, carbonate concentrations and any other relevant derived quantities

▲ capability to simulate solid solutions;

▲ capability to simulate sorption;

▲ an advanced GUI, which means that models can be set up quickly;

▲ a suite of tools for plotting and presenting outputs.

As well as leading edge modelling capabilities, CABARET is easy to set up and use. A combination of the software's efficient solver, the GUI and the tools for presenting outputs means that the overall process of setting up simulations, running them and interpreting the outputs is much more rapid than with other software. Consequently it is beneficial to use CABARET to explore alternative barrier options and sensitivities to uncertainties (e.g. uncertainties in thermodynamic data).

2. Notes (Please provide following information if possible.)

- Technology readiness level (including cases of application, not limited to nuclear industry, time line for application)

CABARET is available for use immediately. The software has so far been used to simulate cement-bentonite interactions in barrier systems for deep geological repositories for radioactive wastes. CABARET is based upon the general-purpose QPAC software. QPAC has been very widely applied to simulate many different processes including: chemical and physical evolution of engineered barriers in radioactive waste repositories (both in the near-surface and deep sub-surface), gas evolution in radioactive waste repositories, gas migration though the cores of AGR nuclear reactors, behaviour of CO_2 in underground reservoirs, and leaching of contaminants from materials used to stabilize underground cavities. The projects in which QPAC has been employed have been undertaken for many clients in the UK and internationally, including JAEA, Andra, Nagra, NDA RWMD, EDF Energy and LLWR Ltd.

- Challenges

Run times of coupled reactive transport models may become very long as the number of chemical components and / or phases simulated increases and/or as the spatial discretization of the modelled system becomes more complex. This challenge may be addressed by a combination of:

▲ 'offline simulations / calculations' in order to identify only those aspects of the system that are relevant to the problem of concern (e.g. to carry out independent chemical speciation calculations using a software package such as PHREEQ to identify which chemical species are important and hence need to be included in the CABARET simulations);

▲ adopting a modelling strategy in which simplified models of parts of the system of interest are developed initially to gain understanding of the processes of interest, such that optimized simulations of the full system can then be developed.

- Others (referential information on patent if any)

CABARET is Quintessa Limited's Intellectual Property (IP). Licenses for bespoke versions of the software could be supplied, subject to negotiation. CABARET allows specific models to be developed with bespoke GUI's that allow users to vary key parameters, and then exported as standalone 'player' models that can be freely distributed.

【Areas of Technologies Requested】
  (1) Accumulation of contaminated water (Storage Tanks, etc.)
  (2) Treatment of contaminated water (Tritium, etc.)
  (3) Removal of radioactive materials from the seawater in the harbor
  (4) Management of contaminated water inside the buildings
  (5) Management measures to block groundwater from flowing into the site
  (6) Understanding the groundwater flow