Development of Process Coupling System for the Numerical Experiment of High Level Radioactive Waste

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Abstract: Numerical experiment is the only available approach to demonstrate long-term complex evolution of a high-level radioactive repository. Designer and performance assessor of a repository have to consider coupled processes due to thermal, hydrology, mechanical, mass transport and geochemistry in the deep underground. However it is very difficult to construct coupling program, because it has to analyze individual program of each process. A coupling system was developed and was used to demonstrate temporal and spatial variations in the chemistry for one-dimensional column by using existing reactive and transport code. Verification was carried out in order to confirm the applicability of coupling process by using the system COUPLYS(coupling of PHREEQE and transport model) and HYDROGEOCHEM. The results show that, the use of a prototype coupling system like COUPLYS is very effective to improve the efficiency and quality for development of coupling codes.

Key-Words: coupling system, HLW, geochemical, mass transport, COUPLYS, numerical experiment

1. Introduction

The Japanese disposal concept for high-level radioactive waste (HLW) repository considers the use of metal over-pack, compacted bentonite and natural rock for barrier function [1]. In order to design and evaluate performance for engineered barrier system which include over-pack and compacted bentonite, it is necessary to understand near-field processes such as groundwater flow, reaction of rock with groundwater, stress, radionuclide migration and retardation and thermal conductivity. It is very difficult to carry out experimental test such a system for a long-term period. Therefore, actual design work adopted the approach that an independent processes analysis code was used under consideration of conservatism. In the Yucca Mountain project, which is the HLW disposal project of USA, the coupling analysis includes Thermal-Hydrology-Chemistry (THC) [2], [3]. The mechanical analysis in Yucca Mountain project is omitted from the coupling system because there is no buffer material in the Engineered Barrier System (EBS), and no need for the stresses analysis on bentonite swelling or any other processes concerning the EBS. A coupling analysis of Thermal-Hydrology-Mechanical (THM) was carried out to evaluate maximum temperature in the bentonite due to the heat output of vitrified waste and resaturation time (time to reach saturation in the compacted bentonite after emplacement of the EBS) due to the groundwater infiltration [1]. Since the detailed requirements of design for underground repository includes the long-term behavior analysis of processes such as dissolution and precipitation of minerals and their effect on the porosity, it is important to add the reactive transport coupling. The new approach we are developing to evaluate the repository design is Thermal-Hydrology-Mechanical-Chemistry (THMC). This paper presents a useful and integrated tool for the analysis of the coupling processes affecting the HLW repository design. The coupling code are verified and compared to well-known codes used for analyzing such processes. Section 2, presents the strategy used to construct the coupling system, section 3 presents design concept. Section 4 presents the verification of the coupling system. Finally section 5 gives the concluded remarks of this study.

2. Strategy for development of prototype coupling system

A coupling system is mainly designed to support and verify the different codes used in the HLW repository design. In order to develop a strategy for the coupling system, it is important to understand the different processes occurring and to choose the relevant parameters that affect such processes, and their relationship with each other. In the near field of the repository, especially EBS, the processes such as groundwater flow, reaction of the rock with groundwater, heat generation, stresses due to heat deformation, stresses due to the water saturation, radionuclide migration and geochemical reaction in bentonite should be coupled. Figure 1, shows the expected processes in the near field of the HLW repository. In the early work, the coupling system, which was THM, was compared to a heat conductivity code and it proved that, this heat conductivity code is conservative [1].

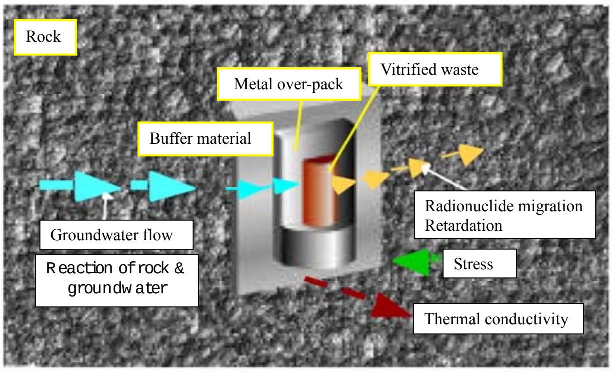

Fig.1 Expected processes for the HLW disposal system [1].

It is necessary to acquire some information of coupling issues for each process to develop coupling analysis code. For example, the purpose of this requirement for coupling issues is to introduce change in porosity due to dissolution and precipitation of minerals in the coupling code [4].

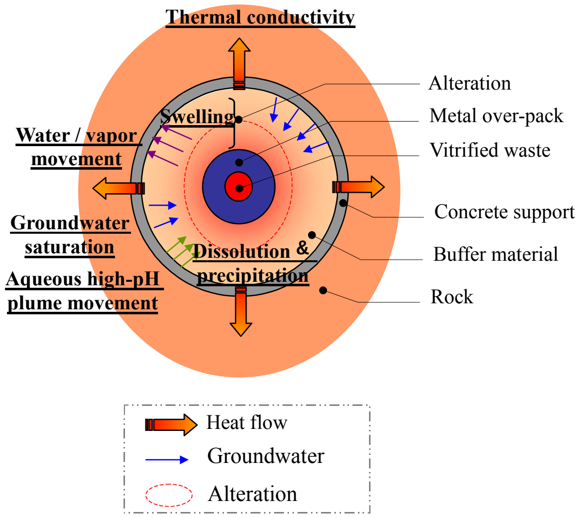

Fig.2 THMC processes in the Near-Field for the HLW disposal system.

It is very difficult to construct coupling code by using individual process codes in a short time, because we have to modify each code in detail. This research developed prototype platform (COUPLYS) to built coupling analysis shown in

Fig.2 in a short time. This paper presents the prototype system of a coupling analysis platform. And a reactive transport coupling analysis was performed for verification to confirm the applicability of the system.

3. Design concept of prototype coupling system

The selection of the technique was done by using the existent analysis codes from the efficiency of work to develop the coupling analysis code and the viewpoint of the correctness by this research. The technique, which was not depending on the programming language of the existing analysis codes, was adopted to secure the efficiency and the correctness of the work. A Fig.3 shows the design concept of the platform of coupling analysis system.

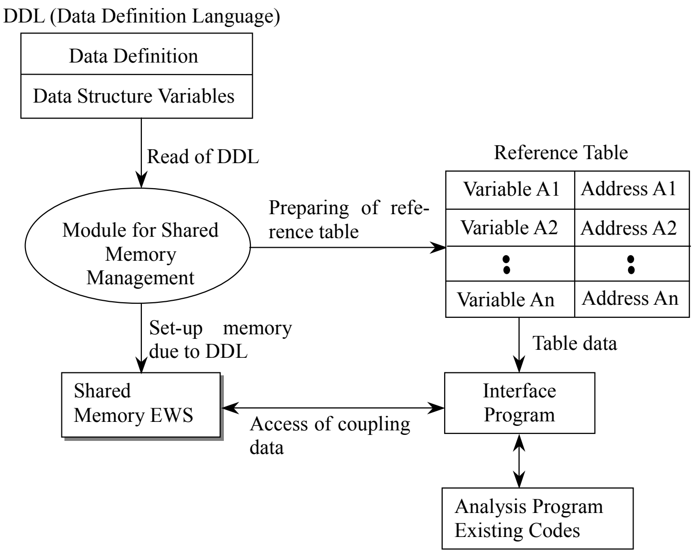

Fig.3. Design concept of prototype process coupling system

Coupling data are able to acquire by this concept at high speed. Block of data definition is that end-user will define structure of shared memory based on the variable information for coupling. This data definition includes variable name, variable type and dimension size for each variable by text format. This technique is using Data Definition Language (DDL) as a language to describe the data for coupling data relation with each individual code. Module of shared memory management will prepare reference table to access data for coupling between each existing code. Also this module will ensure memory area based on the information of DDL. Reference table will control the relation between variable name and address in the shared memory. Interface program has a function of reading of information in the reference table by using command of “get” or “set” in the existing program. And then interface program will exchange coupling data between existing codes through shared memory.

4. Development of prototype coupling system

An existing reactive transport analysis code was used based on the basically concept of the Fig.3.

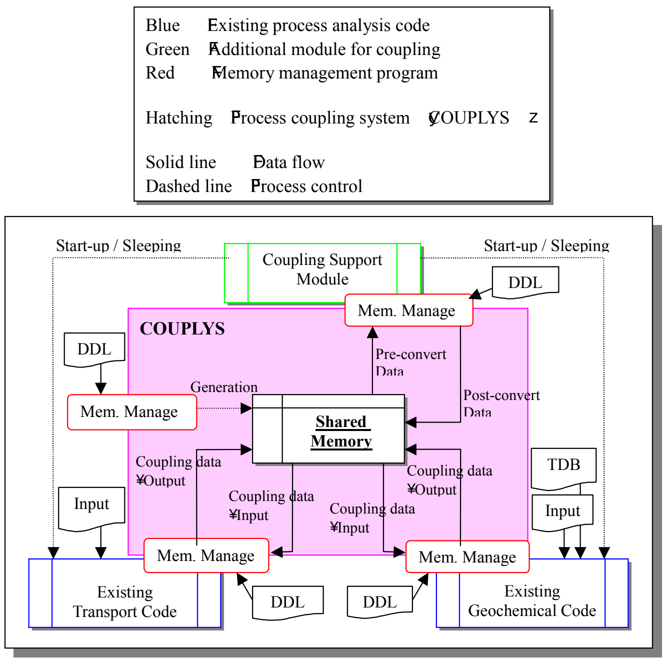

Fig.4. Prototype of coupling system for reactive transport model using existing analysis codes

The part of transport in the coupling used the mass transport module of HYDROGEOCHEM [6], and the part of geochemistry adopted a code PHREEQE [5]. The structure of coupling analysis code is shown in the Fig.4.

A coupling support module shown in Fig.4 has a function about the start-up and sleeping of the existing analysis code. And, it has the function of the input data which are necessary for and dependent on what coupling code we develop. For example, one of option is a set up of the precipitation candidate mineral. It has also the control function of a result of output. The coupling information, which should be necessary for geochemical analysis code PHREEQE, is total concentration (aqueous species concentration plus precipitation concentration), pH and Eh. The coupling information, which should be necessary for mass transport analysis code HYDROGEOCHEM, is equilibrium aqueous species concentration and equilibrium precipitation concentration. Therefore the above command (“set” and “get”) was inserted in the existing source program by FORTRAN language in this research. This prototype system is implemented on a SUN ULTRA, DEC-• and SGI workstation.

5. Verification of prototype coupling system

Comparison with existing reactive transport analysis code was done in order to confirm the applicability of the prototype process coupling system. A verification analysis case is that calcite is filled within one-dimensional column dissolved from one side. Mass transport due to the diffusion was dealt with one-dimensional column. Geometry of one-dimensional column is shown in the Fig.5. And, medium material in the column, an initial condition and a boundary condition for elements of Ca and C are shown in the Table.1. This test case is that calcite dissolves in the end part of column gradually, and it is exhausted, because boundary is a pure solution in the end (nodal point 21) of the column. And, since calcite is exhausted at the end part, total aqueous concentration of Ca and C become smaller than dissolution equilibrium of calcite, and it becomes smaller than pH of the equilibrium dissolution of calcite. This interpretation is shown in Fig.6, 7 and 8.

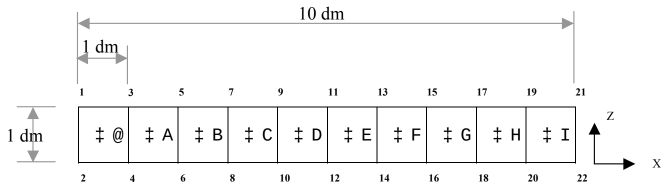

Fig.5. Calculation model for reactive transport: one-dimensional column system

Table.1. Parameter for transport and geochemistry analysis

Parameter	Unit	Value
Effective Diffusion Coefficient	m^2/sec	3×10^{-10}
Porosity in the column	–	0.33
Boundary total concentration Nodal point 1, 2, [Ca, C]	mol/l	1×10^{-2}
Boundary total concentration Nodal point 21, 22, [Ca, C]	mol/l	1×10^{-10}
Initial total concentration Nodal point 3•20, [Ca, C]	mol/l	1×10^{-3}

Figure 6 shows the results of the pH of the column, in which the results of comparison with existing coupling code and the prototype system are taken into account. The pH distribution at early stage and sixty years are shown in this figure. We have confirmed agreement between the result of existing coupling code (HYDRO-GEOCHEM) and prototype coupling system (transport of HYDROGEOCHEM and PHREEQE).

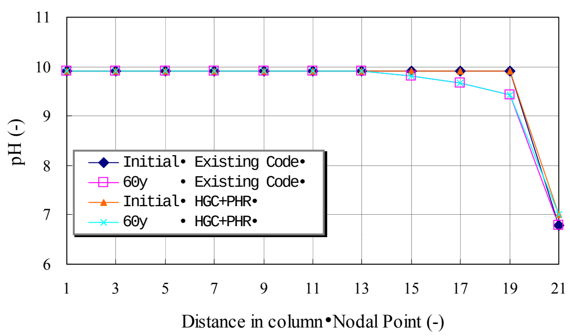

Fig.6. Verification result: distribution of pH in the column

Figure 7 shows the results of the precipitation concentration of calcite (solid phase of $CaCO_3$) distribution in the column, in which the results of comparison with existing coupling code and the prototype system are taken into account. The calcite distributions at early stage and sixty years are shown in this figure. We have confirmed agree between the results of both codes.

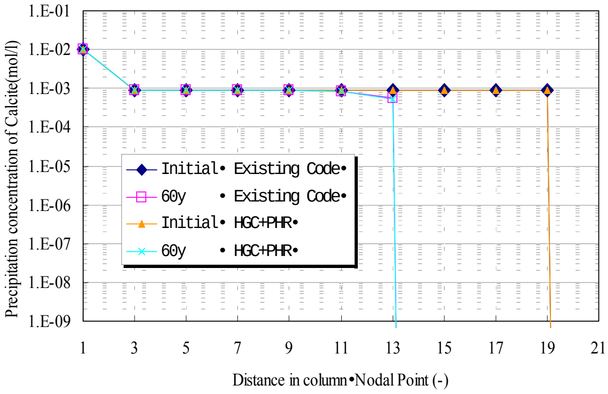

Fig.7. Verification result: distribution of calcite concentration in the column

Figure 8 shows the results of the aqueous species total concentrations of Ca and C distributions in the column, in which the results of comparison with existing coupling code and the prototype system are taken into account. The total aqueous Ca and C distributions at early stage and sixty years are shown in this figure. We have confirmed agreement between the results of both codes.

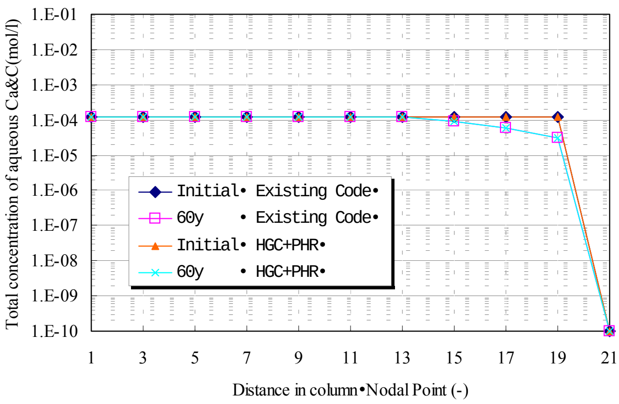

Fig.8. Verification result: distribution of aqueous concentration in the column

6. Conclusion

The applicability of the prototype coupling system by DDL to develop the coupling frame using existing codes was shown by using demonstration of the design concept and results of verification for test case of the reactive transport. The use of the prototype coupling system like COUPLYS is very effective to improve the efficiency and quality of development for coupling code. Two processes, mass transport and geochemistry, were coupled by using the prototype system and verified by comparison with the existing code. However, we have to consider to extend several processes from the viewpoint of the increase in reality. Future issues are as follows;

(1) Development of process management system to control some existing code (coupling of thermal-hydrological-mechanical-transport-chemistry)
(2) Parallel distributed processing for high-speed calculation.
(3) Development of coupling instruction system from the viewpoint of the use for the advanced knowledge and the working efficiency.

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