Development of Modeling Interface for a Process-Based Total System Performance Assessment of a Geological Disposal System

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1. Introduction

Until recently, only a system-level safety assessment model was generally used for the safety assessment of a geological disposal system in Korea. For instance, KAERI developed K-PAM (KAERI Performance Assessment Model), a system-level safety assessment model [1], and used it for the safety assessment in its safety case [2].

The system-level safety assessment is a kind of conservative approach and has the advantage of short computation time. However, it has limitations to reflect short- and long-term evolution of the disposal system and to realistically simulate thermal, hydraulic, mechanical, and chemical complex phenomena. Because many important processes are highly abstracted in the system-level models, the advanced knowledge from state-of-the-art researches is seldom applied into the safety assessment. In addition, it is impossible or very difficult to verify the total system models owing to the absence of the system-scale experimental data.

To cope with the limitations of the total system models shown above, the US has been trying to use high-performance computational codes to move the total system model closer to the process model level [3], and the EU has developed and been using a multiphysics simulation framework by coupling COMSOL Multiphysics and PHREEQC [4]. Although the process-based total system performance assessment requires a lot of computational resources and computation time, the computational efficiency can be improved through parallel computation that takes advantage of recent high-performance computers.

To keep up with the trends, KAERI has also recently proposed developing a process-based total system performance assessment model for a geological disposal system (APro). As the first step of development of the model, the modeling interface was designed in this study.

2. APro

APro stands for "**A**dvanced **Pro**cess-based total system performance assessment framework for a geological disposal system". APro employs a bottom-up approach unlike a system-level model which uses top-down approach. APro was basically designed to be able to simulate all the processes that can be occurred in a geological disposal system including thermal, hydraulic, mechanical, chemical, and radiological processes. The flowchart of APro is depicted in Fig. 1.

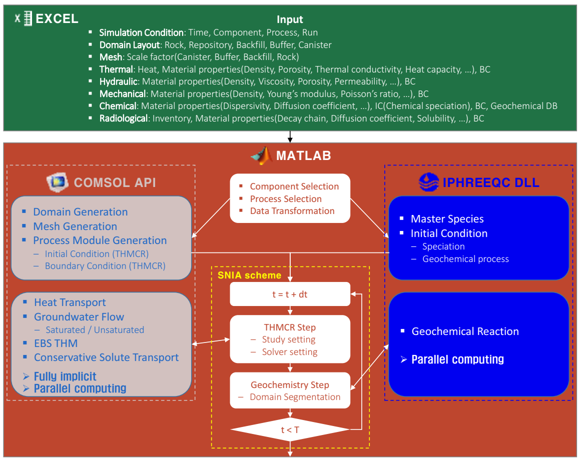

Fig. 1. Flowchart of APro.

2.1 Input

All input data are defined in an EXCEL file. The input EXCEL file consists of "Simulation Condition", "Domain Layout", "Mesh", "Thermal", "Hydraulic", "Mechanical", "Chemical", "Radiological" sheets.

2.1.1 Simulation Condition. From "Simulation Condition" sheet, time-related parameters, components and processes to be considered in the simulation, and output options are defined.

2.1.2 Domain Layout. The target repository considered in APro is typical KBS3-type including both vertical- and horizontal types. From "Domain Layout" sheet, the numbers of repositories, tunnels, boreholes and canisters, and dimensions of them can be defined.

2.1.3 Mesh. From "Mesh" sheet, the scale factors for each components are defined to control mesh size.

2.1.4 Thermal. From "Thermal" sheet, the input data related to the thermal process, such as heat source, density, porosity, thermal conductivity, heat capacity, etc., are defined. Each parameter can be defined as not only a constant but also a function of time or temperature.

2.1.5 Hydraulic. From "Hydraulic" sheet, the input data related to the hydraulic process, such as water density, viscosity, porosity, permeability, etc., are defined. Each parameter can be defined as not only a constant but also a function of temperature.

2.1.6 Mechanical. From "Mechanical" sheet, the input data related to the mechanical process, such as density, Young's modulus, Poisson's ratio, etc., are defined with respect to the linear elastic model.

2.1.7 Chemical. From "Chemical" sheet, the input data related to the geochemical process, such as dispersivity, diffusion coefficient, initial condition, boundary condition, thermodynamic DB, etc., are defined. The initial and boundary conditions and thermodynamic DB are defined as separated PHREEQC files which should be in a subfolder.

2.1.8 Radiological. From "Radiological" sheet, the input data related to the radiological process, such as inventories for each repository, radioactive decay properties, diffusion coefficients and solubilities of radionuclides, etc. are defined.

2.2 Computation Procedure

The overall computation is mainly managed in MATLAB workspace by controlling COMSOL API and IPHREEQC DLL.

Firstly, input data are loaded and rearranged in MATLAB workspace. Secondly, model domain and mesh are constructed using COMSOL based on the selected components. Thirdly, COMSOL physics are defined based on the selected processes. In case of the "Chemical" process, the chemical speciation of the initial and boundary conditions is calculated by IPHREEQC DLL and transferred to the COMSOL physics. Finally, the computations are iterated with COMSOL API and IPHREEQC DLL for each time step.

In each time step, heat source, radionuclide inventory, etc. are updated, and THMC process including heat transport, groundwater flow, EBS THM, non-reactive transport, etc., are computed by COMSOL. And then, radioactive decay is computed in MATLAB workspace, and the geochemical reactions for each mesh nodes are computed in parallel by using PHREEQC DLL.

3. Conclusion

As the first step of development of a process-based total system performance assessment model, APro, the modeling interface was designed in this study. After configuring the interface, each specific processes as module-type will be embedded into the overall framework step by step, and the coupled effects will additionally be evaluated. In the future, APro is expected to contribute to improving the reliability of the safety assessment in combination with the system-level safety assessment model (e.g., K-PAM).

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