A Review of Process-based Total System Performance Assessment Model for A Geological Disposal System

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1. Introduction

A geological disposal system of radioactive wastes generally consists of multiscale components, such as engineered barrier system (EBS), natural barrier system (NBS), etc., and multiphysical processes are involved in the system. Thus, the general performance assessment process can be represented as a pyramid in Fig. 1 [1]. Based on the massive information and knowledge, detailed process models are developed and tested. The detailed process models are abstracted and then finally the total system models can simulate the integrated behaviors of the entire disposal system [1].

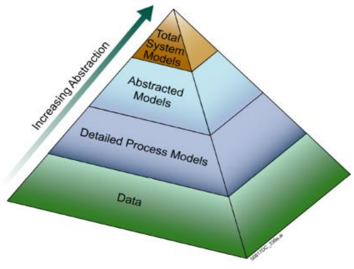

Fig. 1. Performance assessment pyramid [1].

In the most disposal projects, the post-closure safety assessments have been conducted by using the total system models until recently. KAERI's post-closure safety assessment tool was also the total system model developed with GoldSim until now.

Since many important processes are highly abstracted in the total system 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 due to the absence of the system-scale experimental data.

To cope with the total system models' limitations above, US has been trying to use high-performance computational codes to move the total system model closer to the process model level [2] and EU has developed and been using a multiphysics simulation framework by coupling COMSOL Multiphysics and PHREEQC [3]. To keep up with the trends, recently, KAERI has also proposed developing a process-based total system performance assessment (TSPA) model for a geological disposal system.

In this study, therefore, some precedent studies abroad were reviewed and the general considerations in the process-based TSPA model development were stated.

2. General Considerations in Multiphysics

2.1 Multiphysics system [4]

Multiphysics system can be classified by whether the multi-components in the system are coupled in the bulk (bulk-coupled multiphysics system) or on the lower dimensional interface (interface-coupled multiphysics system). The reactive transport in subsurface flows and the fluid-structure dynamics would be a typical example of bulk- and interface-coupled multiphysics systems, respectively.

Multiphysics application can be considered from algorithmic and architectural perspectives. Both mathematical analysis and computational complexity would be dealt with algorithmic perspective, and both software and hardware environments with architectural perspective.

2.2 Multi- concepts in multiphysics system [4]

2.2.1 Multi-scale. Lifting is the coarse-to-fine transformation which may means populating an ensemble of particles according to a distribution, and restriction is the fine-to-coarse transformation which may means averaging.

2.2.2 Multi-rate or multi-resolution. A chemical kinetics in the reactive transport model where the relaxation time should be modulated is the typical example of multi-rate.

2.2.3 Multi-level. The modeling system may be distinguished by only different mathematical formulations or even different discretizations.

2.2.4 Multi-model. Even single component may be analyzed using systems of partial differential equations of different types.

2.3 Operator splitting (OS)

Operator splitting (OS), where numerical computations are separated for each components and/or processes, is generally considered in multiphysics problem due to its expeditiousness. The general algorithm of OS is as follows [4]:

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Given initial values $\{u_1(t_0), u_2(t_0)\}$
for $n = 1, 2, \ldots, N$ do
  Evolve one timestep in $\partial_t u_1 + f_1(u_1, u_2(t_{n-1})) = 0$ to obtain $u_1(t_n)$
  Evolve one timestep in $\partial_t u_2 + f_2(u_1(t_n), u_2) = 0$ to obtain $u_2(t_n)$
end for
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Among various OS techniques [5], the appropriate OS scheme for the multiphysics should be decided keeping in mind the error propagation.

3. Process-based TSPA Models

3.1 PFLOTRAN

PFLOTRAN is “A recently developed code for modeling multi-phase, multi-component subsurface flow and reactive transport using massively parallel computers” from US’s national laboratories [2]. It is written in Fortran, and the reactive transport equations can be solved using either a fully implicit Newton-Raphson algorithm or OS method [2]. Followings are current capabilities of PFLOTRAN [6]:

- Richard’s Equation
- Thermo-Hydro-Chemical
- Multiphase Water-Supercritical CO2
- Surface Flow
- Discrete Fracture Network
- Aqueous Complexation
- Sorption
- Mineral Precipitation and Dissolution
- Multiple Continuum for Heat
- Subsurface Flow-Reactive Transport Coupling
- Multiphase Ice-Water-Vapor Flow

And, followings are under development in PFLOTRAN [6]:

- Community Land Model Coupling
- Surface-Subsurface Flow Coupling
- Geomechanics
- Multiple Continuum for Reactive Transport

3.2 iCP [3]

iCP is a numerical interface “Which couples two standalone simulation programs: the general purpose Finite Element framework COMSOL Multiphysics and the geochemical simulator PHREEQC” by Amphos 21, Spain. Fig. 2 is the iCP’s computing algorithm.

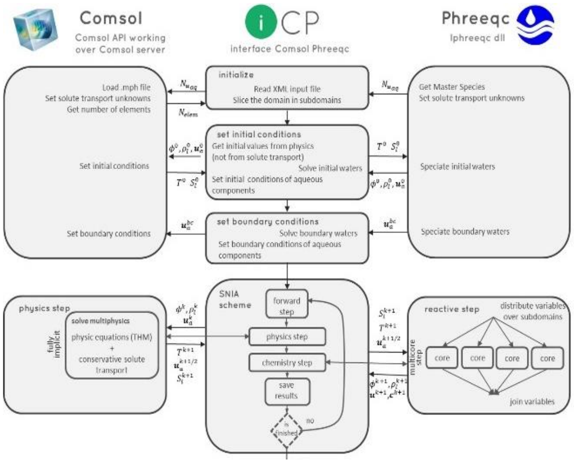

Fig. 2. iCP’s computing algorithm [3].

4. Conclusion

The current trend of process-based TSPA model will contribute to the diversity and robustness of the post-closure safety assessment tools as well as will decrease uncertainty.

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