



## Design for integrated pyroprocessing plant level simulator



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### ABSTRACT

Pyroprocessing has been studied for a decade as one of the promising fuel recycling options in Korea. Most studies have focused on test-based research, which is often limited, expensive, and time-consuming. Thus, modeling and simulation studies began to complement or overcome test-based research. The Korea Atomic Energy Research Institute (KAERI) suggested a modeling architecture for pyroprocessing consisting of three-tiered models: unit process, operation, and plant-level models. The unit process model can be addressed using governing equations or empirical equations as a continuous system (CS). In contrast, the operation model describes the operational behaviors as a discrete event system (DES). The plant-level model is an integrated model of the unit process and an operation model with various analysis modules. An interface with different systems, incorporation of a different code, the database design, and the implementation of a dynamic material flow are discussed as components for the framework of the plant-level model. This paper addresses the current status of the pyroprocessing modeling and simulation at KAERI, and discusses its path forward.

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### 1. Introduction

Next-generation nuclear fuel cycles require innovative features such as an environmental load reduction, safety, efficient recycling of resources, nuclear proliferation resistance, and economics. From these viewpoints, the pyrometallurgical processing of spent nuclear fuel (SF) is now considered as one of the most promising options for future nuclear cycles in Korea (Kim, 2006). The Korea Atomic Energy Research Institute (KAERI) has been developing pyroprocessing technologies, which can reduce the increasing amount of spent nuclear fuel and dramatically decrease the disposal load, through recycling and destroying toxic waste such as long-life fission products in spent nuclear fuel (You et al., 2007).

Pyroprocessing technology has not been fully demonstrated in terms of commercialization and technology maturity. To navigate the right direction of pyroprocessing technology development, a demonstration in an integrated facility is certainly a tangible

solution, but it is too costly and time consuming to construct a fully integrated facility including all unit processing and remote handling equipment. Therefore, a technology assessment and breakthrough by modeling and simulation would be preferable. Plant modeling and simulations are now widespread among the manufacturing, semi-conductor, steel, and refinery industries. However, they focus on layouts, assembly, automation, remote control of the process flow, and so on.

Currently, there are neither commercialized nor integrated pyroprocessing facilities around the world. KAERI is constructing an integrated demonstration facility, and thus expects to contribute to boosting the pyroprocessing technology and step toward a realization of spent nuclear fuel recycling. Nevertheless, pyroprocessing technology has been confronted by many problems that are currently awaiting solutions.

The expected potential benefits of modeling and simulation in the field of nuclear recycling systems include the following: to reduce the process and facility development, optimize the system designs, and reduce the risk of material diversion. Actually, modeling and simulation enhance an understanding of known systems, provide qualitative and quantitative insights and guidance for experimental work, and produce quantitative results that replace difficult, dangerous, or expensive experiments (DePaoli, 2011).

Pyroprocessing contains various unit processes and various types of nuclear materials that flow in and out of these unit processes. It is a batch type process in overall terms, i.e., the receipt and shipment of materials among the unit process; however, the unit process itself features a continuous chemical or electro-chemical process.

*Abbreviations:* ASCI, Advanced Strategic Computing Initiative; CS, continuous system; DES, discrete event system; DLL, dynamic link library; EcWinSim, FORTRAN code name of electrowinning model; IPSCs, Integrated Performance and Safety Codes; KAERI, Korea Atomic Energy Research Institute; NEAMS, Nuclear Energy Advanced Modeling and Simulation; LCC, liquid cadmium cathode; Pu, plutonium; PUREX, plutonium–uranium extraction; PyroFlow, ExtendSim model for an integrated pyroprocessing material flow; RAR, residual actinide recovery; RE, rare earth; RPTK, Reprocessing Plant ToolKit; SciDAC, Scientific Discovery through Advanced Computing; SF, Spent nuclear Fuel; TRU, TRansUranic; U, uranium; PRIDE, Pyroprocessing Integrated inactive DEMonstration Facility.

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The unit process may have a different batch capacity and different processing time. In addition, there are recycling routes of the output material on a unit process into a prior unit process. In addition, nuclear elements may take different routes as the process goes on. Owing to this complexity, it is difficult to understand the dynamic behaviors of the material flow during pyroprocessing. With this background, this study was undertaken. The simple material flow during pyroprocessing can be easily understood based on the equilibrium mass balance. However, a simple material flow based on the equilibrium mass balance cannot give insight into any dynamic behavior of the material flow since it cannot take into account changes according to time and events. EXCEL-like software is widely used to establish the equilibrium mass balance of the overall process, but it is very restrictive in that it can only see the accumulated mass balance based on a specific time. To implement a dynamic material flow, two methods are proposed in this paper. One is a semi-dynamic material flow, which can be achieved by an algorithm based on a discrete event system (DES). The other method is a fully dynamic material flow, which can be achieved through unit process modeling.

This study suggests a three-tiered modeling architecture for an integrated pyroprocessing plant level simulator. To successfully build the pyroprocessing simulator based on the modeling architecture, there are some technical issues to settle from a software engineering aspect. A skillful management of two different systems such as a continuous system (CS) and DES might be of great concern, as might a database design for a unit process model. A detailed solution will be addressed with a sample problem.

## 2. RandD status

### 2.1. US

Motivated by the challenges and needs of nuclear energy systems that can be addressed by modeling and simulation, the Office of Nuclear Energy of the US Department of Energy has articulated a vision for a Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. NEAMS is aimed toward building on the success of recent programs in advanced scientific computing, namely, Advanced Strategic Computing Initiative (ASCI) and Scientific Discovery through Advanced Computing (SciDAC), with a focus on very different challenges. These challenges include the need for nuclear energy systems to be licensed by regulators and moving advanced technologies out of the research environment and into the hands of the engineers who will design, build, and operate the new nuclear energy systems. NEAMS will provide a comprehensive solution, and is organized into the following five elements:

- Integrated Performance and Safety Codes (IPSCs), end-to-end codes to understand the detailed, integrated performance of new nuclear systems, including the following: Nuclear Fuels, Reactor Core and Safety, Separations and Safeguards, Waste Forms and Near-Field Repositories.
- Fundamental Methods and Models.
- Verification, Validation, and Uncertainty Quantification.
- Capability Transfer Enabling Computational Technologies.

Through the NEAMS-IPSC, the US is devoting to developing a reprocessing plant level toolkit named RPTk (Reprocessing Plant Toolkit), which uses an open-source platform to accommodate legacy codes across the US (McCasky et al., 2011). RPTk implements a data flow architecture, which is the source of the system's extensibility and scalability. Data flows through physicochemical modules sequentially, with each module importing data, evolving them, and exporting the updated data to the next downstream module. This

is accomplished through various architectural abstractions designed to give RPTk true plug-and-play capabilities.

### 2.2. Japan

A decade ago, Japan developed an analysis code (Okamura and Sato, 2002) using the object-oriented software ExtendSim (Diamond et al., 2010) for an estimation of the material balance for the system design of the pyrochemical reprocessing plants consisting of batch processes. This code can also estimate the radioactivity balance, decay heat balance, and holdup, and can easily cope with an improvement of the process flow. The study describes the outline of the code and an estimation of the material balance in an oxide electrowinning reprocessing system under consideration of the solvent recycling time. However, it is difficult to determine the current activity with respect to the modeling and simulation of a SF recycling facility in Japan.

### 2.3. Republic of Korea

To analyze the operational issues in a pyroprocessing head-end facility, a discrete event modeling approach was applied (Lee et al., 2009). Also, a code development study on the dynamic material flow in an integrated pyroprocess was carried out under the DES environment (Lee et al., 2011). This paper addresses the plant-level framework in detail including a previous dynamic material flow study.

## 3. Semi-dynamic material flow

A basic plant-level model for an integrated pyroprocessing facility is a dynamic material flow. Since most analyses are related to a material flow, a plant-level model should include a framework to implement a dynamic flow. The mass balance can be calculated anywhere and anytime, in other words, at any unit process and at a specific time. Pyroprocessing is a batch-type process, which is unlike an aqueous system such as plutonium (Pu)–uranium (U) extraction (PUREX). The material flow between unit processes is not seamless, and thus it is better that such behavior be modeled as DES and not a continuous variable system. However, looking inside the unit process operation itself, its chemical reaction or electro-chemical reaction is modeled as a differential or difference equation that is time-dependent. Unless there is unit process model to represent the output of the SF composition according to time and stream, the fully dynamic behavior of the unit process model can be replaced with a semi-dynamic material flow. A semi-dynamic material flow is not concerned with material changes during the unit process, but rather the final results after the unit process finishes. Even though reliable unit process models have not yet been developed at present, a semi-dynamic material flow can be obtained only if there is an equilibrium mass balance at a specific time. Currently, a baseline pyroprocessing flowsheet including the equilibrium mass balance for a one-year operation is being revised based on current technology at KAERI. In 2009, the so-called PyroFlow (Lee et al., 2011) was developed, which represents semi-dynamic material flows according to all streams by modeling many operational events such as the material's arrival and departure, equipment failure, and repairs changing the state of the unit process into idleness, operation, or breakdown. Given the information on the batch capacity, process time, preparation time, post-process time, and equipment failure rate, an integrated pyroprocess material flow can be modeled as DES.

The following equation addresses the processed amount of mass in process  $P_j$  given the voloxidation equivalent batch capacity

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