Development of Integrated Operation Model for Pyroprocessing (IOMP)

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1. Introduction

There have been some studies on modeling and simulation of integrated pyroprocessing to see complex dynamic material flow [1-4]. They are dealing with their own flow-sheet based model that reflects their own country's pyroprocessing technology. The Korea Atomic Energy Research Institute (KAERI) has been developing the multi-purpose integrated pyroprocessing operation model. Consulting with process developers, facility designers, and safeguards researchers, key requirements for so-called integrated operation model for pyroprocessing (IOMP) has been developed. The distinguished features of IOMP are element-wise mass tracking in an element as well as chemical basis, linebalancing, resource optimization, and random mass balance area selection for safeguards research purpose. IOMP v1.0 will be released soon to KAERI personnel for receiving review feedback. It is expected that IOMP can give insight into pyroprocessing technological direction as it makes the complex integrated operational behavior of pyroprocessing more foreseeable.

2. IOMP Purpose

The objectives of IOMP development give insight into optimized operation with various process parameters to enable process line balancing analysis to design an efficient process line and give insight into the configuration of the process line. The following decision variables such as number of equipment, number of human operators, number of material handling systems, size of work-in-progress (WIP) storage, separation ratios could be determined to be values close to optimized values through the repeated simulations. IOMP can shows the consequences of overall and individual cell lead times, final product and waste generations, concentration of a nuclide species in molten salt, and element trace through all material streams.

3. Methods and Results

IOMP just handles not unit process model but unit operation model and plant-level model in the three tiered modeling architecture [3]. The unit operation model in the second level, and their integration based on the material flow in a discrete event system (DES) environment.

3.1 Development Procedures

Requirements for the multi-purpose IOMP were aggregated from expected potential users from various areas [5]. Before starting the construction of IOMP, lots of domain knowledge needed to be reproduced to deliver pyroprocess domain knowledge to modeling experts. The KAERI's flowsheet [6] was revised to make it clearer. The operation sequences for integrated material flow and process flow map were produced so that unit operations and their interdependency can be easily understood. The conventional mass balance file was broken down to the unit operation's mass balances to build mass balance calculation scheme in the model.

3.2 Required Software and File

IOMP has been constructed in the ExtendSim v.9.2 platform [7]. It consists of model file, library file, and EXCEL import file for model's user-defined parameters.

3.3 IOMP Configuration

IOMP has a hierarchical modeling structure. The top window shows only cell configuration so that there are 8 cells such as truck bay area, head-end cell, oxide reduction cell, electrolytic recovery cell, product storage cell, waste form storage cell, and off-gas cell, and inter-connections among such cells. There also exist user interfaces to track dynamic historical material flow in a chemical mass basis, to import lots of user parameters, to see final product and waste forms. There also exist work-in-progress summary and cell lead time block to analyze each cell's capability.

The second level window of IOMP consists of several functions and display of results. There are user interfaces to adjust resource size and to display utilization, lead time of unit operation. Especially, nuclides concentrations within molten salt of equipment can be historically tracked according to the number of batch operation on a nuclide basis.

A user can drag into the third level of window if one unit operation represented in a box is double-clicked. Detailed logic model and equations to calculate mass flow is represented in this level. There exist user interfaces of the corresponding unit operation in this level such as failure and recovery rate of equipment, process operation and transfer times.

3.4 Run IOMP

Running IOMP follows the sequences: (1) select spent nuclear fuel (SNF) composition, (2) modify

parameters, (3) enable/disable element tracking, (4) enable/disable element trace, and (5) run simulation. To select SNF composition, a user needs to assess inside truck bay H-block and select one of embedded SNF compositions. By default, IOMP includes 7 SNFs with different burn-ups and enrichments. There are 3 methods to modify model parameters: Import from Excel import workbook, modify the values at 2nd or 3rd level user interface directly, and modify the values in the database. IOMP can get random values as model input parameters is to modify the values in the database.

To run IOMP with external input parameters, a user needs to open 'IOMP Import Parameters.xlsx' Excel file and adjust the parameter values in 3 tabs such as 'Independent Process Parameters', **'Operation** Parameter', and 'Transfer Parameter' and save and close the file. If a user click [Import all tables] button in the top window of IOMP, all import parameters will be loaded in the corresponding DB tables in IOMP. In order to change parameters at UIs in the 2nd and 3rd level, a user needs to access a corresponding cell and process operation. A user may double click a cell to open 2nd level UI for selected cell and enter the desired values for the parameters on 2nd level UI. If more information needs to be input, a user may double click a process operation H-block to open 3rd level UI for selected process, and enter the desired values for the parameters on 3rd level UI or click [Separation Ratio] button to open up Separation Ratio table and enter the desired values for the parameters.

3.5 Element-wise Mass Tracking

A user needs to make the element tracking check box enable to analyze dynamic mass flow. A user can decide a random mass balance area (MBA) from the popup list containing unit operations and cells as default MBAs, or make his own MBA. Setting time window is needed to calculate sum of inputs, sum of outputs and remaining mass at the end of time window. Options of level, chemical form, select, and mass basis is required to show that mass balance is valid for the selected options. In the bottom pane there are mass balance results are displayed for the selected nuclide species and chemical form. All results will also be checked in the report tables by clicking [Generate Report Tables] and [Generate all saved reports]. For example, let's set an MBA as Op3-6 Low Temperature Voloxidation that converts UO2 pellets to U3O8 powder by pulverization process. It has four input streams from WIP1-Op3-5, WIP2-Op3-5, oxygen supplier, and filter supplier and four output streams to WIP1-Op3-6, WIP2-Op3-6, SWIP for filters, and Off_Gas_Cell, and only one storage, i.e., Op3-6 itself. When the Op3-6 is selected as an MBA, four inputs, log files for five outputs and one storage are listed on the table in the top part of the dialog window as shown in Fig. 4. If a user clicks [Generate Report Tables], compound mass balance

report and element mass balance report tables are appeared. The tables show a total of 9 in- and outstreams, and storage. The last column of the table is the verification column of mass balance equation as follows.

net mass change =
$$\sum_{j=1}^{n_i} I_j - \sum_{k=1}^{n_o} O_k - \sum_{l=1}^{n_l} R_l$$
 (1)

where n_i , n_o , and n_l are the number of input stream, output stream, and remaining storage within MBA, respectively, and I_j , O_k , and R_l are accumulated j-th input during the time window, accumulated k-th output during the time window, and current amount at l-th remaining storage, respectively.

In the Fig. 4, UO_2 has positive, whereas U_3O_8 has negative values in the remaining storage, Op3-6. The table shows the 'converted from' compound as a positive value (UO_2 is consumed in Op3-6, same as stored in Op3-6) and the 'converted to' compound as a negative value (U_3O_8 is produced in Op3-6). If the net mass change is always zero, it means net mass change in Eq. (1) is zero under the condition of given MBA and time window.

3.6 Line-Balancing of Integrated Process

One of the main analysis functions of IOMP is to analyze if integrated process is well balanced. For such purpose, we firstly make each cell capable of having equivalent processing capacity by adjusting cell's capacity. To check capacity of each cell, cell lead time will be investigated by clicking the [Cell Lead Time]. If a cell lead time is much less than most of cells, that cell should be improved by adjusting capacities of unit operations such as batch size and process time. The lead time is defined as difference between operation complete time and operation start time. As a result of simulation with default parameters, the electrolytic recovery (ER) cell lead time is longer than others so that a user may investigate what unit process in the ER cell is so-called rate determining step. Clicking ER cell leads to open ER cell H-block where lead times for all unit operations in the ER cell will be shown. Op5-9 LiCl-KCl purification operation is considered the rate determining step in ER cell. In order to make all unit operations have almost same capacity, a user needs to perform design of experiment (DOE) for analysis with detailed scenarios. For such purpose, IOMP provides scenario manager that can designate process time and batch size as factors and lead time as response. Detailed explanation for DOE exceeds over the scope of this paper.

4. Conclusions

As IOMP has been developed based on the KAERI's up-to-date pyroprocessing flow-sheet, pyroprocessing experts including process designers were equipped with a powerful analysis tool for understanding dynamic behavior of complex integrated pyroprocessing. It is definitely an excellent simulation model capable of multi-purpose analyses such as dynamic mass flow analysis of a specific nuclide, reliability of equipment, line balancing, resource optimization, and monitoring of molten salt concentration. This very first version of IOMP will be released soon within KAERI experts to get real user's feedback for improvement of IOMP.

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REFERENCES

[1] N. Okamura, K. Sato, Computer code system for the R&D of nuclear fuel cycle with fast reactor-IV. Development of an object-oriented analysis code for estimation of the material balance in the pyrochemical reprocessing process, Cycle system technical report 3, pp.1–10, 2002.

[2] H. J. Lee, Discrete event dynamic system (DES)-based modeling for dynamic material flow in the pyroprocess. Ann. Nucl. Energy, Vol.38, pp.860–875, 2011.

[3] H. J. Lee, W. I. Ko, I. T. Kim, and H. S. Lee, Design for integrated pyroprocessing plant level simulator, Ann. Nucl. Energy Vol.60, pp.316–328, 2013.

[4] L. E. Maggos, J. Figueroa, J. L. Willit and M. A. Williamson, Development of AMPYRE - A Dynamic Pyroprocess Model, Integrated Pyroprocessing Research Conference(IPRC-014), Oct.19-23, 2014, Idaho Falls, ID.

[5] H. J. Lee, H. S. Im, and B. H. Won, Requirement of an Integrated Operation Model for Pyroprocessing (IOMP), KAERI/TR-6445/2016, 2016.

[6] H. S. Im et al., Korea's Pyroprocessing Baseline Flowsheet v5.19, 2016.

[7] <u>www.extendsim.com</u>



Fig. 1. Main window of IOMP with several cells and user interfaces.



Fig. 2. Second level window of oxide reduction cell with user interface and unit operations



Fig. 3. Third level window of unit operation of oxide reduction with user interfaces to adjust user parameters and to display results.



Fig. 4. Element wise mass tracking dialog window (top) to set MBA and see if mass balance is valid in the MBA (bottom)