Discrete Event System Based Pyroprocessing Modeling and Simulation

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Abstract: The pyroprocessing operation-modelling is characterized as complicated batch type operation and tangled material flow logic, and handling many numbers of chemical elements. Discrete event system modeling was performed to build an integrated operation model, a simulation of which showed that a dynamic material flow was implemented. All data related to a dynamic material flow were recorded in database tables, and used for verification and validation in terms of material balance. Compared to equilibrium material balance, dynamic mass balance showed that the amount of material transported upstream and downstream in the unit process satisfied the mass balance equation at every batch operation. This study also showed that a dynamic material flow, which is a basic framework for an integrated pyroprocessing simulator, was well working. The integrated model built thus far will be improved in a few years toward an integrated simulator with safeguards assessment, technical feasibility, and economic feasibility modules.

1 INTRODUCTION

The Korea Atomic Energy Research Institute (KAERI) has been developing pyroprocessing technologies, which can reduce the increasing amount of spent nuclear fuel (SNF) and dramatically decrease the disposal load, through recycling and destroying toxic waste such as long-life fission products in the SNF. 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. Actually, modelling and simulation enhance an understanding of known systems, provide qualitative and quantitative insight and guidance for experimental work, and produce quantitative results that replace difficult, dangerous, or expensive experiments (DePaoli, 2011). Therefore, a technology assessment and breakthrough by modelling and simulation would be preferable even in pyroprocessing technology development. In this study, the main concern is to build a consolidate framework able to describe the material flow of an integrated pyroprocessing facility and to build a model on that. This study is on-going mid-term research to aim at a multi-purpose integrated pyroprocessing simulator. As a basic frame of the simulator, the material flow modelling and mass balance management were carefully designed and applied to the simulator. Mass balancing model was studied about iron ore terminal example by using mixed discrete and continuous model (Béchard, 2013). In this study, a discrete event based system (DES) appropriate to build a model of a batch type process is applied to the configuration of the pyroprocessing material flow. Dynamic in-out material balance in the unit process is managed in the database whenever events according to the material flow occur. The progress on the simulator was verified in terms of rigorous implementation of operation logic and mass balance.

2 PYROPROCESSING

An integrated pyroprocess is under consideration to

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process the spent oxide fuel discharged from PWRs and fabricate metallic fuel containing transuranic (TRU) elements for a future sodium cooled fast reactor (SFR) (Yoo et al., 2008). The process includes head-end process, electrolytic reduction, electro-refining, electro-winning, and a salt waste treatment system.

The pyroprocessing also includes many complex recycling flows. Since it almost consists of batch-type processes even though some are more like continuous processes, a discrete event system is preferred to model it. A lot of effort has been put into an investigation of principle (Song et al., 2010; Lee et al., 2011). Since current experimental studies focus on the unit process technology, and not an integrated process, it is hard to predict the overall behaviour and mutual influence. However, modeling and simulation can make it possible to see unforeseeable behaviour.

3 MODELING AND SIMULATION

3.1 Operation Model

3.1.1 Discrete Event and Hybrid System

The operation model in the pyroprocessing simulator is located between the process model and facility model (Lee et al., 2013). Although the process model is involved in a pyrochemical reaction within a batch, the operation model is engaged in states in border of batch, that is, states driven by the start and end of the batch operation. The state transition driven by event in the operation model is what the DES modeling describes the best. On the other hand, a time-dependant state in the process model can be well described in a continuous variable dynamic system (CVDS). This is why the pyroprocessing simulator is a hybrid system. In this paper, the operation model is focused more than in the process model because the process modelling and hybrid system modelling was explained in a previous study (Lee et al., 2013).

3.1.2 Operation Procedures

We do not have as much information on the pyroprocessing operation as a real existing facility operation. Therefore, gathering the operation information is limited. However, baseline operation procedures for a rational process operation can be drawn by professionals involved in the process development. Since pyroprocessing often has recycling and complex operations, to build an operation model to meet such requirements is not that simple.

For example, the oxide reduction process (Karell and Gourishankar, 2001; Herrmann et al., 2005; Hur et al., 2008) includes three unit processes such as electrolytic reduction (P2-1), cathode processing (P2-2), and LiCl purification (W4-1) as shown in Figure 1. P2-1 converts two types (pellet and fragment) of oxide fuels into metal ones by electrolytic reduction, P2-2 evaporates and recovers entrained salt in a cathode product carried from P2-1, and then recycles the recovered salts during the first campaign (1st through 40th batch) but sends them to W4-1 after the first campaign (41st batch ~). The recovered salt is added in P2-1 every other batch (3rd, 5th, 7th, … 39th batch) operation during the first campaign. The recovered salt is regenerated in W4-1 to be recycled to P2-1 from the third campaign (81st batch ~). During the second campaign (41st batch through 80th batch), P2-1 needs new salt to compliment insufficient salt corresponding to entrained salt accompanied by a cathode product, and P2-2 holds the recovered salt until it reaches an amount sufficient to feed W4-1. From the third campaign, P2-1 receives the regenerated salt during every other batch operation, and new fresh salt can then be added if it is insufficient.

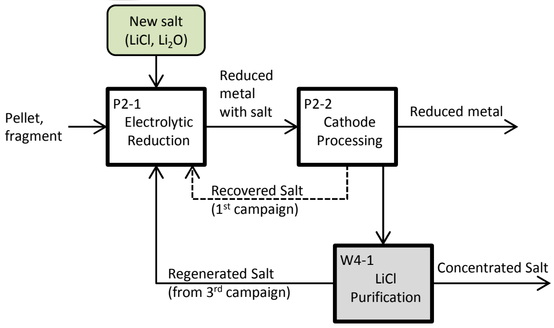


Figure 1: Material flow diagram for oxide reduction.

The above operation requirement is changed according to the batch operation number. Consequently, the material flow direction changes. To reflect such complex flow change in a model, a well-designed logic based model should be built.

3.1.3 Operation Modeling

Operation logic in 3.1.1 was implemented in an ExtendSim^{TM} v8. Routing modeling is built based on DES, as shown in Figure 2, as a feed material for one batch is considered to be an item. The oxide reduction model begins with the transport block that

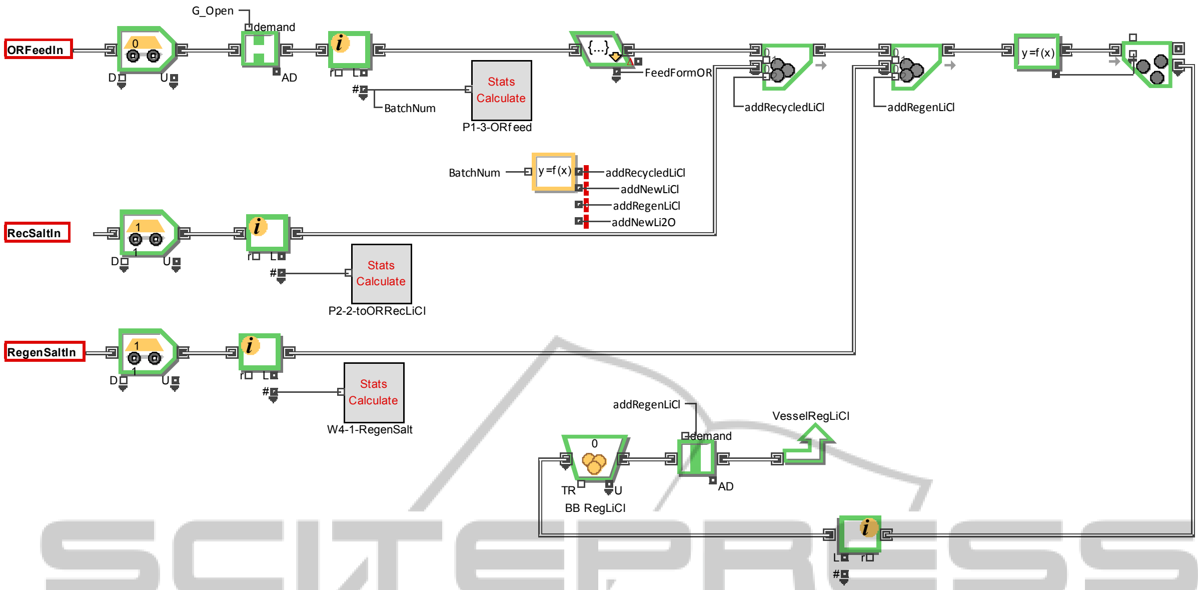
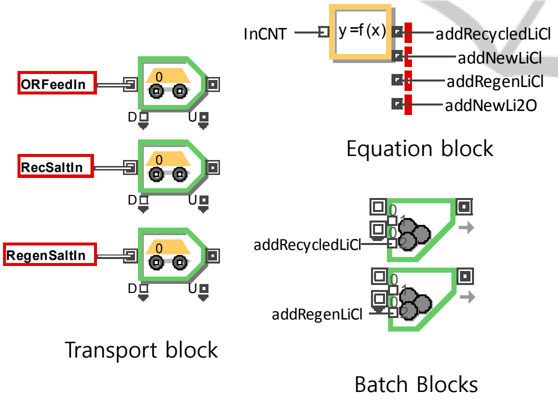


Figure 2: Logic model of feed material receipt in P2-1.



Equation block

Transport block

Batch Blocks

Figure 3: Blocks needed for operation logic.

represents three types of feed material (SNF, recovered salts, and regenerated salts) receipt. SNF is always needed for every batch operation. However, the recovered salts and regenerated salts can be received or not according to the batch operation number. Such routing logic is implemented by an equation block and batch blocks, as shown in Figure 3.

Equation block includes complex logic behaviour describing the operation condition, for example, whether the current batch operation requires the addition of new, recovered, or regenerated salt. If an addition is needed, a corresponding batch quantity in the batch block is set to TRUE. The pseudo-code for the equation block is as follows:

```
// Batch #: 1
if(BatchNum == TRUE)
    addNewSalt = TRUE;
    addRecycledSalt = FALSE;
    addRegenSalt = FALSE;
// Batch #: 3, 5, 7, ... ,39
else if((BatchNum <= 40) &&
(Realmod(BatchNum-1, 2) == 0))
{
    addNewSalt = FALSE;
    addRecycledSalt = TRUE;
    addRegenSalt = FALSE;
}
// Batch #: 2, 4, 6, ... ,40
else if((BatchNum <= 40) &&
(Realmod(BatchNum, 2) == 0))
{
    addNewSalt = FALSE;
    addRecycledSalt = FALSE;
    addRegenSalt = FALSE;
}
// Batch #: 41, 43, 45, ..., 79
else if(BatchNum >= 41 && BatchNum <=
80 && Realmod(BatchNum, 2) == 1)
{
    addNewSalt = TRUE;
    addRecycledSalt = FALSE;
    addRegenSalt = FALSE;
}
// Batch #: 42, 44, 46, ..., 80
else if(BatchNum >= 41 && BatchNum <=
80 && Realmod(BatchNum, 2) == 0)
{
    addNewSalt = FALSE;
    addRecycledSalt = FALSE;
    addRegenSalt = FASLE;
```

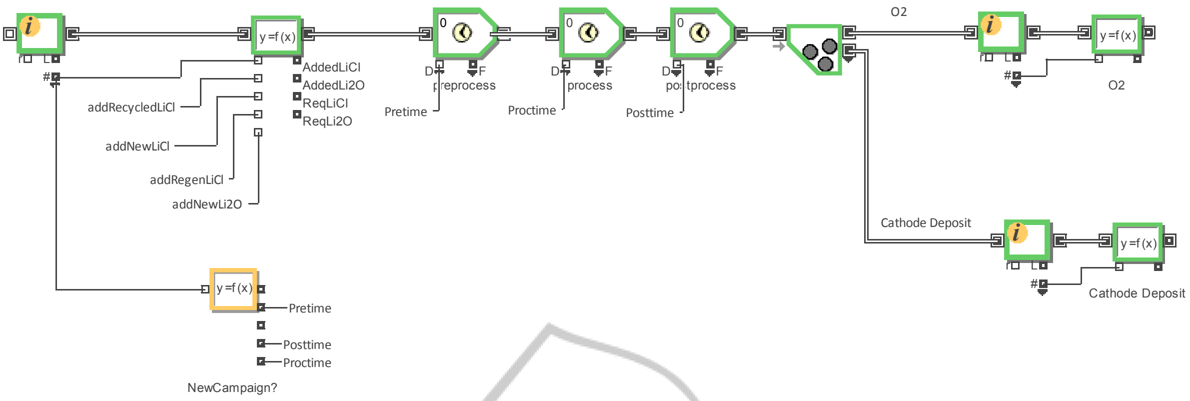


Figure 4: Mass composition calculation of feed (input) and product materials (output) in P2-1.

```
}
// Batch #: 81, 83, ....
else if(BatchNum >= 81 &&
Realmod(BatchNum, 2) == 1)
{
    if(ReqSalt > RegSalt)
        addNewSalt = TRUE;
    else
        addNewSalt = FALST;
    addRegenSalt = TRUE;
    addRecycledSalt = TRUE;
}
```

The first inputs of two batch blocks are for the receipt of pellet/fragment, which starts from the ORFeedIn connector. The batch blocks merge the first and second input items into one new item. The second input item number is controlled by the equation block to be set to 0 (FALSE) or 1 (TRUE). In the case of FALSE, the batch block converts only the first item into one new item.

A receipt of regenerated and recycled salt means the P2-1 process has a recycling material flow from another unit process. In this way, complex recycling is easily incorporated into a routing model through equation and batch blocks.

3.1.4 Material Flow Management

Material dealt with in the pyroprocessing simulator consists of 52 elements for SNF and 23 elements for chemical additives needed for pyroprocessing. A total of 75 elements are calculated and written in a record of the database table whenever each event occurs. To access ExtendSim's internal database table, equation blocks for the mass balance calculation are inserted at an appropriate position in the model. The first equation block in Figure 4, which is an item equation block different from the equation block in Figure 3, calculates the salt composition in a bath when an item passes through the equation block after receiving and merging a pellet/fragment with recovered or regenerated salt, and the item then passes through pre-process, process, and post-process sequentially. Because an electrolytic reduction generates two types of products such as O_2 and cathode product, the material should be separated into two products. An unbatch block plays a role of an item separation and each equation block actually calculates each product composition, as shown in Figure 4.

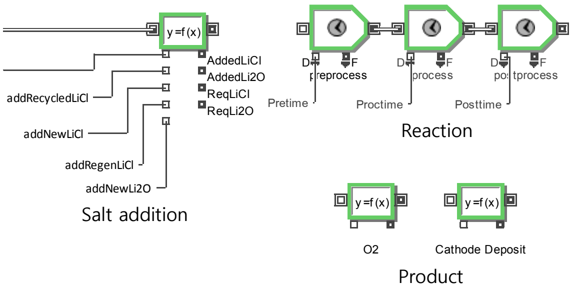


Figure 5: Blocks for mass calculations and process operation delay.

Figure 5 shows equation blocks to calculate an in-bath salt composition after receiving the feed material, and product composition after process operation. The codes in the equation blocks for mass composition calculation directly access the database tables to write, read, delete, and create data. The equation blocks in Figures 4 and 5 are item blocks and are able to be located anywhere in the item flow. Therefore, a mass composition can be timely calculated according to the material flow and event driven modelling for a material flow to be possible.

Process operation (electro-chemical reaction) is simply modelled with three activity blocks so that each activity (pre-processing, processing and post-processing) consume each specific time. In this part, the processing activity block can be replaced with a process model if it exists.

3.2 Material Balance

3.2.1 Equilibrium Material Balance

The integrated pyroprocessing simulator is designed on a basis of dynamic material balance. On the other hand, a flowsheet study (Lee et al., 2012) is based on equilibrium mass balance at a specific time, for example, at the end of year. Since equilibrium material balance simply indicates the accumulation of material transported through steam at a specific time, the calculation of equilibrium mass balance after a long period has an average effect such that transient changes are diminished over time. An equilibrium material balance represents the overall static characteristic, but a dynamic one shows the exact material balance change at any specific instance in time. An equilibrium mass balance in process P2-1 is shown in Table 1. This result is obtained from the accumulated transported mass via input and output streams after 200 batch operations, which correspond to 10 tons/year of annual throughput, have finished.

Table 1: Equilibrium material balance in P2-1.

Material via Stream	type	SNF mass (kg)
new salt	feed	-
pellet/fragment	feed	11,331
recovered salt	feed	5
regenerated salt	feed	6
Input Sum		11,341
cathode product	product	9,997
O_2	product	1,331
Output Sum		11,328
remaining salt	hold-up	13

Since equilibrium mass balance shows accumulated results over numerous batches, a difference of each batch is ignored. Process P2-1 has a total of four inputs and two outputs. Sums of inputs and outputs are not the same. However, considering that process P2-1 can hold a small amount of SNF in its bath, the mass balance is satisfied. We cannot predict from the equilibrium mass balance any result affected by the operation procedure described in section 3.1.1.

3.2.2 Dynamic Material Balance

Table 2 represents the mass of inputs and outputs calculated whenever every process batch operation is completed. Process P2-1 receives 50 kgHM/batch from a previous process. The second column in Table 2 represents the mass of pellet/fragment oxide. Excluding the oxide weight, it becomes 50 kgHM/batch. The operation procedure in sections 3.1.1 and 3.1.2 indicates that the recovered salt is added at every other batch during the first campaign, and the third batch operation expects a receipt of the recovered salt from P2-2. However, in the third batch operation, P2-1 does not receive the recovered salt because P2-2 has not prepared another recovered salt by then. Such a dedicate behaviour cannot be estimated in the equilibrium mass balance.

Table 2: Dynamic material balance in P2-1.

batch #	fragment/ pellet (kg)	recovered salt (kg)	regenerated salt (kg)	remaining salt (kg)	cathode product (kg)	O2 (kg)
1	56.67	-	-	0.28	49.72	6.67
2	56.67	-	-	0.54	49.73	6.67
3	56.59	0.02	-	0.83	49.74	6.59
4	56.67	-	-	1.08	49.75	6.67
5	56.59	-	-	1.33	49.75	6.59
6	56.67	-	-	1.57	49.76	6.67
7	56.59	0.05	-	1.85	49.77	6.59
8	56.67	-	-	2.08	49.77	6.67
9	56.59	0.08	-	2.38	49.78	6.59
…						
41	56.59	-	-	10.25	49.97	6.59
42	56.67	-	-	10.27	49.98	6.67
43	56.59	-	-	10.30	49.97	6.59
44	56.67	-	-	10.32	49.98	6.67
45	56.59	-	-	10.35	49.97	6.59
46	56.67	-	-	10.37	49.98	6.67
47	56.59	-	-	10.40	49.97	6.59
…						
81	56.59	-	0.08	11.03	49.99	6.59
82	56.67	-	-	11.04	50.00	6.67
83	56.59	-	0.08	11.13	49.99	6.59
84	56.67	-	-	11.13	50.00	6.67
85	56.59	-	0.08	11.21	49.99	6.59
86	56.67	-	-	11.22	50.00	6.67
87	56.67	-	0.08	11.30	49.99	6.67
…						
194	56.67	-	-	13.30	50.05	6.67
195	56.67	-	0.11	13.37	50.04	6.67
196	56.67	-	-	13.32	50.05	6.67
197	56.67	-	0.12	13.39	50.04	6.67
198	56.67	-	-	13.34	50.05	6.67
199	56.67	-	0.12	13.41	50.04	6.67
200	56.67	-	-	13.36	50.05	6.67
sum	11,331	5	6	13.36	9,997	1,331

It shows that regenerated salt is provided at every other batch operation from the third campaign (81th batch ~) in the 4th column in Table 2, as expected in section 3.1.1. Since the remaining salt always exists in the bath of P2-1, the 5th column in Table 2 indicates the current accumulated state in the bath. The amount of products increases as the campaign increases because a small amount of SNF elements accompanied by regenerated salts is added in P2-1 from the 3rd campaign. A summation of the input and output materials over 200 batch operations in Table 2 means accumulated transported mass through input and output streams. The accumulation of each batch operation results is exactly the same as the equilibrium mass balance in Table 1. Compared to the equilibrium mass balance, the dynamic mass balance gives a lot of information on the state at a specific instance in time, i.e., how much material has been processed, how many products have been produced, how much of the material has been held up, and how much material remains in temporary storage while waiting for the next process.

4 VERIFICATION AND VALIDATION

4.1 Models & Codes

Logics and models for operation modeling are verified from a material flow point of view. Many debugging tools and utility blocks support the building of an integrity model. Debugging the item flow and equation are necessary to detect problems and fix them to accomplish the completeness of a model. In the model level, a pausesim block is located anywhere and stops the simulation progress at a user intended point. In the code level, a set break point will stop the programming code in the equation block running at a user intended point. The integrated pyroprocessing model includes a very complicated item flow, and thus a debugging process is needed to guarantee item flow logic. It also includes many equation blocks to build a complicated operation procedure and calculate the mass composition. Therefore, to debug such equations is also necessary. Whenever a unit process model is developed, not only is the model itself debugged, the integrated operation model is also verified.

Validation is quite difficult to perform at this moment because there is no existing integrated facility using SNF. However, lab-scale based experimental results using simulated fuels, which are not real SNF but are able to simulate real SNF to a certain degree, can be validation data. Such results have already been used in the model to obtain material composition of the product. Therefore, the material composition of every product should be checked at every batch operation to satisfy the separation factor as obtained in the experiment.

4.2 Material Balance

Once the unit process is modelled, the mass balance equation must be satisfied for every batch operation through an investigation into the related database tables.

$$\sum_{i=1}^{m} I_{i,k} = \sum_{i=1}^{n} O_{i,k} + (H_k - H_{k-1}) \tag{2}$$

where m is the number of inputs, n is the number of outputs, k is the current number of batch operations, $I_{i,k}$ is the k-th input amount of mass transported through the i-th upstream, $O_{i,k}$ is the k-th output amount of mass transported through the i-th downstream, and H_k is the hold-up until the k-th batch.

The bracket in equation (2), which represents the difference between the current and previous hold-up, means the contribution by only the current batch operation because a hold-up inherently involves accumulation. For example, for the 9th batch operation in Table 2, the mass balance equation (2) is satisfied as follows:

Table 3: Mass balance equation in the 9th batch operation.

9-th inputs		9-th outputs	8-th hold-up	9-th hold-up
56.59		49.78	2.08	2.38
0.08		6.59		
0.00				
56.67	=	56.37	+	0.30

After the current batch (9th batch), an operation hold-up represents 2.38 kg, but the contribution by the current batch operation is exactly 0.30 kg. Any other batch operation satisfies the mass balance equation as the result of the 9th batch operation. The above results must also be satisfied even though a gross mass decomposes into the type and element level. The proof is skipped in this paper due to limitations.

5 CONCLUSIONS

The integrated pyroprocessing features are a batch type operation, complicated recycling, and tangled operation logic. An item flow model based on DES enables a flow control, mass balance calculation, and basic framework of an integrated pyroprocessing simulator. Compared to a static or equilibrium material flow, a model-based dynamic material flow provides detailed information and thus a careful analysis of every batch is necessary to confirm the mass balance results. Verification and validation regarding the model built thus far has been performed in terms of the mass balance calculation, and shows the completeness of the model. However, the modeling has not been finished but is still under progress.

To improve the operation model toward a multi-purpose integrated pyroprocessing simulator, various modules must be incorporated at a facility level. One of the issues on a new recycling process such as pyroprocessing is to guarantee integrated safeguards in terms of material accountancy and security. Mass tracking is the most fundamental requirement for a model to cope with for safeguards assessment. Since the material flow framework in the current model can support a perfect mass tracking on an element basis, a safeguards module is expected to be developed without difficulty and to be added in an integrated simulator. Technical feasibility can also be supported by an integrated simulator to determine or recommend process operation conditions by adding an optimization module. Compared to other reprocessing technologies, economic feasibility must be tested in a simulation by developing a cost evaluation module. It is expected that an integrated pyroprocessing simulator fulfilling the above described functions by add-on modules will be released in a few years.

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