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A FACILITY MODEL FOR THE LOS ALAMOS PLUTONIUM FACILITY*

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ABSTRACT

The Los Alamos Plutonium Facility contains more than sixty unit processes and handles a large variety of nuclear materials, including many forms of plutonium-bearing scrap. The management of the Plutonium Facility is supporting the development of a computer model of the facility as a means of effectively integrating the large amount of information required for material control, process planning, and facility development. The model is designed to provide a flexible, easily maintainable facility description that allows the facility to be represented at any desired level of detail within a single modeling framework, and to do this using a model program and data files that can be read and understood by a technically qualified person without modeling experience. These characteristics were achieved by structuring the model so that all facility data is contained in data files, formulating the model in a simulation language that provides a flexible set of data structures and permits a near-English-language syntax, and using a description for unit processes that can represent either a true unit process or a major subsection of the facility. Use of the model is illustrated by applying it to two configurations of a fictitious nuclear material processing line.

I. INTRODUCTION

The Los Alamos Plutonium Facility contains more than sixty unit processes utilizing both aqueous chemistry and pyrochemical methods, and it is called upon to process a wide variety of nuclear materials including most known forms of plutonium-bearing scrap. The complexity of the facility and the variety of the feeds it receives create a significant challenge in generating processing schedules and maintaining a comprehensive picture of the flows of nuclear materials within the facility, particularly because detailed knowledge of the status of various sections of the facility is usually fragmented among a number

of different people. However, failure to maintain a comprehensive overview of facility operations can result in processing inefficiencies, and can impede the detection of abnormal situations affecting material control. The management of the Los Alamos Plutonium Facility recognized that a facility model could aid in integrating the extensive body of information concerning the facility in a fashion that would be useful for planning and operational purposes and for the evaluation of the effects of technological innovations, and is sponsoring the development of a computer model to achieve these ends.

The purpose of this paper is to describe the features of the facility model that is being developed and to illustrate some of its potential applications. As an example, we use the model to examine the operational characteristics of two versions of a fictional but realistic pyrochemical plutonium metal processing line. In the first version of the line all by-products of the pyrochemical processes are either discarded or are retained for aqueous chemistry recovery; and in the second version a number of internal pyrochemical recovery steps are added, in an attempt to reduce the quantity of material that must be processed by aqueous chemistry methods. The model is used to simulate operation of each of these metal processing lines for a 3-month period to determine how incorporation of the recycle steps affects product and waste generation.

The structure of the model itself is described in the next section. Section 3 presents the two versions of the metal processing line that are studied, and the results of the process simulations for these two lines are given in Section 4. Planned enhancements for the model are discussed in Section 5.

II. FEATURES OF THE MODEL

Considerable attention was given to design of the logical structure for the model in an effort to achieve the greatest flexibility and ease of maintenance possible. In particular, the following were identified as important attributes that the model should possess.

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- (1) It should be easy to update the information the model contains about the numbers, types, and interconnections of the facility's unit processes.
- (2) The model should allow the facility to be represented at any desired level of detail.
- (3) The facility representation in the model should contain not only numerical parameters but also the process structure of the facility in a form that can be read and interpreted by other computer programs.
- (4) The model and its data files should be written so they can be read and understood by a technically qualified person familiar with the chemical processes but lacking modeling experience.

These characteristics are desirable because the structure of the Plutonium Facility is not only complex but also changes relatively frequently; because both long- and short-range planning studies are to be done within one modeling framework; because facility optimization and technological innovation studies are to be done that involve variations in process structure as well as process parameters; and because the analysts developing the model do not wish to spend the rest of their lives assisting in its use! These goals are achieved within the model by the following methods.

1. The model is structured so that all facility information is contained in data files. No facility information of any kind is contained in the model program itself, though the program does reflect—and limit—the kinds of facility information that are utilized in the model. The data files themselves are currently in human-readable text form with descriptive legends identifying the items of facility information contained in the files. This form for the data files allows the facility description to be maintained by technically qualified process personnel who are not familiar with the details of the model program itself. The human-readable text files will soon be replaced by binary files maintained by a menu-driven "front-end" program to simplify maintenance of the facility description even further.

2. The model is formulated in a simulation language that permits a near-English-language syntax and that provides a large, flexible set of data structures. The near-English-language syntax makes it possible to write the model program in a form that can be read by computer-literate process personnel who have no modeling experience. The flexible set of data structures allows one to place the facility information in data files and then generate at execution time the descriptor variables required by the program.

3. A unit process is treated in the model as an operation that transforms an input nuclear material item into a set of output items (a product and possibly one or more by-products), and

that requires a set of human and equipment resources and some period of time to achieve the transformation. This representation makes it possible to treat any desired subset of the facility from a true unit process to an entire process line as a "unit process" for purposes of modeling. Consequently, detailed facility planning and optimization studies can be performed by using the model program and a facility data file that contains facility information at a true unit-process level; and long-range projections can be made by using the same model program with a process data file that treats entire process lines as "unit processes" with appropriate input and output material flows, and with batch sizes and process times adjusted to represent extended processing periods such as weeks or months.

The model program has been constructed to permit inclusion of most types of facility information that might be expected to affect operation. These include provision for

- Multiple operating shifts, each with its own set of break and meal periods for process personnel;
- Multiple feeds and products for each unit process with each feed/product having its own characteristics;
- Several flexible material selection schemes for unit processes that draw feeds from the vault;
- Multiple alternative destinations for process products with actual choice of destination determined by priority order and by space availability;
- Multiple steps in the functioning of each unit process with each step having its own requirements for time and process personnel.

This framework has proved to be flexible and easy to use in the applications of the model made thus far and has been completely adequate to describe the process information of interest.

III. EXAMPLE PROCESSES: A PLUTONIUM METAL PROCESSING LINE

The model is demonstrated using two example processes. Both examples are fictional plutonium metal processing lines. The first contains no recovery processes. The second is the same line with several pyrochemical recovery processes added. The recycle steps in the second example are currently under development, and have not been demonstrated on a production scale. Information used in the models is a composite of data from several references.¹⁻⁹

Table I contains a listing of the unit processes with the product yields, process personnel ("operator") time requirements, and total operating time requirements. The unit processes are described below. Example 1 contains Direct Oxide

Reduction (DOR), Vacuum Casting, and Electrorefining (ER). Example 2 uses these three unit processes plus DOR Salt Recovery, ER Salt Recovery, and Pyroredox. In both cases, oxide generated by casting is recycled to DOR.

TABLE I
EXAMPLE PROCESS INFORMATION

Unit Process	Yield (%)*	Hours	
		Operator	Total
Direct Oxide Reduction	99.5	2.0	12.0
Vacuum Casting	95.0	8.0	8.0
Electrorefining	82.0	10.0	77.0
DOR Salt Recovery	**	5.0	15.0
ER Salt Recovery	96.0	4.75	12.75
Pyroredox	99.0	8.25	36.25

$$*Yield = \frac{(\text{Plutonium in product})}{(\text{Plutonium in feed})} \times 100.$$

**This step is for solid waste reduction, not plutonium recovery.

Direct Oxide Reduction (DOR)

In DOR, batches of >85% plutonium oxide are taken from the vault to form a charge of 800-1000 grams of the oxide for each process unit. There are five process units available. DOR produces impure metal that is sent to vacuum casting, if space is available, or to the vault for storage otherwise. By-product materials include DOR salts, and crucibles that are below discard limits and are sent to waste storage. The complete process includes four steps: setup, loading, reaction, and breakout. Each step has its own operator time and processing time. Five operators are available to run DOR.

Vacuum Casting

Batches of impure metal are taken from DOR or the vault to form a load of 5-6 kg of plutonium metal. Only one process unit is available. Vacuum casting produces a plutonium metal anode which is sent to electrorefining or to the vault. A by-product of the casting process is >85% oxide which is recycled to DOR. The casting process is one step; the one available operator must be present for the entire operating time.

Electrorefining

An anode is transferred from vacuum casting or the vault to ER and used as a charge for electrorefining. There are no restrictions on the size of the charge since that is fixed in casting. One ER process unit is available. The product of electrorefining is pure metal, which is sent to the vault for storage. By-products include an anode heel and ER Salts, which are sent to the vault for recovery. Crucibles, another by-product, are assumed to be below discard limits and

are sent to waste storage. The ER process is composed of four steps: setup, start-up, stop process, and breakout. Each step has its own operator and process times. One operator is available to run ER.

DOR Salt Recovery

DOR salts are below discard limits but constitute a large volume of waste. This process regenerates the salt and sends the required amount back to DOR for reuse. The excess salt (about 20%) is sent to waste storage. Additional waste is generated in the form of crucibles. Five process units and three operators are available for DOR salt recovery. DOR salt recovery has four steps: setup, loading, reaction, and completion. Each step has its own operator and processing times.

ER Salt Recovery

ER salts contain a significant amount of plutonium, which must be recovered, and present a processing problem for aqueous recovery. This process removes most plutonium from the salt as metal for recycle to vacuum casting. Two types of salt are generated: white salt is recycled to ER; black salt is sent to the vault for recovery. One process unit is available. This process requires the same operator as ER. ER salt recovery has four steps: setup, heating, reaction, and breakout. Each step has its own operator and processing times.

Pyroredox

Pyroredox is a combination of several reaction steps. It is used to purify the anode heel by-product from electrorefining. The product of this process, impure metal, is recycled to vacuum casting for fabrication into anodes. By-products are zinc waste and salt and crucible, which are all below discard limits and are sent to waste storage. One unit of this process is available; a new operator was added to run this process. Pyroredox has ten steps: setup 1, start-up 1, oxidation, liftout, cooldown, separation, setup 2, start-up 2, reduction, and breakout. Each step has its own operator and processing times.

At the beginning of the simulation for each version of the metal processing line, the vault contained a quantity of >85% oxide great enough to feed the line for the duration of the simulation period, and none of the unit processes contained any material. Consequently, on the first day of the simulation only the DOR units operated; on the second day of the simulation casting began to operate; and on the third day of the simulation ER began to operate. The simulation period chosen was 10/1/86 through 12/31/86, with account taken of weekends but not holidays. Among the process parameters monitored were unit process utilization, throughput by unit process and feed type, product and by-product generation by unit process and product type, and accumulation of materials in the vault. The next section discusses the results obtained from the two simulations.

IV. RESULTS AND DISCUSSION

The simulation examples are not intended to represent the actual operations of any particular facility and are intended only for illustration purposes. The numerical results are probably not applicable to real-life processing but give an idea of how this simulation program can be used. Only a pyrochemical metal processing line is considered; we have not considered process time and waste generated in recovering pyrochemical scrap through an aqueous recovery line. Furthermore, as noted earlier, the recycle processes added in example 2 are still under development and have not been completely demonstrated on a production scale.

Results for both examples are summarized in tables II-IV. Process utilization information is given in Table II. The "average number used" is calculated as the number of units in use times the hours in use divided by the number of hours of operation of the active shift. Because the units may remain active after the operating shift ends, the "average number used" can be greater than the actual number of units. Notice that of the three major processes only casting showed a change in usage by adding the recycle steps. In example 1 casting is underutilized, that is, it just wait for DOR to produce more impure metal; in example 2, anode heels and ER salts contribute additional impure metal so more material can now be processed through casting. An interesting point about utilization that is not given in table II is that addition of ER salt recovery increased the utilization of the ER operator by about 50% without interfering with the operation of ER. (Remember that the ER operator is used for both ER and ER salt recovery).

TABLE II
PROCESS UTILIZATION

Process	Number Units	Average Number Used	
		Ex. 1	Ex. 2
DOR	5	6.04	6.04
Casting	1	0.60	0.65
ER	1	2.61	2.61
DOR Salt Rec	5	-	5.93
ER Salt Rec	1	-	0.41
Pyroredox	1	-	1.12

The number of batches, total kilograms of plutonium, and total kilograms of bulk processed by each unit process are listed in Table III. Bulk refers to the total mass of material including plutonium. The increased usage of casting in example 2 is observed in Table III as the increased number of batches processed. Although the total amount of material processed by casting increased in example 2, the average batch size

decreased. This shows up in the decrease in the amount of material processed by ER. Casting requires 5-6 kg of bulk before process initiation; seven DOR impure metal batches are required to achieve this amount in example 1; however, only six DOR impure metal and one recycle batch (from ER salt recycle or pyroredox) activate casting in example 2. The combined batches with recycle material are always smaller than the seven batches from ER thus yielding a smaller anode from casting when recycled impure metal is used. A possible means of avoiding this problem and perhaps increasing the throughput of ER is to combine two or three recycle batches before transfer to casting, thus giving larger casting charges when recycle material is used.

In Table IV is a listing of process, scrap, and waste materials generated during the simulation and remaining in the vault at completion of the simulation. It can be seen that ER is a bottleneck for the metal processing line. In example 1, it processed only 16 anodes (as seen from the number of batches of ER salts produced) and has 19 anodes waiting for processing. Addition of the recycle steps in example 2 caused a further increase in the number of anodes in the vault, since ER could not handle the increased throughput of casting.

In both examples the scrap materials in the vault require further processing. In example 1, all scrap is intended to be processed by aqueous recovery. In example 2, only black salt is intended for processing by aqueous. Waste can be discarded. The addition of pyroredox in example 2 reduced the number of anode heels in the vault to zero, thus eliminating the need for aqueous processing of the heels and eliminating an inventory term in the materials balance equation. The same is true for ER salt recycle; ER salts were eliminated. DOR salts are discarded in example 1 and regenerated in example 2; salt regeneration reduces the amount of waste salts, which often constitute a measurement problem for safeguards.

All of this occurs at some expense. Both of the scrap recovery operations in example 2 generate scrap and waste that may present more of a problem for accounting than the original materials they process. Another problem that these examples do not address is the impact of the process changes in pyrochemical processing on the rest of the facility. For example, even though the recycle steps reduced the amount of scrap and waste from the pyrochemical line and allowed rapid turnaround of recycle material, it generated scrap that may present more of a problem for aqueous recovery. The problem is compounded if some of the waste generated by the recycle steps really does not fall below the discard limits. To determine the complete impact on processing, all aspects of the facility would have to be incorporated into the simulation. Other parts of the facility need not be represented in the detail used in these examples; the data for entire process lines could be entered as one unit process. The pyroredox unit process is an example of this.

TABLE III
MATERIAL PROCESSED

Process	Batches		kg Pu		kg Bulk	
	Ex. 1	Ex. 2	Ex. 1	Ex. 2	Ex. 1	Ex. 2
DOR	245	245	195.8	195.4	226.6	226.1
Casting	35	39	190.8	203.6	195.2	208.6
ER	16	16	80.2	77.8	82.6	80.2
DOR Salt Rec	-	194	-	0.8	-	1102.0
ER Salt Rec	-	16	-	5.6	-	30.4
Pyroredox	-	15	-	7.9	-	9.6

TABLE IV
VAULT HOLDINGS AT THE END OF THE SIMULATION

Material	Batches		kg Pu		kg Bulk	
	Ex. 1	Ex. 2	Ex. 1	Ex. 2	Ex. 1	Ex. 2
Impure Metal	0	0	0.0	0.0	0.0	0.0
Anodes	19	22	91.6	106.3	94.4	109.5
Anode Heels	16	0	8.7	0.0	10.5	0.0
Pure Metal	16	16	65.7	63.8	65.7	63.8
ER Salts	16	0	5.8	0.0	30.6	0.0
Black Salt	-	16	-	0.2	-	0.7
Wastes:						
Crucible	97	113	0.0	0.0	187.7	198.9
Salt & Crucible	-	209	-	0.2	-	306.9
Zinc Waste	-	15	-	0.04	-	3.6
DOR Salts	245	46	1.0	0.2	1390.9	260.4

Pyroredox is actually two processes as described in the process steps in the example data set, and in a "real-life" facility could be as many as four or five processes; but in this example it is treated as one unit process.

By building material measurements into the simulation, one can estimate the impact of process changes on materials accounting. This could be particularly useful for large or rapidly changing facilities as well as for planning. Additionally, the model can be used as a scheduling tool so that, for example, only the needed materials would be removed from a vault for processing, thus reducing processing conflicts and the amount of in-process storage.

V. PLANNED ENHANCEMENTS TO THE MODEL

The model is now sufficiently complete so that it can be used for process simulations but is still under development. Work is under way to replace the human-readable data files the model program uses by binary files that are maintained by menu-driven auxiliary programs; this change will not only simplify development and maintenance of a facility description but will reduce the time

required for input of facility data when the program executes. A more flexible method of handling conflicting requests for process personnel will soon be incorporated into the program. In addition, we are still experimenting with the content of the output reports generated at the conclusion of a simulation, and continually discover the need for additional items of information not previously calculated and/or reported by the program. When the definitions of the printed reports have stabilized somewhat, we plan to develop graphical presentations for those items of simulation information that can benefit by such display.

We also plan to extend the scope of the model to include material measurement simulations. The model can then be applied to material control and accounting studies and in particular can be used to determine approximate values for inventory difference variances for process operations that are not in a steady state. Determination of non-steady-state material measurement variances by means other than simulation is often extremely difficult.

Finally, we note that, though the model has been developed specifically for the Los Alamos Plutonium Facility, its design probably will permit it to be adapted with relative ease for use at other nuclear material processing facilities that operate in batch mode. In fact, alterations to the program itself will be needed only when the new facility to be modeled contains generic features not present at the Los Alamos Plutonium Facility, and the number of such features can be expected to be small. Most of the adaptation will only require the construction of an appropriate set of data files for the new facility.

REFERENCES

1. W. S. Moser and J. D. Navratil, "Review of Major Plutonium Pyrochemical Technology," *J. Less. Com. Met.* 100, 171-187 (1984).
2. J. D. Navratil, "Plutonium and Americium Processing Chemistry and Technology," *Inorg. Chem. Acta* 94, 263-269 (1984).
3. L. J. Mullins and J. A. Leary, "Fused-Salt Electrorefining of Molten Plutonium and its Alloys by the LAMEX Process," *Ind. Eng. Chem. Process Design Develop.* 4, 394-400 (1965).
4. L. J. Mullins, D. C. Christensen, and B. R. Babcock, "Fused Salt Processing of Impure Plutonium Dioxide to High-Purity Plutonium Metal," Los Alamos National Laboratory report LA-9154-MS (1982).
5. L. J. Mullins, A. N. Morgan, S. A. Appar III, and D. C. Christensen, "Six-Kilogram Scale Electrorefining of Plutonium Metal," Los Alamos National Laboratory report LA-9469-MS (1982).
6. K. W. Fife, D. F. Bowersox, and E. D. McCormick, "Comparison of Phosgene, Chlorine, and Hydrogen Chloride as Reagents for Converting Molten $\text{CaO}\cdot\text{CaCl}_2$ to CaCl_2 ," Los Alamos National Laboratory report LA-10523-MS (1985).
7. D. C. Christensen and L. J. Mullins, "Salt Stripping, A Pyrochemical Approach to the Recovery of Plutonium Electrorefining Salt Residues," Los Alamos National Laboratory report LA-9464-MS (1982).
8. J. A. McNeese, D. F. Bowersox, and D. C. Christensen, "Recovery of Plutonium by Pyrore-dox Processing," Los Alamos National Laboratory report LA-10457 (1985).