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MODELING OF BATCH OPERATIONS IN THE DEFENSE WASTE PROCESSING FACILITY AT THE SAVANNAH RIVER SITE (U)

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ABSTRACT

A computer model is in development to provide a dynamic simulation of batch operations within the Defense Waste Processing Facility (DWPF) at the Savannah River Site (SRS). The DWPF will chemically treat high level waste materials from the site tank farm and vitrify the resulting slurry into a borosilicate glass for permanent disposal. The DWPF consists of three major processing areas: Salt Processing Cell (SPC), Chemical Processing Cell (CPC) and the Melt Cell. Separate models have been developed for each of these process units using the SPEEDUP™ software from Aspen Technology. Except for glass production in the Melt Cell, all of the chemical operations within DWPF are batch processes. Since the SPEEDUP software is designed for dynamic modeling of continuous processes, considerable effort was required to devise batch process algorithms. This effort was successful and the models are able to simulate batch operations and the dynamic behavior of the process. In this paper, we will describe the SPC model in some detail and present preliminary results from a few simulation studies.

INTRODUCTION

Approximately 300 million liters of high level radioactive waste is stored in the SRS tank farm. This waste exists as sludge, salt cake and supernate within the tanks. The site is actively engaged in the process of removing waste from storage and treating it for final disposal. To accomplish this mission, processing in the tank farm is first done to the salt and sludge. Salt cake is redissolved and soluble radionuclides, such as Cs and Sr, are precipitated. Sludge is also pretreated by dissolving aluminum and washing out the soluble components to reduce the volume of glass produced. Concentrated precipitate and sludge are sent to the DWPF for further treatment and vitrification. Tests in DWPF using simulated wastes are currently in progress with radioactive operations scheduled to begin in late 1995.

An integrated flowsheet model of SRS waste processing operations has existed for several years (Choi *et al.* 1991). This model was developed using the du Pont Company's proprietary process simulation software CPES (Chemical Process Evaluation System). The model has over 1,700 process streams and 650 unit operations and tracks 183 chemical species. The model includes detailed waste processing chemistry and performs vapor-liquid equilibrium calculations. This model has been used to plan waste removal operations and allow permitting of plant operations. However, the simulation treats the processes as continuous steady-state operations and provides no information on system dynamic behavior or batch cycle operation.

Recently a model of waste tank farm operations at SRS that considers batch processes has been developed using SPEEDUP (Gregory *et al.* 1994). This model simulates the tank farm and in-tank processes in detail; however, DWPF operations are treated as a simple continuous process to estimate glass product and recycle streams. Only mass balance calculations for liquid and solid phases are performed and, with 27 chemical species, the treatment of reaction chemistry is limited.

To compliment the existing process models, a detailed model of the DWPF operations is under development. This model will perform dynamic material and energy balances around all process vessels, consider both liquid and vapor phases and use detailed chemistry models to simulate process operations. In addition, the model will accurately reflect batch operating sequences in the process. A preliminary version of this model (simplified process chemistry is still used) is now available and will be presented in this paper.

SALT CELL PROCESS SIMULATION

To focus the discussion, this paper is limited to a description of the SPC model, which represents about half of the entire DWPF process. Figure 1 shows process components included in the model. The primary processing vessels in the SPC are a precipitate reactor where hydrolysis reactions are carried out and an organic evaporator where organic materials from the precipitate reactor overheads are collected and concentrated. Both vessels have condenser-decanter units (PRCD and OECD, respectively) to separate the aqueous and organic phases boiled off during steam stripping. Vapors from the condenser-decanter units pass through a secondary condenser (SCVC) prior to venting. The SPC has several other tanks associated with the process that feed raw materials and collect products. In all, the SPC model simulates batch operations through 9 tanks and the condenser systems. The model has 16 chemical species, and treats the vapor phase and aqueous and organic liquid phases. Figure 1 also shows all control valves included in the model. When a schematic flow meter is attached to a valve, the user specifies the volume of material that will flow when the valve is opened; else, valve actuation is controlled by conditions in the sending and receiving tanks.

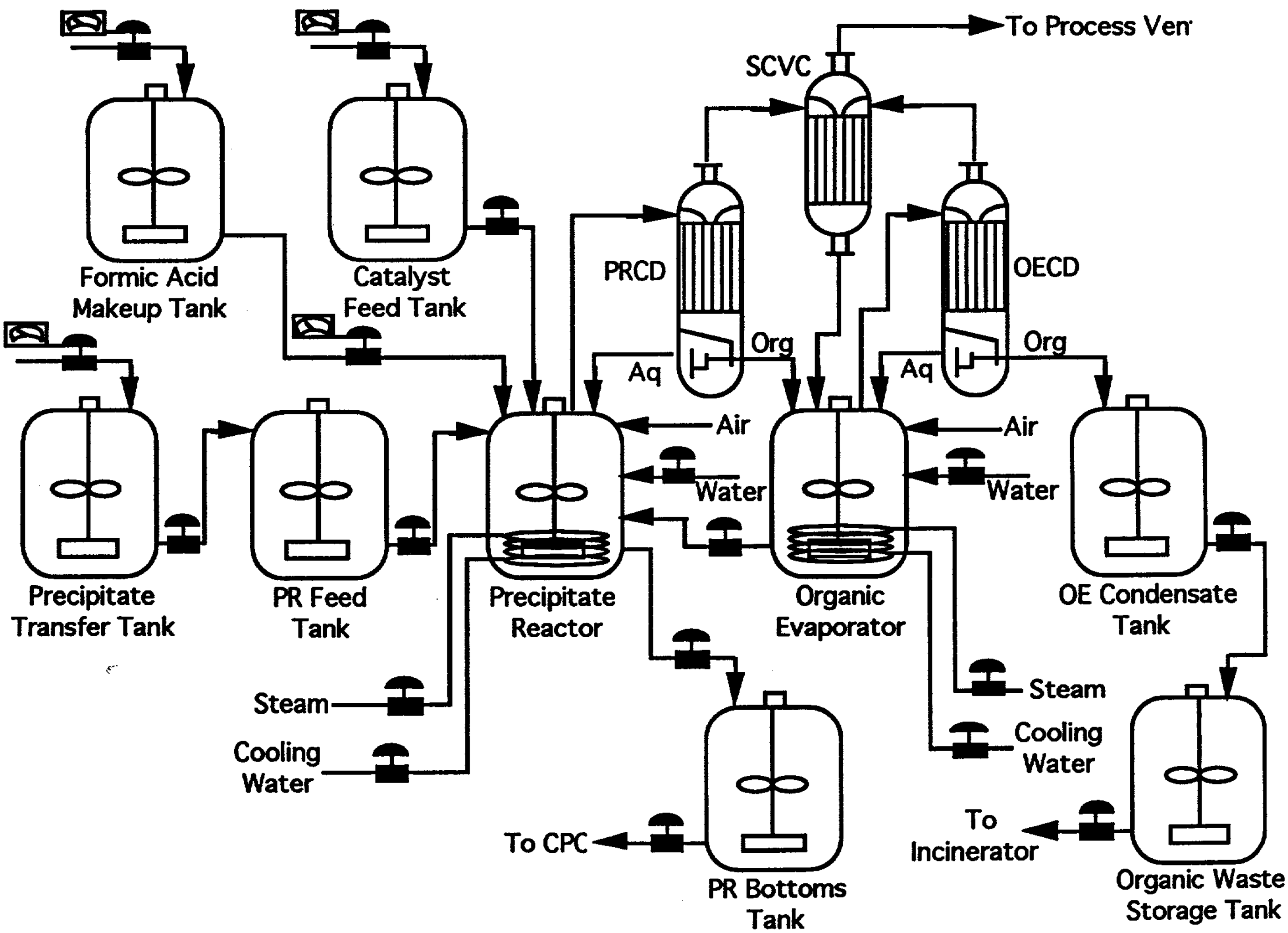

Figure 1. Schematic diagram of DWPF Salt Processing Cell showing model features.

To start an SPC run, precipitate feed from in-tank salt processing is charged into the Precipitate Transfer Tank and from there into the PR Feed Tank. Copper catalyst solution and formic acid are made up in their respective feed tanks. The SPC process then consists of a Precipitate Reactor (PR) cycle followed by an Organic Evaporator (OE) cycle. PR cycle steps are:

1. If a previous SPC batch has been completed, the OE heel is transferred into the PR.
2. A predetermined volume of 40% formic acid is added to the PR.
3. The contents of the catalyst feed tank are transferred into the PR.
4. The PR is heated to 55° C using steam.
5. Precipitate slurry is added to the PR while maintaining a 55° C vessel temperature.
6. If the volume of the PR batch is below the level of the heating coils, water is added to cover the coils.
7. The PR is heated to boiling where hydrolysis reactions release benzene from tetraphenyl borate ions in the salt solution by:

   $$\phi(C_6H_5)_4B + HCOOH + 3H_2O \rightarrow \phi COOH + B(OH)_3 + 4C_6H_6$$

   where ϕ = Cs, K, Na or NH_4
8. When the benzene concentration falls below the desired limit or if the heating coils become uncovered, the PR is cooled down to 50° C and the contents transferred into the PRBT.

Model simulation of the PR cycle is shown in Fig. 2 where the reactor liquid volume and solution temperature are plotted as functions of time.

As the PR is boiled, vapors are condensed and the organic and aqueous phases separated in the PRCD. Once the decanter fills, organic overflow is sent to the OE. After completion of the PR cycle, material collected in the OE is concentrated by boiling. Concentrated organic from the OE boilup is condensed and separated in the OECD and collected in the OE Condensate Tank. The aqueous phase is recycled back to the OE. Boiling is stopped if the tank level falls below the top of the heating coils or if the benzene concentration falls below a preset limit. When the condensate tank is full, its contents are transferred to the Organic Waste Storage Tank. At the end of the OE boilup, the heel is transferred into the PR. Model simulation of the OE cycle is shown in Fig. 3 where the volume of liquid in the evaporator and the solution temperature are plotted.

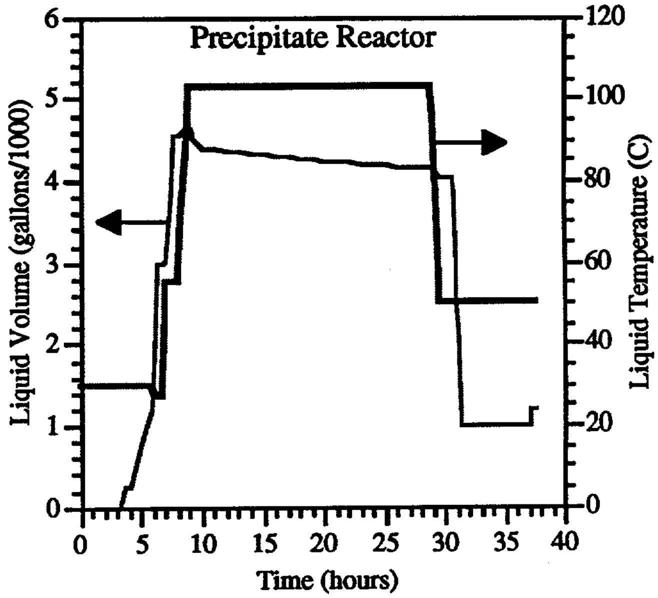

Figure 2. Simulation of PR cycle.

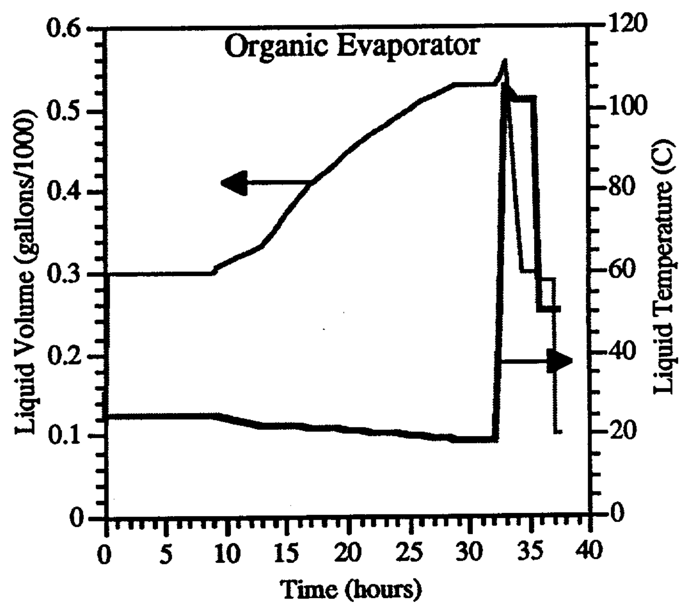

Figure 3. Simulation of OE cycle.

The process model predicts chemical compositions in the vessels and in the vent system and calculates pressures and temperatures throughout the process. Figure 4 shows pressure profiles in the PR and OE through the process cycle. As expected, during boiling, the vessel pressure increases and there is some interaction between the vessels since the vapor spaces are connected through the vent system. The results shown in Fig. 4 use a simple model of the vent system assuming constant loss coefficients for the vapor flow. These results have not been tuned to match real process operations which actually maintain a slight vacuum in these tanks.

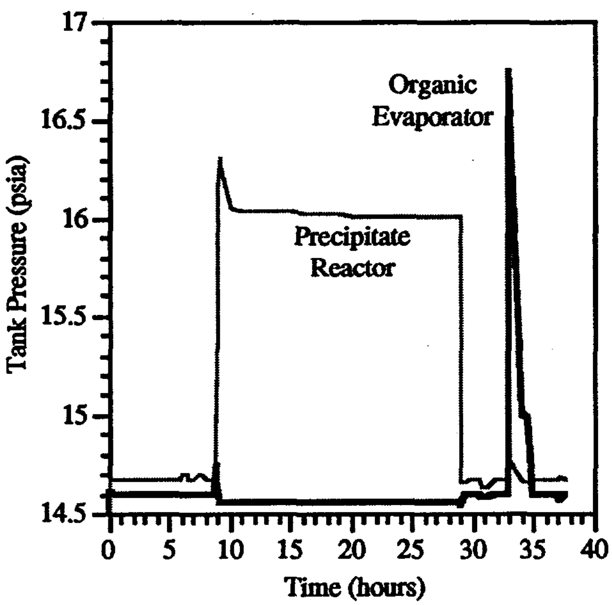

Figure 4. Vessel pressures.

BATCH PROCESS MODELING IN SPEEDUP

The SPEEDUP software is a convenient vehicle for the development of dynamic process simulations. The user need only write the appropriate material balance equations to construct models of unit operations and then connect the units in a process flowsheet. However, for batch processes, control logic to sequence batching operations must be supplied by the user. Since SPEEDUP is designed to solve the flowsheet as a continuous process, supplying functional batch control logic is a significant task.

Several approaches are available to solve this problem. The modeler can use the External Data Interface (EDI) in SPEEDUP to access coding outside of the flowsheet solution to effect batch control. A SPEEDUP simulation using the EDI approach has previously been presented by an SRS group at this conference (Gregory *et al.* 1994). The EDI approach suffers from the drawback that the external coding can only be called at predetermined times in the simulation. If the timing of the batch steps is known before hand this presents no problem. However, in general, we will not know in advance the time when a batch step will be initiated or the step duration. This requires iteration between the SPEEDUP solver and external code to locate points where conditions change and accepting some error in the control logic. The external coding can also become quite complicated in attempting to model batch control.

To develop the DWPF model, we have taken the approach of incorporating batch control directly into the SPEEDUP simulation coupled with simple FORTRAN procedures. Using procedures linked directly to the simulation solution allows us to program conditional tests that sequence batch operations based on process conditions. We use the converged SPEEDUP solution to signal when to start and stop batch steps. This approach greatly simplifies the required control logic. One disadvantage of the procedure based approach is that procedures are called and must be converged at each time step in the solution along with the other model equations.

We find that a convenient batch control strategy is to use simple time delays to separate process steps. In SPEEDUP notation, the appropriate model equations are

```
$Elapsed_Time =
        Input_Signal * (1 - Output_Signal)
        - Reset_Signal * Tau * Elapsed_Time;

If Elapsed_Time > Delay_Time Then
        Output_Signal = 1
Else
        Output_Signal = 0
Endif;
```

where the $ prefix indicates a time derivative. We initialize the model with all control signals set to zero. Setting the Input_Signal of a time delay model equal to one then starts integration of the Elapsed_Time variable. When the value of Elapsed_Time reaches the specified Delay_Time, integration stops as the Output_Signal is set to one. Setting the Reset_Signal to one will drive the Elapsed_Time variable to zero at a rate governed by the constant Tau. The Output_Signal is used to start the next batch step or control other process operations. For example, after catalyst is added to the PR, the Input_Signal to the associated time delay is changed from zero to one. When the Delay_Time is reached, steam flow to the PR cooling coils is enabled by the Output_Signal.

Using output from time delays to indicate that batch steps have been completed has several advantages. The time delay Output_Signal remains at a value of one until it is reset for the next batch. This allows us to, for example, refill the catalyst tank in preparation for the next batch while the PR is in operation. The flowsheet would naturally interpret a filled catalyst tank as ready to feed the PR and restart catalyst transfer as soon as the tank is ready. We use the time delay output signal to prevent this from occurring until the batch in progress is completed. Time delays also represent actual process operations. After materials are batched to a vessel, there is usually a time delay to allow mixing or to prepare for the next process step. The user can specify time delays of any duration to match actual operating procedures.

Figure 5 illustrates an application of this batch control scheme in the SPC model. At the start of the simulation, 3500 gal of solution is added to the Precipitate Transfer Tank (PTT) at a rate of 75 gpm. After mixing for 0.5 hour, precipitate is transferred into the PR Feed Tank (PRFT) leaving a 1000 gal heel in the PTT. Refilling of the tank to its 3500 gal capacity is immediately started. The PRFT is mixed and waits until the PR is ready to accept a transfer. After 1500 gal is transferred into the PR (leaving a 1000 gal heel) the PRFT is refilled to maximum capacity (3500 gal) from the PTT. The PTT is then also refilled and both tanks wait for completion of the SPC cycle before further transfers are made. Control of these batch steps is accomplished by using one delay timer in the PTT

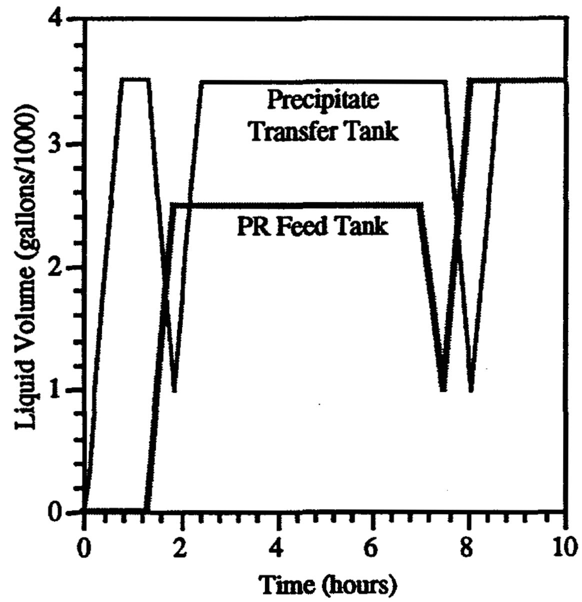

Figure 5. Batch operation of feed tanks.

while the PRFT requires two timers and a counter to indicate the local batch number.

A related problem is that of sensing the completion of batch cycles for individual vessels so that time delays can be reset and the next cycle initiated. A simple method to track batch cycles is best explained through an example. Each vessel has associated with it the number of the batch that is currently being processed. To decide if the PRFT should receive feed from the PTT we compute

Feed_Added = 1 - Feed_Signal
= Feed_Batch - Batch_No;

where Feed_Batch is the batch number in the feed tank and Batch_No is the batch number in the receiving vessel. Initially all vessels are processing batch number 1. When the PTT batch number is incremented to 2 (Feed_Batch = 2) the above calculation in the PRFT (Batch_No = 1) signals that feed has been added (Feed_Added = 1) and sets the feed control signal off (Feed_Signal = 0). When the PRFT completes batch 1 and increments its batch counter to 2, the feed signals are reversed and the PTT can again send material to the PRFT when it has progressed to the next batch. The above algorithm can be modified to allow more than one feed batch to be added before the receiving tank completes a batch.

The final problem that must be addressed is incrementing batch counters for each vessel. Because of the continuous nature of the SPEEDUP solution no simple method to implement this directly within SPEEDUP was found. Placing an equation of the form

$$n = n + 1$$

directly inside SPEEDUP would increment n at every time step. Actually, this exact equation would be indeterminate in SPEEDUP; but, for illustration purposes, we use this example. Placing an IF test around the equation does not solve the problem since, once the IF test branches to the equation, n will again be incremented at every time step until the other branch of the IF test is satisfied. We need a scheme that will increment a number only one time when signalled to do so. With our models, this task is performed in a FORTRAN procedure (equivalent to a subroutine) where it is easier to program the required logic. Basically, the successful scheme uses an IF test and a logical variable to decide if the batch number should be incremented. A signal that the batch is completed, often obtained from a time delay model, increments the batch number and sets the logical variable to true. As long as the signal does not change the batch number is not incremented. When the signal is turned off, the logical variable is reset but the batch number is not incremented until the signal is turned on again. This easily programmed method allows step changes at the correct time in all vessel batch numbers.

CONCLUSIONS

A set of 733 algebraic and differential equations describing mass and energy balances are solved using the SPEEDUP software to simulate operation of the DWPF Salt Cell process. Simulation of one batch cycle through the entire SPC process requires approximately 15 min of CPU time on a VAX 8550 (with some screen printing enabled). This represents several days of process operating time. The model can easily be ported to faster computers (IBM RISC/6000 or CRAY) to significantly improve simulation timings. Future improvements to the model will involve extending the number of chemical species treated and including more details of the process chemistry. For development purposes, the model currently uses a set of simplified physical property subroutines that assume ideal solutions. These will eventually be replaced with Aspen Properties Plus routines that model aqueous electrolyte solutions.

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BIOGRAPHY

Dr. Smith earned a Bachelor of Science degree from the University of Louisville, a Masters degree from the California Institute of Technology and an Sc.D. from the Massachusetts Institute of Technology all in the field of chemical engineering. Dr. Smith has worked at the Savannah River Site since 1981 and is currently a Principal Engineer in the Savannah River Technology Center.