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PROCESS SIMULATION: SUCCESSES AND FAILURES

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ABSTRACT

This paper discusses the application of discrete simulation to batch processes in the chemical industry. The advantages and difficulties of batch processes are presented and related to some of the barriers in the application of discrete simulation in the chemical industry. Examples from the literature are cited and four actual industrial simulations are described and their impact evaluated.

1 BACKGROUND

Most chemical manufacturing processes consists of a raw material supply system, various reaction and separation steps, and final product handling. They differ from other manufacturing processes in that the materials being handled are "bulk" materials as opposed to discrete items. A specific "pound" cannot be identified as it goes through the process without special effort to keep it segregated. Storage of most materials must be in relatively expensive tanks. Even a discrete item such as a bag or batch of material loses its identity when put in a tank with other material. The resources of concern are generally: equipment, heating utilities, cooling utilities and operators. Processes are categorized as continuous, batch or batch semi-continuous (BSC).

Continuous processes are very efficient and economical for high volume products. In highly competitive markets where margins may only be a few cents per pound, they are a virtual necessity. The widespread use of batch processes for high value added, specialty process results from several inherent advantages which include:

1. They are relatively easy to design, even if the knowledge of the process is limited.
2. If the basic process is sound, the plant can usually be made to work, even if some errors were made in the design.
3. Multiple operations in one piece of equipment and ease of shutdown and startup make operation at low volumes practical and economical.
4. The manufacture of more than one product in a single facility is often possible even if the processes are somewhat different.

On the other hand, there are more than a few significant problems associated with batch processing. Some of them are obvious, some not quite so obvious. Anyone who has worked with a batch process for very long could probably add to the following list:

1. They are labor intensive. The use of automated sequencing and material handling can reduce the number of operators needed, but the unsteady state nature of batch processing still requires careful monitoring and manual intervention at times.
2. Different operators have various ways of operating. Operating instructions for the typical batch process which covered every detail would be the size of an encyclopedia. Usually, details which are <u>assumed</u> to be unimportant are left to the discretion of the operator.
3. The amount of data required to define the processing of a specific batch is voluminous: all the same data which would exist on a continuous process multiplied by a time dimension with discontinuities and discrete events thrown in for good measure.
4. Data is recorded at some instant in time. Critical happenings can be missed.
5. If something unusual occurs, the opportunity to observe, sample or get additional data may be gone quickly and may not happen again on the next batch.

6. There is a great deal of random variation in batch processes and the effect tends to be cumulative.
7. Since 2 batches are seldom exactly the same, it can be very difficult to identify the significant deviations.
8. Temperatures, pressures, pH, etc. vary over wide ranges, causing maintenance, corrosion and control problems.
9. It is an accepted fact that problems such as line pluggage, upsets, mistakes and equipment failure tend to occur on startup and shutdown. A batch process is always starting up or shutting down something.
10. Since conditions are always changing, a rapid change in an instrument indication does not call attention to a possible control problem. As a result, confidence in instrumentation may be low.
11. Sequencing and scheduling can affect production, quality and cost. Planning ahead is important.
12. Sequencing problems or wide variation in cycle times may create capacity limitations. The result may seem to appear at another point in the process as an apparent bottleneck.

Discrete simulation has the potential to be a very powerful tool for engineers in the chemical process industry. A good simulation can provide a controlled environment for experimentation which would be impossible to achieve in an operating process. The management of noise and other process conditions make it possible to state with confidence that "All other conditions being the same, the overall effect on the process of reducing the reactor cycle by increasing the excess of monomer is ...." Computer aided design is highly advanced for the steady state, continuous process. However, the majority of chemicals produced in the world on a numerical basis are produced in batch, discrete processes. Reklaitis (1989) presents an excellent summary of the state of the art in computer aided batch process design. Most of the actual design of batch chemical processes is still done using pragmatic approaches. Engineers working on batch processes often feel consigned to simple calculations and educated guesses based on experience.

2 BARRIERS TO SIMULATION

This suggests one reason why simulation of batch processes is not done more frequently. Many "batch process people" are not comfortable with computer aided design and analysis. There is seems to be a feeling that it cannot be that complicated and a good engineer ought to be able to figure it out. Budgets for the operation of batch processes are relatively low due to the lower volume of production and several months of technical effort for a quality simulation can be a significant blip. In spite of the fact that batch processing is widely used in chemical manufacturing, it is often lacks emphasis in the undergraduate Chemical Engineering curriculum, especially low-tech simulation approaches. Several exceptions are Felder (1983) at North Carolina State University and Schultheisz and Sommerfeld (1989) at Georgia Institute of Technology. To quote Richard Bronson (1978), "To fully appreciate the scope and power of simulations, one must become a practitioner."

The other major hurdle to overcome in increasing the application of discrete simulation to batch chemical processing are the gaps in knowledge of exactly how the process is operated. The engineers closest to the operation who might realize just how beneficial a simulation might be are very aware of this. As noted in items 2 and 3 above, a lot of decisions are left to operating personnel. Although there is some latitude in using the simulation for sensitivity analysis to determine how critical consistent operation is in some areas, in every simulation I have been involved in there have been numerous questions about operating procedure which took considerable research (go ask the operators) to get correct answers. We often fail to realize how little we know about a thing until we attempt to simulate it on a computer (Knuth 1973). There may be a tie-in between the computer dis-comfort of "batch process people" and gaps in process knowledge. The use of proprietary Unit Operations and Equipment simulation programs for batch processes is also quite low. Many batch processes involve uncommon materials for which the physical properties and other data required by the Unit Operations and Equipment simulation programs are unavailable in the literature and would require extensive and costly laboratory work to obtain. It probably is not realized by the "non-practitioner" that data for discrete simulation can usually be obtained through records, observation and analysis.

As Frederick Brooks (1987) said in his classic "No Silver Bullet" article, "The complexity of software is an essential property, not an accidental one. In most cases, the elements interact with each other in some nonlinear fashion, and the complexity of the whole increases much more than linearly. [Simplification] does not work when the complexities are of the essence." At times it is difficult to get clients to grasp this. After completion of a successful project, the client often comments that the definition was as useful as the model. It is important to publicize success stories. Unfortunately, it is sometimes hard to get "good press", especially if the answer is not what the client wanted. Sometimes they shoot the messenger. As pointed out by White (1989), close involvement of the client personnel is very important. The more clients understand about discrete simulation, the better. A short tutorial for everyone involved early in the project is very worthwhile. Clear simulation code which can be easily comprehended by the client also helps. For example: a single ADVANCE block may be satisfactory from a simulation standpoint, but breaking it down into a series of steps meaningful to the customer will aid understanding. Entity names using the acronyms and names used by the process engineers and operators makes it simple for them to follow the flow. Production of customized output reports in the clients "language" promotes acceptance of the results. The work involved in defining the system, model and data is significant. "The hard thing about building software," Brooks (1987) claims, "is deciding what one wants to say, not saying it." Describing the work involved in a model before the client is sold on the benefits may kill the project. All of this can be summarized as the need for user "buy-in" at a very early stage.

3 SOME TECHNIQUES FOR GPSS

Many batch processes will have one or more continuous units making it a batch semi-continuous (BSC) process. These can usually be simulated with sufficient accuracy by creating "mini-batches" with a processing time of 5 minutes to an hour. Since discrete simulations of batch processes will deal with a batch, and then pounds and then batches again, it is easy to end up with a lot of active transactions. At best, this will make the model costly and/or slow to run and may cause the model to run out of common and crash. Terminate unneeded transactions or put them on user chains. Use the Number of Units parameter on the ENTER block where possible to fill storages with pounds from a single batch. SPLIT blocks can create "mini-batches" or pounds where required.

Many batch process simulations are self starting. Batches in the first unit are started as soon as the unit is available by using a GENERATE block with no mean time or spread modifier. Just make sure the next block will refuse entry. There is not much point to trying to fit a distribution to batch cycle data. For an existing process, tabulate cycles off batch sheets and set up a function card for an empirical distribution. For a new process, triangular or Beta distributions as suggested by Taha and Stephen (1984) using the PERT approach of a weighted average of optimistic, pessimistic and expected values gives good results; see p. 230 of Hiller and Lieberman (1967). Downtime is an important consideration in many simulations since one of the purposes of intermediate storage tanks is to prevent disruption of the process flow when downtime occurs. Downtime records are often kept with regard to total number of hours/month and number of occurrences due to a particular cause. In other words, only the mean duration and mean interarrival time are known. The exponential distribution wins by default since only the mean is needed to characterize the distribution.

If operators are included in the model, a utilization of 25% is about right. That is the wisdom of a number of manufacturing managers. Animation of simulations is possible using products such as PROOF from Wolverine Software, but for process simulation, is more interesting than informative. Graphical history plots can be very useful. Importing output results into spreadsheets for graphics or using SASGRAPH works well.

4 SOME SUCCESSES AND FAILURES

There have been some examples of process discrete simulation reported in the literature. A GPSS simulation of a beet sugar refinery was described by Stephenson, Dewsnup and Templeton (1978). An Exxon Chemical Company plant in Linden, New Jersey was simulated with GASP IV by Miner and Wortman (1980). A simulation of specialty chemical operations using GASP IV was reported by Felder (1983) and Felder, McLeon and Moldin (1985). Tomato processing was simulated with SLAM by Starbird and Ghiassi (1986). A simulation of a large-scale, multiproduct batch processing system using SIMSCRIPT II.5 was reported by White (1987). Kenvin and Sommerfeld (1987) described the simulation of Poliomyelitis Vaccine production with GPSS. Terry et al. (1989) simulated a multiproduct batch plant using BATCHES, a simulator specifically for chemical processes. DDT manufacture was simulated by Blaylock, Morgan and Sommerfeld (1986) using GPSS. Batch wastewater treatment was simulated with GPSS by Glenn, Norris and Sommerfeld (1990).

This paper will present overviews of 4 actual simulations, all using GPSS. From a technical standpoint, they were all successes, accurately depicting the operation of the chemical process. The actual impact on the operation differed significantly.

4.1 Raw Material Supply

The major raw material is supplied to a large, continuous manufacturing unit by barge. Tank cars of raw material are also kept on hand, but facilities for unloading limit the rate of use. Storage requires costly pressurized tanks. A limited amount of storage is currently available. A project to expand production was being considered. The barges are subject to weather and traffic related delays but raw material outages are currently infrequent. The process downtime is of frequency and length to cause barge unloading delays. The objective of the simulation was to determine if the existing storage facilities were adequate at increased production rates.

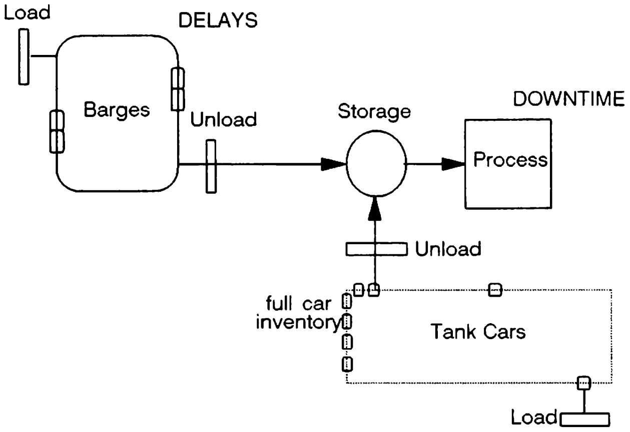

Figure 1: Raw Material Supply

A prototype model was quickly developed after a visit to the plant site to develop the model logic and review the required data. Data was available on barge round trip times, production rates and production downtime. There were 5 sections to the model: barge movement, barge unloading, tank car unloading, production operation and production downtime. Review of the prototype led to much more complex barge delay and barge unloading sections. There were 2 barges per tow. If the second barge could not be unloaded within a specified time frame, it would be left and the tug would make a trip with one barge. This required some "look ahead" to determine if the barge probably would be unloaded in the specified time frame. The barge delays were changed to make the model more realistic. Tank car unloading also required a certain amount of "look ahead". Based on the projected barge arrival time and estimated raw material usage, tank car unloading had to be started before inventory was too low since the unloading of tank cars could not keep up with production.

The simulation results indicated that the existing storage would not be adequate and that adding tank cars to the fleet would not be of significant help. Even adding additional storage was only marginally effective and would result in unloading many more tank cars. Tank car shipment was both more expensive and hazardous. Additional runs revealed that adding additional barges to eliminate one barge trips would be both more economical and effective. These were not the answers the clients wanted to hear. Eliminating one barge trips would require changes in the way things were currently done and taking a hard look at some operational and safety questions.

4.2 Compounding

A plastic extrusion operation requires preparation of containers of custom blends of materials for the extruder feeders. Orders are received from customers and entered into the system requiring a specified recipe of bulk materials and small additives. Steps in the process are: bulk addition from bags and hoppers, weighing small adds from small containers, blending, sampling and analysis, extrusion, and container washing and drying. A new system was being designed using an AGV to move the containers from step to step. Multiple recipes are being extruded at one time on different feeders. All containers for a given order may not be complete when the run is started. Containers for future runs are usually in preparation. Containers may require rework if they fail analysis. Not all containers are analyzed. To minimize load on the waste treatment from washing, the number of containers used for a run is limited (containers reused for the same recipe do not have to be washed). The original objective for the simulation was to determine if one AGV would be sufficient.

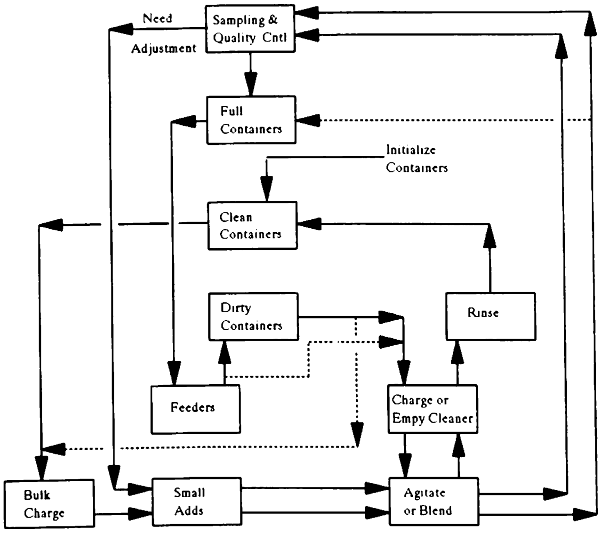

Figure 2: Compounding Flow

A short Fortran program was written to generate a random file of orders for a 3 month period based on a statistical analysis of order history. It contained the order time, number of containers required, the amount of bulk addition, the number of small adds and production rate for each order. This was a JOBTAPE file to generate transactions representing the orders. The simulation was complex from the standpoint of synchronizing the container preparation, feeders and production operation making use of MATCH blocks in several places. A Fortran HELP block was used to do the bookkeeping on clean, dirty, full and MT container inventory. Rules for analysis, rework, run sequencing, and off specification material all added to the complexity of the model.

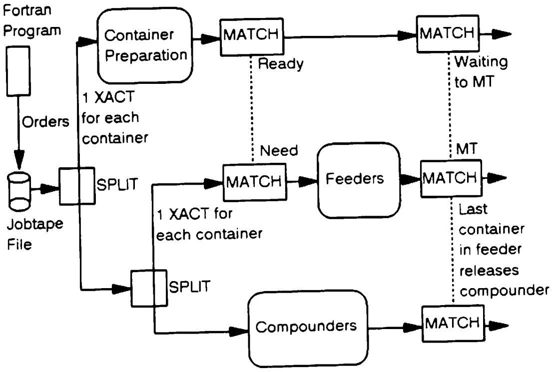

Figure 3: Compounding Simulation

It was obvious after a few runs that one AGV was more than adequate. With the initial set of rules for operating the system, the system was capable of gridlock. These situations were analyzed and appropriate rules for prevention developed. This was very helpful in the design of the system. Throughput through the system was lower than expected and various modifications were investigated to improve throughput, successfully bringing it up to the project basis. There were requests for changes in the method of operation from the manufacturing as the design progressed. These were evaluated with the model to predict the impact on throughput. Due to the limited original objective, there was a lot of growth to the model. This resulted in poor organization and clarity.

There was always a validity question with the model. Since it was for a new system, there was nothing with which to compare the results. The model was so complex that only the developer understood it completely and it was difficult to grasp the operation of the model as a whole. When something went wrong, it took careful study to determine if it was a bug or really the way the system would work. This left the design people with a very uncomfortable feeling. But they quickly realized that they had nothing better on which to depend. This was particularly difficult when some of the results were counter-intuitive. For example, it was difficult to convince the design engineers that they could have too many containers in the system. The model was useful, perhaps essential in the design work, but nobody was very satisfied with it.

4.3 Intermediate Storage I

The objective of this model was to investigate the impact of maximum inventory level of a hazardous intermediate on the production rate of the using operations. The material is produced as a byproduct of a continuous unit. All of the using operations are batch. If the storage is full or at the maximum level, the excess material is burned for the fuel value. The continuous unit has essentially 100% on-stream-time except for scheduled turnarounds. The using units have approximately 10% random downtime. Good data was available on downtime, rates and raw material usage. The model was straightforward GPSS. The continuous unit was approximated with 15 minute "mini-batches".

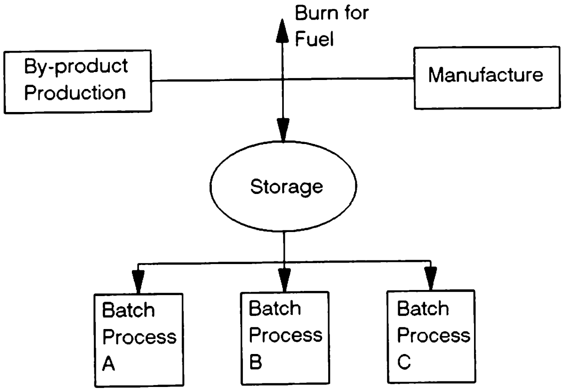

Figure 4: Intermediate Production and Use

SAS was used to produce plots of storage level vs. time with various limits on maximum level. The output included a custom report with statistics on the percent of the intermediate produced which was burned and percent downtime due to raw material shortage. Priorities were used to allocate raw material between using departments. Schedules could be set for the using departments at less than capacity. Acceptance of the model was good. Understanding of the model by everyone involved was also good. The actual percent burned was not measured but the model reported about what conventional wisdom said it was. The model indicated that a substantial reduction in maximum inventory was possible without impacting production. Reduction of the inventory to near zero levels as some people wanted would have been a disaster.

The model went through a number of revisions over a period of several years as different proposals were made to increase the amount of intermediate available. One proposal for additional direct manufacture of the material was incorporated in the model and it was obvious that turndown capability of the new facility was critical. After details of the turndown were available, the model was revised to check the adequacy of the minimum rate and the speed with which the rate could be changed. The model has proven to be very useful in the management of this facility.

4.4 Intermediate Storage II

This model was similar in many respects to the previously described model. The objective was similar, to investigate the effect of maximum storage level on production rates.

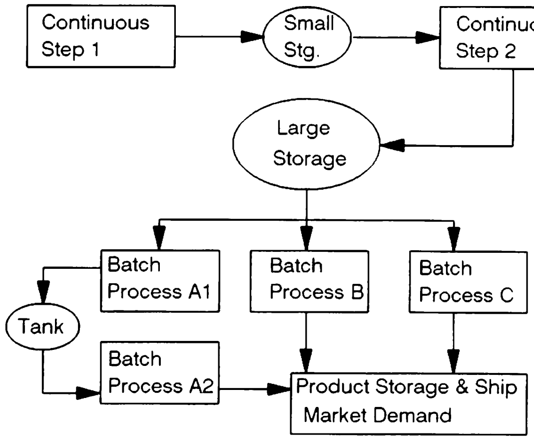

Figure 5: Intermediate II Flow Sheet

The intermediate in this case was not a byproduct. This simulation had much more detailed models of both the supply and using processes. Much of the required data was unavailable and had to be estimated. Some of the procedures for controlling the supply department were not documented and were developed for the model. Although there was general agreement that the logic of the model was a reasonable representation of the real world, the level of confidence in the results was reduced by the relatively poor data. But it was realized that based on the available data, it was the best prediction of expected impact on production of various inventory levels. The model indicated that maximum inventory levels could be substantially reduced without significant impact on production. Actions were taken to reduce the maximum level of inventory based on the simulation predictions.

5 CONCLUSIONS

Discrete simulation can be a very useful tool in overcoming some of the problems associated with the design and operation of batch chemical processes. The available tools are quite adequate to provide an accurate representation of complex processes. Barriers to the wider application of discrete simulation to chemical processes include the lack of knowledge on the part of Chemical Engineers about discrete simulation and the potential benefits and gaps in the knowledge about the process operation. The success and acceptance of simulation projects is related to the involvement of the process engineers and ability to document the key aspects of the process operation.

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