Monte Carlo Simulation to Propose Improvements of an Alkyd Resin Process

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Abstract: - This paper reports findings of a study of a batch chemical process using simulation. A model of an alkyd resin plant is presented and used to carry out improvement studies, to evaluate changes in plant operating conditions. With the proposed changes, in the simulation studies, productivity could be improved to around ten percent.

Key-Words: - Monte Carlo simulation, alkyd process modeling, probabilistic models, activities duration, simulation improvements.

1 Introduction

Computer simulation has been widely used in a variety of applications since the early days of computer development. With the rapid growing of power and speed of hardware and software technologies, simulation is used as a standard tool to evaluate and design equipment and processes in the chemical and petroleum industries. Modeling and simulation is employed to study the sensitivity of a system to variations in the input variables and parameters, to observe and reduce bottlenecks and delays that limits productivity, to solve problems which are not amenable to analytical solutions and, in the academia as a powerful tool for teaching [1].

Modeling and simulation are complementary activities. Simulation involves the development of a model of a real or proposed system, and the experimental manipulation of it; while a model is a logical or mathematical description of how a system, process or component behaves [2]. Computer simulation refers to experiments using numerical, logical or procedural models in a computer. So the behavior of the system under specific consideration may be studied. In these way models are used to represent, explain, predict, or estimate the behavior of a system.

Running a simulation differs from running a conventional experiment, in that simulation requires a model of the system to work with, rather than the actual system. The main reason for using simulation is that it provides a suitable framework to imitate the behavior of the actual system, using software, without the time, expense, or risks involved in experimenting with the actual system [3].

Computer simulation can be classified as discrete-event simulation or as continuous simulation. In discrete-event simulation the system (or more precisely the simulation model) changes its state only at discrete moments of time. Queuing problems (like the waiting-in-line for service in front of a teller window in a bank), are emulated as discrete-event simulation [3]. Whereas in continuous, simulation the system changes its state continuously with time. An example of continuous simulation would be a model of the heart and blood circulation system. This paper describes a batch chemical process and how discrete event simulation is used to improve it.

In order to arrive to a representation of a system by a simulation model, the system itself has to be defined. The system is viewed as a collection of related entities or elements. Associated with each entity there is a set of attributes or variables that characterize their operations. These operations or activities interact with each other according with the functional relationships between them [4].

The system state is the collection of attributes or state variables that represents the entities of the system. The events are instantaneous changes, something that happen and changes the entities states, for example, start of machine loading, end of machine loading, etc. Thus an event marks the initiation or termination of an activity. The occurrence of an event affects the state of one or more entities and alters the state of the whole system, which is reflected by the changes in the attribute's values of the system's entities. Furthermore, a particular sequence of activities defines a process, being possible to have several processes in parallel, series, series-parallel or in feedback connection in a given system. Entities, attributes, events activities and the interrelationships between these components are defined in the model of the system.

In a batch chemical process an event could be the reaction termination and batch discharge to a separation unit. In this case the reactor and the separation unit (two different entities), are affected. The attributes of each entity might be the reaction and discharge times for the reactor and the separation time for the separator. The reaction itself is an activity that has some duration. The duration can be a constant, a random value from a probabilistic distribution, or the result of an equation. A simulation that uses models with random variables is known as stochastic or probabilistic simulation.

Problems in batch processing are due to the uncertainty of occurrence of an event. Since the probabilistic nature of each activity, it is common to find delays and bottlenecks. For example, after a batch reaction terminates, and it is ready to discharge, if the separation unit is not available, a delay occurs. Due to this delay of an unavailable down stream facility, the overall process productivity is affected [5, 7-8]. In a batch manufacturing process if the average batch time is reduced, the annual plant throughput increases.

Unpredicted variations, like the one just described, convey to significant variation in productivity from one batch to another. Simulation can provide valuable insights into the complexities inherent in batch processing. One of the main purposes to use simulation is to identify the critical activities, those that can cause considerable delays or bottlenecks, and test possible modifications to cancel out its effect and to increase the productivity and/or to improve the use of resources (e.g. labor, utilities and raw materials), while reducing the operating cost.

A batch process may be viewed as a queue network, the output of one unit operation as one queue, comprising the input to another. Queues are characterized by an arrival pattern, a service mechanism, and a queue discipline; analogically, process units are characterized by the preparation, operation, discharge, and cleaning activities. Each modeled by a probabilistic distribution. A procedure called the Monte Carlo method makes use of sampling from probabilistic models to perform discrete-event simulations.

2 The Simulation Process

A simulation can be written in any computer language like FORTRAN or Visual Basic. There are several specialized languages, like GASP, Simscript III, and GPSS [6]. In fact the study presented in this paper was made using FORTRAN.

The simulation algorithm follows a cycle of steps until a number of batches had been run. After defining the initial conditions and parameters to control de simulation, the repeated part of the algorithm follows the scheme given by [5], and is based on the particular values of the attributes which reflects the state of the system, called the system image. Depending upon the system image, the algorithm determines the events that might take place next and test if they can be executed. By executing those activities that has no restriction for any event to occur, the simulation clock advances in discrete steps, (typically of unequal size) and the system image is updated.

Executing and activity is actually a statistically sampling with a model. Sampling takes place by the Monte Carlo method and the use of random numbers.

3 The Alkyd Resin Process

Alkyd resins are used for the preparation of varnishes and lithographic printing ink. The manufacturing of alkyd resins is essentially an estherification process. The main ingredients of the alkyd resin are pine tar, anhydride maleic and pentaerythritol. Reactions are carried out at elevated temperature in a single reaction kettle. A batch begins by charging the pine tar in the kettle reactor. Batch preparation and melting of the pine tar requires about four hours. Then a stream of inner gas is bubbled through a perforated ring below the surface of the liquid mix. The prime reason for an inert gas addition (usually nitrogen or carbon dioxide), is to prevent side reactions resulting from oxygen contamination. Then the gas content in the reactor is removed by a vacuum pump.

After an inert atmosphere is obtained, the maleic anhydride is added for the estherification preparation. A maleic anhydride adduct of the polyunsaturated carboxylic acids, which composes about 95 per cent of the rosin material, is obtained.

Then the reactor content is agitated thoroughly for about 60 min. After homogenization is complete, pentaerythritol is added in three steps while determining the reaction progress by testing the acid number of the mixture. Resins compositions having acid numbers greater than 35 are not accepted. In order to carry out the estherification reaction, the temperature is elevated to 270 ºC and held at that value for one hour to obtain a homogeneous mix.

Again vacuum is made inside the kettle, to produce the alkyd resin. To guarantee the product quality, samples are taken for laboratory verification until final specification is obtained. Finally the mixture is cooled down and the product is discharged. The processing of a batch is completed in approximately 18 h. A schematic diagram of the sequence of activities is shown in Fig. 1. The block diagram of Fig. 1, represents the sequence of activities of the process, those activities with random variation in their time duration are linked to a circle by arcs, pointing out the possible state of random waiting.

operating time for some activities were considered fixed.

The cumulative frequency distributions of some of the activities are shown in Table 2, integer values of time are used for simplicity. The frequency distributions of activities A, F, I, and L do not follow any of the known probabilistic distributions; the cumulative distributions were used to model each activity.

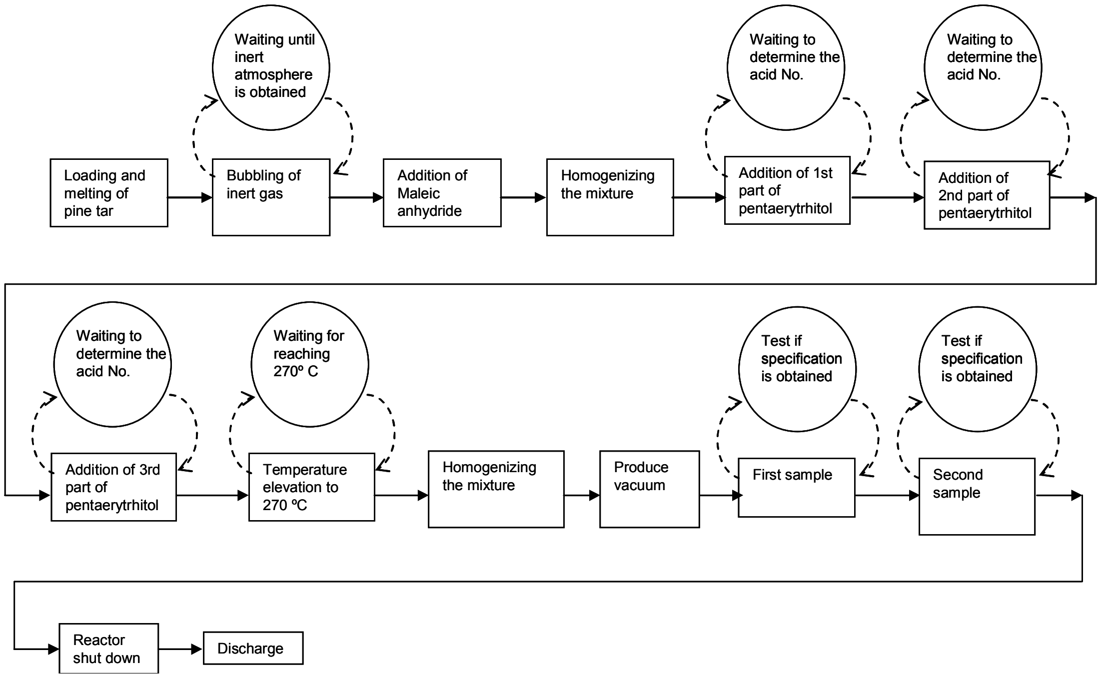

Figure 1. Schematic sequence of activities for the resin process manufacture.

3.1 Building the model

The objectives of the study were:

1. To identify those activities that delays the overall process.
2. To test the effects of varying the operation time for activities that delays the process, and
3. To determine process design parameters that reduces the duration time of the critical activities, to improve productivity.

To derive the models for each activity in Fig. 1, historical data from the plant was obtained. Table 1 summarizes the activities of the process and their duration time, in this table a code is assigned to each activity to facilitate the analysis. Note that the

Table 1
Activities of the process

Activities	Code	duration
Batch preparation & tar melting	-	240 min
Bubbling inert gas	A	variable
Addition of maleic anhydride	B	variable
Homogenizing the mixture	C	60 min
First addition of pentaerytrhitol	D	15 min
Second addition of pentaerytrhitol	E	15 min
Third addition of pentaerytrhitol	F	variable
Temperature elevation to 270 ºC	G	variable
Homogenizing the mixture	H	60 min
Vacuum the reactor	I	variable
First sample	J	variable
Second sample	K	variable
Reactor shutdown	L	variable
Reactor discharge	M	15 min

By operating 24 hours from Monday to Saturday, about 8 to 9 batches of resin are produced weekly. Taking this into account, the program was designed to run 10 batches and to report some measures of performance such as the average time required for each activity and the overall process duration.

Table 2
Cumulative frequency distributions

Activity A												
Time (min)	55	60	65	70	75	80	85	90	125	130	190	230
Frequency	2	7	13	62	80	84	89	91	93	96	98	100
Activity F												
Time (min)	5	10	15	20	25	30	35	40	45	60		
Frequency	12	23	55	67	83	90	93	95	98	100		
Activity I												
Time (min)	30	45	50	60	65	70	75	80	90	105		
Frequency	4	9	11	84	87	89	91	96	98	100		
Activity L												
Time (min)	5	10	15	20	25	26	30	35	40	55	60	80
Frequency	5	7	17	37	54	56	78	88	93	95	98	100

3.2 Results

A summary of the results obtained from the simulation is detailed in Table 3. It was verified that the model reproduce adequately the alkyd resin manufacture. The simulation confirms the existence of bottlenecks at certain activities of the process.

The delays of type 2 show a difficult to achieve some product specification. The delay of type 3 can be reduced with a better planning of the use of the equipment. So only the other delays of type 1, which is related to physical operations that include heating the reactor, accept modifications.

From the engineering point of view the time required to elevate the temperature can be reduced by adding extra area of heating or using a vapor with greater temperature and pressure. Since the steam generator of the plant is used at its maximum capacity, the only way to reduce the time to elevate the temperature of the reactor is by recirculation of the reactor mixture throughout a heat exchanger outside of the reactor.

Several simulations were run to include a reduction of the heating time, it was estimated that a decrease of approximately 40 % in the duration of activity G, will reduce the overall process time considerably.

Table 4, details the simulation results after the residence time of activity G was reduced by 38 %. Comparing the final time of 10 simulated batches from Tables 3 and 4, a reduction from 10,880 to 9,599 minutes is observed.

Table 3

Results of process simulation, time in min.

Batch	A	B	C	D	E	F	G	H	I	J	K	L	M
1	370	380	440	455	470	495	910	970	1030	1090	1150	1205	1220
2	1525	1535	1595	1610	1625	1630	2030	2090	2150	2210	2240	2270	2285
3	2580	2585	2645	2660	2675	2685	3090	3150	3210	3295	3325	3355	3370
4	3685	3700	3760	3775	3790	3815	4245	4305	4365	4425	4445	4480	4495
5	4805	4815	4875	4890	4905	4935	5325	5385	5430	5490	5495	5525	5540
6	5850	5870	5930	5945	5950	5985	6335	6395	6455	6515	6540	6565	6580
7	6950	6960	7020	7035	7050	7060	7490	7550	7610	7680	7700	7720	7735
8	8045	8050	8110	8125	8140	8155	8530	8590	8650	8710	8715	8735	8750
9	9065	9070	9130	9145	9160	9175	9555	9615	9685	9745	9775	9790	9805
10	10120	10170	10230	10245	10260	10270	10645	10705	10765	10825	10840	10875	10880

From the results obtained we found that the activities with larger delays are:

1. When waiting for the temperature to elevate to 270 ºC,
2. When waiting for the samples to be tested in the lab, and
3. When waiting to discharge.

Using the results as a guidance to propose process improvements, it was considered that the new duration to elevate the temperature to 270 ºC required extra heating, which was calculated taking into account the 38 % reduction of the duration of activity G. A change in the process configuration using the discharged product to preheat the raw material and adding a new heat exchanger was proposed. By implementing these changes the simulation study showed that it is possible to increase process productivity by approximately 10 %, which could save thousands of dollars a week.

Table 4.

Results of process simulation after modifying activity G duration.

Batch	A	B	C	D	E	F	G	H	I	J	K	L	M
1	370	379	439	454	469	494	774	834	894	954	1014	1069	1084
2	1389	1406	1466	1481	1496	1501	1772	1832	1892	1952	1982	2012	2027
3	2322	2328	2388	2403	2418	2428	2703	2763	2823	2898	2928	2958	2973
4	3288	3305	3365	3380	3395	3420	3705	3765	3825	3885	3905	3940	3955
5	4265	4278	4338	4353	4368	4398	4663	4723	4768	4828	4833	4863	4878
6	5188	5206	5266	5281	5296	5321	5572	5632	5692	5752	5777	5802	5817
7	6187	6198	6258	6273	6280	6298	6582	6642	6702	6772	6792	6812	6827
8	7137	7142	7202	7217	7232	7247	7509	7569	7629	7689	7694	7714	7729
9	8044	8050	8110	8125	8140	8155	8418	8478	8548	8608	8638	8653	8668
10	8983	9002	9062	9077	9092	9102	9364	9424	9484	9544	9559	9584	9599

4 Conclusion

A model for the process of manufacturing an alkyd resin, taking into account processing time variability has been build. It was verified that the model reproduce adequately the alkyd resin manufacture. Identification of critical activities that caused delays was done by simulation using the Monte Carlo method. The study resulted in a recommendation of making minor changes in the process configuration, like adding extra heating area required around the reactor. Implementation of this process improvement could increase productivity by eliminating delays of the most critical activity in the reactor, which could save thousands of dollars a week.

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