CONTINUOUS SIMULATION
OF
AN INTERNAL RECYCLE PROCESS

BY

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Summary

The purpose of this simulation is to determine satisfactory parameters for a system to continuously control the concentration of an internal recycle liquor process. The main elements of the process are pigment reactors, filters, raw material storage, a sodium sulfate recovery plant, and a dilution liquor storage system.

The simulation was programmed in FORTRAN IV using portions of IBM's Continuous Systems Modeling Program (CSMP). To solve the system of four simultaneous differential equations two numerical methods were programmed separately, since CSMP does not have a subroutine for such solutions. Integrating elements of the CSMP system with independent program modules proved an effective method of handling this problem.

The hourly update of production variables takes place after the differential equations have been solved for the tank levels and concentrations. At the end of each eight-hour shift the pigment being produced can be changed and settings of the control parameters are randomly altered. Printouts can be obtained every shift, every day or every Nth day.

In our experience to date, about thirty long production runs have brought out design problems in the engineering of the recycle process and provided guidance towards their solution. At present we are attempting to find approximately optimal conditions through repeated use of the simulation.

Introduction and Description of Process

In the Chemical Engineering profession, the start up of even as simple a process as the one described in this paper, used to mean a lot of overtime, short tempers and expensive changes. Over the past few years the development of techniques to simulate continuous processes on a digital computer has given the engineer a tool to test out processes while still in the design stage.

This paper describes the simulation of a process for the control of the concentration of a sodium sulfate recycle stream. This recycle stream is created by and necessary for a pigment production plant. The pigment filter of the production plant produces a strong liquor filtrate stream and a weak wash liquor stream. A portion of these liquors are recycled back to the reactive systems. The excess liquors are sent to the sodium sulfate recovery plant. At present the plant operators attempt to control the concentration of this recycle liquor manually.

The main purpose for the recycle liquor is to keep the concentration of the total liquors as high as possible, thus making the recovery of sodium sulfate more profitable. By controlling the concentration of this recycle we should be able to maintain a more consistent feed to the recovery plant.

The pigment is produced in the pigment reactor using sodium sulfate liquor as a reaction medium. This slurry is pumped to the filters where the bulk of the sodium sulfate liquors are separated and washed out of the pigment. The quantity of sodium sulfate which can be left in the pigment varies depending on the end use of the pigment. This causes variation in the liquor concentrations. Other variations in the liquor concentration come from normal operating variations, such as recycle lag time, reaction variation, etc.

The separation of the liquor from the pigment produces two streams, the filtrate and the wash liquor. In our process terminology these are referred to as the strong liquor and the weak liquor, respectively. The terms "strong" and "weak" refer to concentrations of sodium sulfate in the liquors.

For the proposed recycle system, the strong and weak liquor concentrations are to be monitored by an instrument. The information from the instrument is sent to a switching center which determines whether the stream should go to the weak liquor surge tank or the strong liquor surge tank. Although it is not normal, situations can occur which will cause the strong liquor to be weak enough that it goes to the weak liquor surge tank. Similar reversals can occur for the weak liquor stream.

The recycle liquor is also used as the reaction medium for the sodium silicate, which is a raw material for the pigment production. Whenever the sodium silicate storage tank is full, this plant will stop operating, thus abruptly changing the requirement for recycle liquor. Also, the sodium sulfate recovery plant can be stopped or started independently of the pigment production plant.

The proposed system for production of recycle liquor at a constant concentration will take streams from the strong and weak liquor surge tanks in the proper proportions and blend them to make up the recycle liquor. The blend of the feed to the recovery plant will be controlled by the levels in the two surge tanks. The recycle liquor use has priority over the recovery feed stream, so when the surge tank levels drop to some predetermined level the feed to the recovery plant will have to be stopped. The concentrations and levels of the surge tanks are not controlled, but rather arrive at some level based on what the rest of the process is doing. In order to set up a simulation program for this process we found it necessary to utilize four differential equations which would yield the concentrations and levels at suitable intervals of time. The solution of these equations which would yield the concentrations and levels at suitable intervals of time. The solution of these equations was a vital part of the simulation.

General Features of the Model

The sulfate liquor control system was simulated in sufficient detail to enable the design engineer to find out whether the process would be operable within design limits. It was not necessary to represent the process details within the pigment reactors (See Figure #1)in order to measure changes in concentration and tank levels or demand for concentrated sulfate liquor. The simulation required a set of reaction times and rates, and weak and strong liquor outputs, based on detailed knowledge of the process appropriate to the particular pigment in production. The production run was always set for eight hours; at the start of a new eight hour shift, the filter rate was given a random perturbation. A realistic probability distribution based on production records was used in the simulation to select pigment to be produced for each day, or schedule downtime once every 24 hours. The process variables were updated hourly, and the differential equations were solved once each update period. A variable "step size" in the numerical method of solution permitted adequate control over the level of error for most situations.

The process was considered operable if the tanks did not run over by too much (or run dry). An important measure of design performance was the cumulative total quantity run "down the sewer" from each tank. Another problem to be solved through the use of the simulation model was the correct capacity of the surge tanks (weak and strong liquor).

The model was programmed to add water to the weak liquor and a higher concentrated liquor to the strong surge tank when the respective levels dropped to 1000 gallons. The amounts of each added during a run is a measure of the departure from adequate tank capacity. In the case of the concentrate, only a limited quantity is available from the recovery plant. Thus, excessive demand for the concentrate would indicate design errors regarding capacity.

The variations in flow rates and concentrations show up on the filter as variations in filter rates. Conversely, the program can be run with altered filter rates to study the effect on the sulfate liquor control system. Tests of efficiency of the system were also made through the use of different start and stop levels on the silicate plant and the recovery plant.

The nested character of the various cycles was an important feature of the model. It also proved to be a source of difficulty in getting a working computer program within our original deadline as discussed in later sections of this paper. The main timing features of the simulation are summarized in Figure # 2.

Program Design

The simulation of the sulfate liquor recycle process was originally written in the IBM CSMP/360[1] language and implemented on the S360/40 computer at J. M. Huber. Three sections were programmed:

INITIAL
DYNAMIC
TERMINAL

The INITIAL section was written to provide (i) all the necessary constants such as the starting levels in the surge tanks, the concentrations of the weak and strong liquors and so on (ii) the random number selections to determine which product would be produced for the next eight hour shift (iii) the rate equations for each product.

The DYNAMIC section was to calculate the hourly flows and solve the differential equations for the weak and strong liquor tank levels and concentrations. It also set the switches for operating or shutting down the two auxiliary plants.

The TERMINAL section was designed to provide appropriate run control: it was intended to ensure that some of the variables were re-evaluated every hour, some every eight hours and some every twenty-four hours. For instance, the product on the reactor and its associated rates were to be changed every eight hours.

For the solution of the simultaneous non-linear differential equations each UPDATE period, the IBM Scientific Subroutine (FORTRAN) Package routine 'HPCG' was selected. In the DYNAMIC section of the CSMP program a 'CALL HPCG' statement followed a subsection in which the CSMP variables were transformed and stored in suitable locations for the subroutine. This approach was thought preferable by the authors over attempting to employ the CSMP integration for solution of our particular equations. As will be mentioned in subsequent paragraphs, the method was workable. The complexity of the run control in this simulation resulted in our having difficulties with the TERMINAL section of the CSMP program. It was essential to preserve the important distinctions between hours, shift and days: our limited experience with CSMP did not permit us to achieve this within our original deadline and accordingly we decided to write a FORTRAN program to control the simulation. This meant abandoning the overall system, but taking over as many of its parts as feasible: in the end we used the structural design of the CSMP system to flowchart our simulation and four FORTRAN modules from the CSMP library together with the UPDATE module generated by CSMP in our unsuccessful attempts to get it working.

Continuous Simulation Using CSMP as a Library

The successful program was ultimately composed of FORTRAN subroutines:

1) MAIN
2) INPUTR
3) INITR
4) UPDATE
5) PRINTR
6) HPCG
7) FCT
8) OUTP
9) RNDGEN
10) GAUSS
11) INSW
12) COMPAR

The first five were created, partly, by our incomplete runs using CSMP and partly by rewriting. Numbers 6-8 were taken from the IBM SSP tape[2], except that details of the derivative functions had to be supplied by the user in FCT. Numbers 9-12 were lifted, without change, from the CSMP source program library.

As a result of writing and running a CSMP program for our simulation we acquired a FORTRAN subroutine called UPDATE incorporating all of the DYNAMIC section and some of the INITIAL section. This routine was usable with only a few minor modifications as our program module No. 4. Its purpose was (i) to calculate the hourly changes in flows; (ii) to call HPCG to solve the D.E.'s for tank levels and concentrations; and (iii) to account for overflow as well as starting and stopping the two auxiliary plants under appropriate conditions.

We took the INITIAL section and reworked it into a FORTRAN program 'INITR': No. 3. This was a relatively easy matter as many of the CSMP statements are FORTRAN-like. A branch condition was inserted to allow for correct re-initialization at the beginning of a) the whole run, b) each day, c) each shift.

Program modules No.'s 2 and 5 were the simulation input and output routines respectively. These were written specially for the FORTRAN version of the system. Finally 'MAIN', module No. 1, provided sequencing, length of run, error messages, and print-out option control.

The Equations of the Model

The equations governing the behavior of the system are given below in terms of the weak and strong liquor levels (X_2 and Y_2 respectively); their concentrations (X_1/X_2 and Y_1/Y_2); the weak and strong liquor rates of flow to recycle (X_7 and Y_7); and the weak and strong liquor rates of flow into the 11% stream (X_8 and Y_8).

(5.1) $dX_1/dt = A - (X_1/X_2)*(X_7+X8)$

(5.2) $dX_2/dt = B - X_7 - X_8$

(5.3) $dY_1/dt = C - (Y_1/Y_2)*(Y_7+Y_8)$

(5.4) $dY_2/dt = D - Y_7 - Y_8$

(5.5) $X_7 + Y_7 = S$

(5.6) $(X_1/X_2)*X_7 + (Y_1/Y_2)*Y_7 = 1.011 * S$

(5.7) $X_8+Y_8 = T$

(5.8)(a) $X_8 = Y_8 *(X_2-U)/(Y_2-V)$ if $X_2 > U$ and $Y_2 > V$

(5.8)(b) $X_8 = 0$ if either $X_2 <= U$, or $Y_2 <= V$.

The letters A,B,C,D,S,T,U,V in the above equations represent relative constants, whose values are computed by the program in the hourly UPDATE before beginning numerical solution of the equations. It is not readily apparent from the form of the eight equations what mathematical problems arise in attempting to solve them. For simplification they are recast in the equivalent form:

(5.9) $dZ_1/dt = C_1$

(5.10) $dZ_2/dt = C_2-S*(1.011-Z_4)/(Z_3-Z_4)-H*(Z_2-U)/(Z_1-U-V)$

and $H = \begin{cases} 0 \text{ if } Z_2 <= U \text{ or } Z_1-Z_2 <= V \\ T \text{ otherwise} \end{cases}$

(5.11) $dZ_3/dt = (C_3-C_2*Z_3)/Z_2$

(5.12) $dZ_4/dt = (C_4-C_5*Z_4)/(Z_1-Z_4)$

The four dependent variables Z_1, Z_2, Z_3 or Z_4 are related to the original quantities as follows:

(5.13) $Z_1 = X_2 + Y_2$

(5.14) $Z_2 = X_2$

(5.15) $Z_3 = X_1/X_2$

(5.16) $Z_4 = Y_1/Y_2$

The relative constants S,T,U and V are the same as before; C_1-C_5 are further relative constants known to the program in the UPDATE subroutine through explicit functional relationships, which are not presented here since they do not affect the mathematical solution of equations (5.9) - (5.12).

Run Experience with Modified CSMP Simulation

Obtaining output was easy enough; checking it was another matter. A short run (48 hours) was made and hand calculations were performed using a WANG calculator and replacing HPCG with Euler's method of solving the D.E.'s. These calculations were valuable for showing up glaring errors in the computer program. But they also provided something even better: a check program. We decided to rewrite the UPDATE module No. 4 (also in FORTRAN, of course) with the explicit iterations of the Euler method replacing CALL HPCG section. By running the two versions of the whole system side by side, we were able to discover the subtler bugs and achieve the desired degree of accuracy. After debugging, we discovered that the HPCG version was running six to eight times as long as our 360/40 computer without compensating improvement in accuracy. Hence we decided to use the check program for our long production runs!

At the end of each shift, the current values of the production variables and plant condition variables are shown, the former once only and the latter eight times (since a shift is eight hours). At the end of the shift output, CHECK BALANCES for each of the eight hours are listed: these are the discrepancies in the material balance equation and were used as a primary means of controlling the accuracy of the overall solution.

At the end of each day, cumulative totals of the amounts of water and concentrate demanded, the amount of sulfate produced, and the amounts of weak and strong liquor down the sewer are printed out. In using the simulation for very long runs we found it desirable to have printout every N days only, with N being an additional input parameter. The printout in cases of $N > 1$ includes the complete shift output for the last shift of the day in question.

At the end of the simulation run, a summary of production by pounds of product is printed. Averages and standard deviations of several control variables are also given.

Validation of the Results

One of the most difficult things to do, when a complex process is simulated in big computer programs, is to validate the results in the sense that the numbers produced in the voluminous output really mean what they purport to say. We used a large measure of common sense combined with the thorough familiarity one of use (LEH) had with plant operations to obtain a first-pass validation. Later we added material balance equations to the UPDATE program and printed hourly CHECK BLANACES at the end of each shift at the bottom of the regular shift output. These were quite revealing. When a change of product occurred, or after a strong surge from one of the surge tanks, they would show considerable fluctuations. For the most part, although these balances were frequently far from zero, there did not appear to be any statistical bias in their fluctuations. Furthermore, the amount of variation could be reduced (at the cost of increased run time) by decreasing the step size in the numerical solution of the D.E.'s. These two findings gave us reasonable satisfaction that the simulation output "made sense".

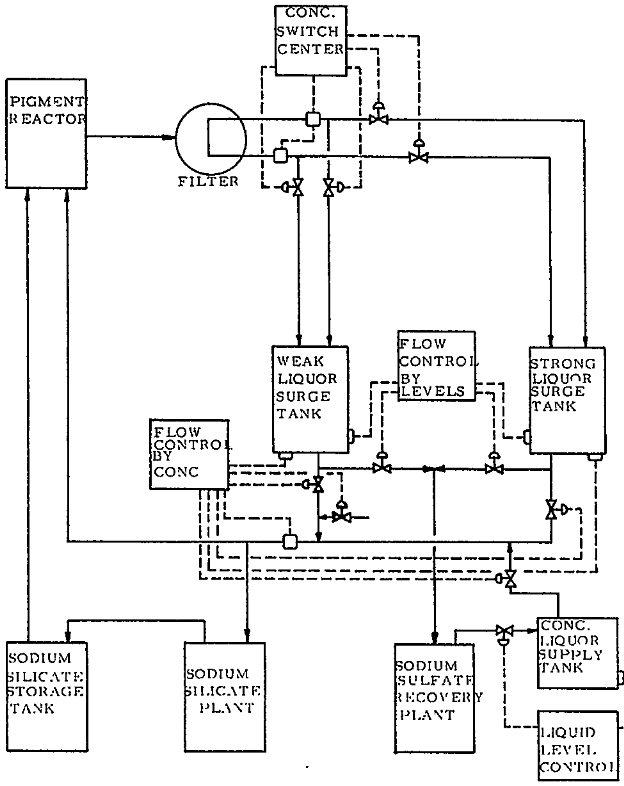
Use of the Simulation

The simulation is being used to study the soundness of the engineering design of the sulfate liquor recycle process, this being the new part of the physical plant. Questions focussing on capacity of storage tanks, frequency of switching on and off of the sulfate and silicate plants, and the amount of the overflow for a specified level of operations are being investigated. Testing of the program has taken longer than we expected; but in the testing phase considerable reshaping of the simulation has occurred and, because of this the resulting program is more general than the CSMP version would have been.

It is intended to use the simulation as a major step towards optimizing the conditions for the recycle process. To date, upwards of thirty long (100 day) runs have been completed with significant improvement of the system's performance. Although the program was not written as an optimization, it is providing strong insights into the effect of capacities, rates and settings on the overflow, surges and consumption of externally supplied material.

References

1. IBM program #360A-CX-16X, Ver. I, Mod. 2
2. System/360 Scientific Subroutine Package (360A-CM-03X) Ver. III



SULFATE LIQUOR CONTROL SYSTEM

FIGURE # 1

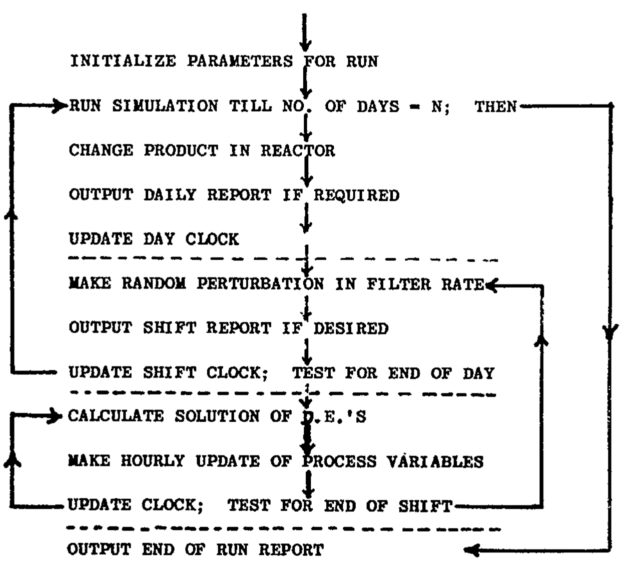


Figure # 2

SHIFT NO. 1 OF DAY NO. 1

PROD	SILLEV
23.0000	23672.9375

SLSLEV	WLSLEV	CSOLEV	SLCONC	WLCONC	SLSCON	WLSCON
36508.4414	55902.8242	10000.0000	1.1280	0.7731	1.1247	0.7847
SLRATE	**WLRATE**	**SLRTSS**	**SLRTWS**	**WLRTSS**	**WLRTWS**	**SOZRX**
7164.2031	9121.3086	7164.2031	0.0	0.0	9121.3086	4925.3359
SOSIPT	**SLRTRC**	**WLRTRC**	**SSOPLT**	**WSOPLT**	**CSORAT**	**SILRAT**
10000.0000	3525.3733	1399.9626	0.0	9225.0898	0.0	0.0
CSORCY	**WATRCY**	**TSOPLT**	**TO11PR**	**SILZRA**	**FR**	**SFTSEW**
0.0	0.0	9225.0898	4925.3359	4815.8828	18241.9922	0.0

SPLOPT	0	0	0	0	0	0	0	1
CSOOPT	0	0	0	0	0	0	0	0
SILOPT	1	2	3	0	1	2	3	0

CHECK BALANCES :

-162.4883 -13.2031 -113.1992 -113.1875 -113.2500 -13.2500 -113.2500 -113.2500

LBS. OF PRD. 23 SO FAR = 0.145936E 06

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SHIFT NO. 2 OF DAY NO. 1

PROD	SILLEV
23.0000	18582.4688

SLSLEV	WLSLEV	CSOLEV	SLCONC	WLCONC	SLSCON	WLSCON
55836.0117	53620.4688	10000.0000	1.1233	0.8588	1.1234	0.8330
SLRATE	**WLRATE**	**SLRTSS**	**SLRTWS**	**WLRTSS**	**WLRTWS**	**SOZRX**
7451.8984	7362.0234	7451.8984	0.0	0.0	7362.0234	4767.2461
SOSIPT	**SLRTRC**	**WLRTRC**	**SSOPLT**	**WSOPLT**	**CSORAT**	**SILRAT**
10000.0000	3086.2786	1680.9675	815.9844	8314.7617	0.0	0.0
CSORCY	**WATRCY**	**TSOPLT**	**TO11PR**	**SILZRA**	**FR**	**SFTSEW**
0.0	0.0	9130.7461	4767.2461	4661.3086	17656.4805	0.0

SPLOPT	0	0	1	1	0	0	1	1
CSOOPT	0	0	0	0	0	0	0	0
SILOPT	1	2	3	0	1	2	3	0

CHECK BALANCES :

5533.1250 0.0 -100.0625 -9.2500 1901.1250 -0.0625 -100.0000 -11.1250

LBS. OF PRD. 23 SO FAR = 0.287188E 06

****

SHIFT NO. 3 OF DAY NO. 1

PROD	SILLEV
23.0000	11569.8750

SLSLEV	WLSLEV	CSOLEV	SLCONC	WLCONC	SLSCON	WLSCON
61362.2695	53218.4844	10000.0000	1.1101	0.7642	1.1137	0.7841

Fig. 3

END OF DAY NO. 10

WATUSE	CSOUSE	PSOPRD	PSLSEW	PWLSEW	CONSPT
0.0	0.0	0.131583E 07	0.374959E 05	0.0	0.0

******************   ******************   ******************

AVERAGE CHECK BALANCE 0.104785E 04

STANDARD DEVIATION 0.222019E 04

TOTAL LBS. OF ALL PRODUCTS = 0.381918E 07

SUMMARY OF PRODUCTION BY LBS. THIS RUN

PRODUCT NO.	LBS.
0	0.0
23	0.279539E 07
35	0.838187E 06
0	0.0
0	0.0
0	0.0
80	0.185603E 06
0	0.0
0	0.0

AVERAGE SPLOPT 0.6333
AVERAGE CSOOPT 0.0
AVERAGE SILOPT 1.6417

AVERAGE SULFATE PLT OP TIME 4.4706

AVERAGE SULFATE PLT DOWN TIME 2.5882

STD.DEV.N OF SULFATE PLT OP TIME 10.6379

STD.DEV.N OF SULFATE PLT DOWN TIME 2.3240

AVERAGE CONCENTRATION TO SULFATE PLANT 0.8249

STD.DEV.N OF FLOW TO SULFATE PLANT 0.0937

END OF SIMULATION RUN

NO.OF DAYS= 10 NO.OF HOURS= 240

Fig. 4