Putting Evaporators to Work:

Dynamic Process Modeling of a Quadruple Effect Evaporation System

The digital simulator was responsible for locating a number of bottlenecks prior to startup, for controlling tuning, and for examining overall system stability.

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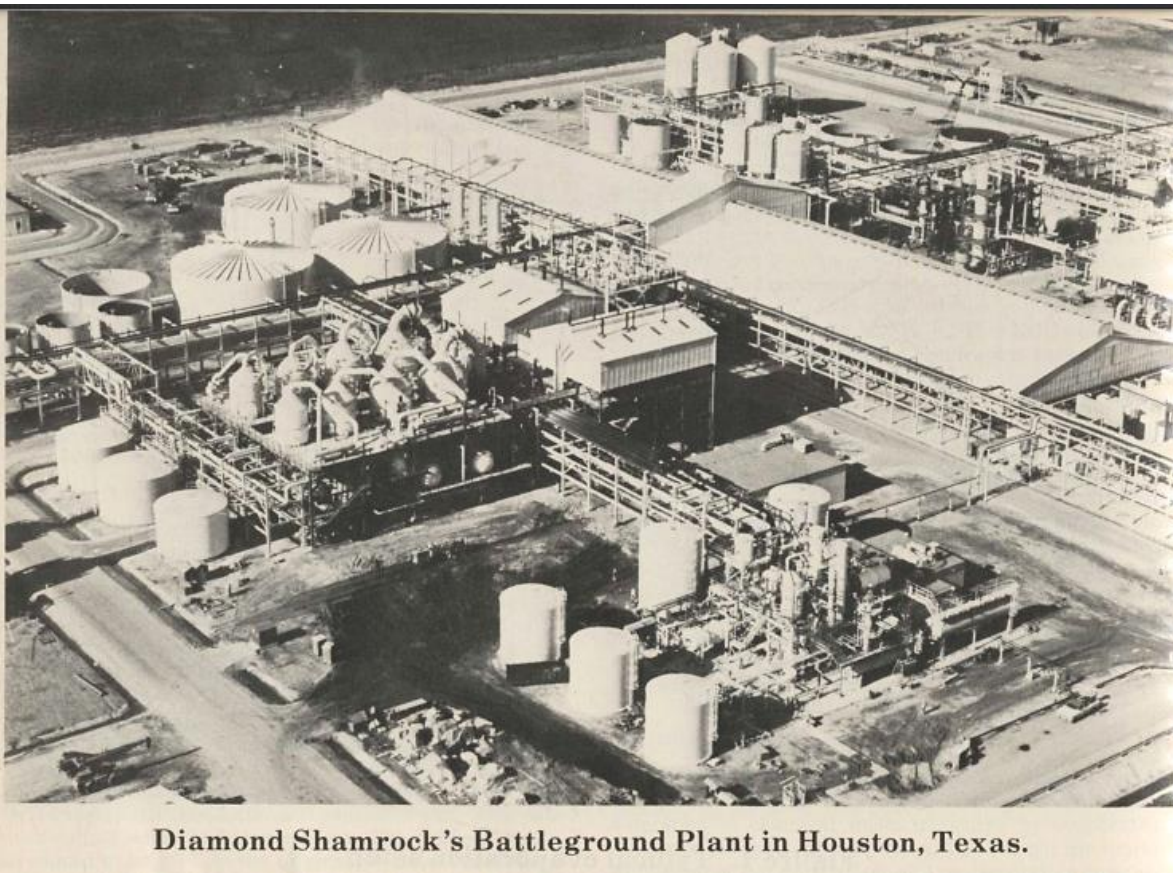
Startup of the first chlorine-caustic plant in the U.S. to operate successfully using a quadruple effect evaporation system was greatly improved by the development and use of a digital simulator before going onstream. The plant is Diamond Shamrock Corp.'s 1,200 ton/day Battleground installation at La Porte, Texas which went into service during the last quarter of 1974. The simulator, developed by Diamond Shamrock's Central Engineering Dept., was responsible for locating several bottlenecks in the system before startup, for controller tuning, for examination of overall system stability, for facilitating startup, and for indicating appropriate washing techniques.

Since the size of the evaporators and appropriate salt handling facilities resulted in relatively large time constants and, since the system is essentially directly connected with little or no surge capacity between the vessels, it was decided that there was a need for a dynamic simulator to determine the system's stability. In fact, at the time the study was initiated, the dynamics of such a system were totally unknown, and it was considered possible that there would be no sets of controller parameters that would result in stable operation utilizing the "as designed" control system.

The original design of the evaporation area's control system utilized proportional-integral (PI) level con-



Diamond Shamrock's Battleground Plant in Houston, Texas.

trollers for all vessels, a PI controller with pressure override for primary steam control and a proportional-integral-derivative (PID) controller for the product composition. These were the major controllers of interest to the scope of the simulator since more modest and relatively external systems such as condensate level control in steam heaters were not considered.

The potential for instability in the system was extremely high since it consisted of seven interacting vessels in series, some of which exhibited considerable time lags. Furthermore, product composition control was essentially unrelated to vessel levels so that the overall system was effectively broken into two noninteracting sets of vessels with each set containing several interacting first order systems.

The intrinsic controllability of such a system is obviously suspect, and the basic need for the simulator was established. As a result, a simulator was desired for the following purposes:

1. Evaluation of alternate control schemes.
2. Controller tuning.
3. Examination of system stability: a) response to load changes, and b) response to set point changes.
4. Identification of equipment limitations.
5. Examination of system response to "deliberate upsets": a) startup, b) shutdown, c) on-line "fly-washing" (i.e., direct injection of water to remove salt deposits while continuing the evaporation process).

General program methods

Included in the analysis of the various control loops was a thorough modeling of the inherently non-linear flow-head relationships and the superimposed interacting heat flows. Analysis of the resultant heat, material and momentum balances is most easily effected on a digital computer; their mathematical complexity, as well as the sheer number of variables made the use of an analog computer impractical. An IBM System 370/158 was chosen for the work.

An efficient dynamic model requires an analysis of loop time constants so that the differential equations modeling those loops with relatively short time constants can be reduced to simple algebraic expressions. The solution to the resultant set of algebraic equations at time zero with the initial conditions of the differential variables is followed by numerical integration over the time step to time $0 + \Delta t$. Updating the values of the differential variables is followed by a second solution of the algebraic expressions.

In the present study, the major differential variables included evaporator body compositions, temperatures and volumes, controller signals, and final control element lags. All evaporator bodies were assumed well mixed so that time was the only independent variable. Other vessels in series with the evaporators were modeled appropriately.

Since the relationship between any controller in liquid level control service and the resultant flow rate includes a direct contribution to the overall loop gain, the calculation of liquid flow rates requires a good deal of accuracy. With reference to Figure 1 (which for proprietary reasons, is not a schematic of the Battleground evaporation area), the modified Bernoulli equation in the absence of any phase changes is:

$$\Delta P_p = (P_2 - P_1) + [(\rho_g)/(g_c)](h_2 - h_1) + \Delta P_f. \quad (1)$$

The friction losses, ΔP_f, may be divided into two parts: the loss across the control valve, and the losses from all other sources including process lines, fittings, and mechanically operated valves.

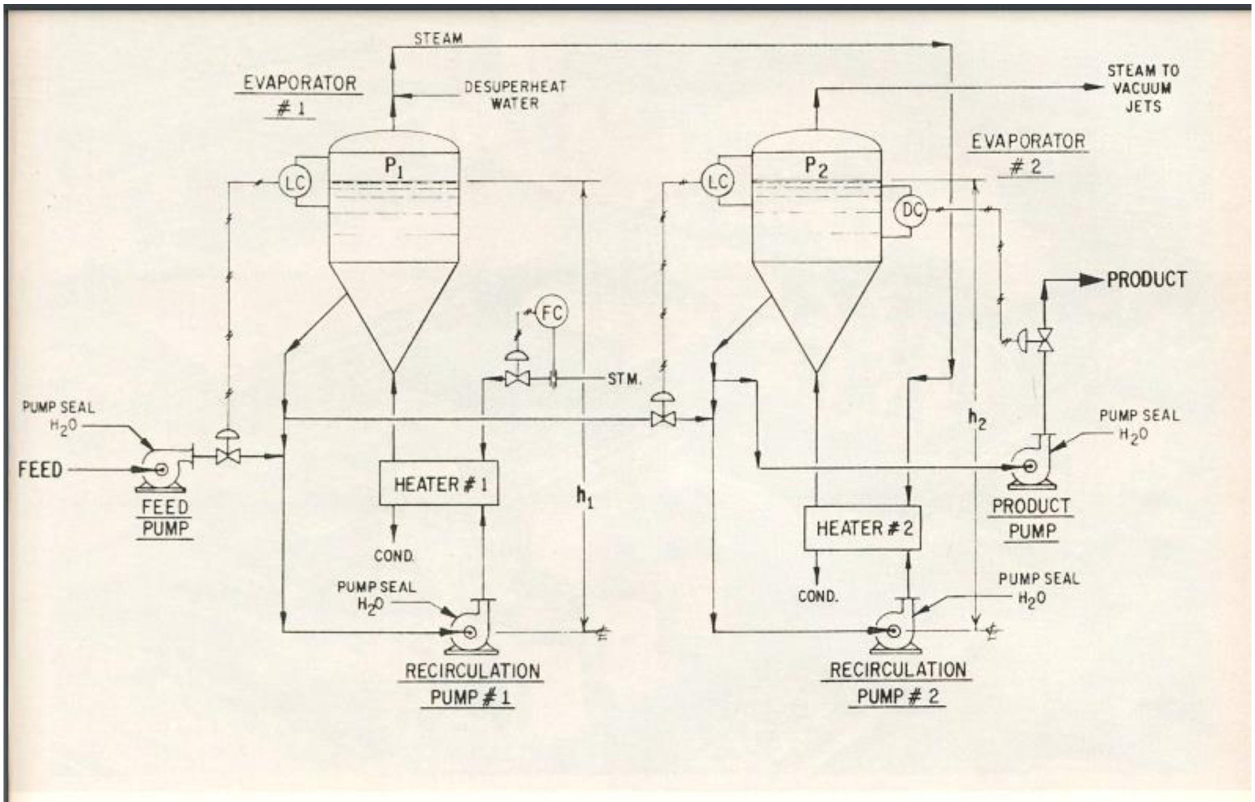


Figure 1. Typical evaporation setup.

Line and fitting losses, ΔP_{fl}, are, of course, estimated from friction factor correlations according to the definition of the friction factor:

$$\Delta P_{fl} = [(\langle v\rangle^2\rho)/(2g_c)]\cdot[(\Sigma L)/(D)]\cdot f \qquad (2)$$

Equation 2 can also be expressed as:

$$\Delta P_{fl} = R_l Q^2 \qquad (3)$$

where R_l is an equivalent line resistance given by

$$R_l = [(\rho\Sigma L)/(2g_c A^2 D)]\cdot f \qquad (4)$$

An expression analogous to equation 2 for the control valve is:

$$\Delta P_{fv} = [(Q)/(C_v)]^2\rho \qquad (5)$$

so that

$$\Delta P_{fv} = R_v Q^2 \qquad (6)$$

where:

$$R_v = \rho[(1)/(C_v)]^2. \qquad (7)$$

Substitution of equations 3 and 6 into equation 1 gives:

$$\begin{aligned}\Delta P_p &= (P_2 - P_1) + [(\rho_g)/(g_c)](h_2 - h_1) \\ &\quad + \Delta P_{fv} + \Delta P_{fl} = (P_2 - P_1) \\ &\quad + [(\rho_g)/(g_c)](h_2 - h_1) \\ &\quad + Q^2(R_v + R_l).\end{aligned} \qquad (8)$$

If Equation 8 is rearranged slightly,

$$\Delta P_p - (P_2 - P_1) - [(\rho_g)/(g_c)](h_2 - h_1) = Q^2(R_v + R_l) \qquad (9)$$

which is analogous to

$$E = IR \qquad (10)$$

results. Such a correspondence gives rise to the "electrical" analog to flow situations.

With the stipulation that "fluid flow" be squared, the analogy between equation 9 and equation 10 for current flow is exact so that all of Kirchoff's laws apply. Such an approach greatly simplifies the solution of complex flow patterns since flows and effective resistances can be determined in the same manner as in electrical circuits of series and parallel branches.

In the present study, ΔP_p, the pump pressure rises, were curve-fitted as functions of flow rate with impeller sizes as parameters. Similarly, control valve flow coefficients, C_v, were curve-fitted as functions of valve stem position. A choice of a reasonable flow rate through a particular process line in an "off-line" calculation fixed R_l/ρ as input data to the simulator since all liquid Reynolds' numbers were sufficiently high during any run to maintain constant friction factors.

Furthermore, at any point in time, the controller output signal fixed the valve stem position and hence R_v/ρ. Since the pump pressure rise is a function of the flow rate, equation 8 and the pump curve were solved simultaneously for every increment in time by a trial and error method to establish the flows between process vessels.

Some calculations were too complex

In some instances, however, multiphase, compressible flow caused by flashing liquor in process lines was a possibility. Such a situation occurred, of course, if there was ever a sufficient drop in pressure so that the prevailing net pressure was equal to or less than the saturation pressure. At first the simulator incorporated a complete subroutine to calculate flow rates under these transient conditions, but it was found that the rather involved calculations consumed an inordinate amount of computer time. Thus, an approximation between incompressible

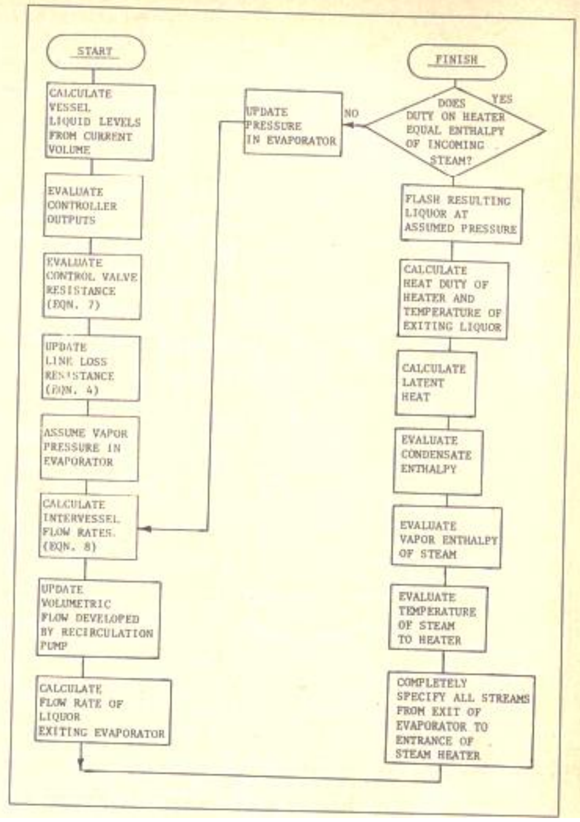


Figure 2. Flowsheet of a typical evaporator subroutine.

flow and critical flow was adopted for situations in which prevailing pressures gave rise to such occurrences.

The sequence of calculations required supporting physical property subroutines. These physical properties included density, solubility, vapor pressure, and enthalpy for both single and multi-phase caustic-water-salt solutions (liquor) and water itself.

The density subroutine calculated specific gravities by corporate data for both saturated and unsaturated liquor as functions of temperature with caustic concentration parameters over a range of 0 to 60% caustic. Average densities of slurries were also calculated.

Whenever a liquor solution physical property was to be determined at a particular temperature and composition, salt solubilities were determined first. Again, corporate data were available for isothermal solubility in the ternary solution, and these data were curve-fitted appropriately. Interpolation between isotherms was accomplished within the solubility subroutine. Although a fourth component, sodium sulfate and its various hydrates and combinations, was always present, the effect of its solubility was determined separately.

Corporate data of Duehring charts along with published data (*1*) served as the basis for vapor pressure data for liquor solutions saturated with salt. The Duehring chart data were available as boiling points of liquor solutions as functions of boiling points of pure water with the salt-free caustic compositions as parameters, and these data were curve fitted appropriately. Again, the vapor pressure subroutine provided an interpolation on caustic composition.

Liquor enthalpy was determined in a separate subroutine via curve fits of published data (*2*) corrected to a

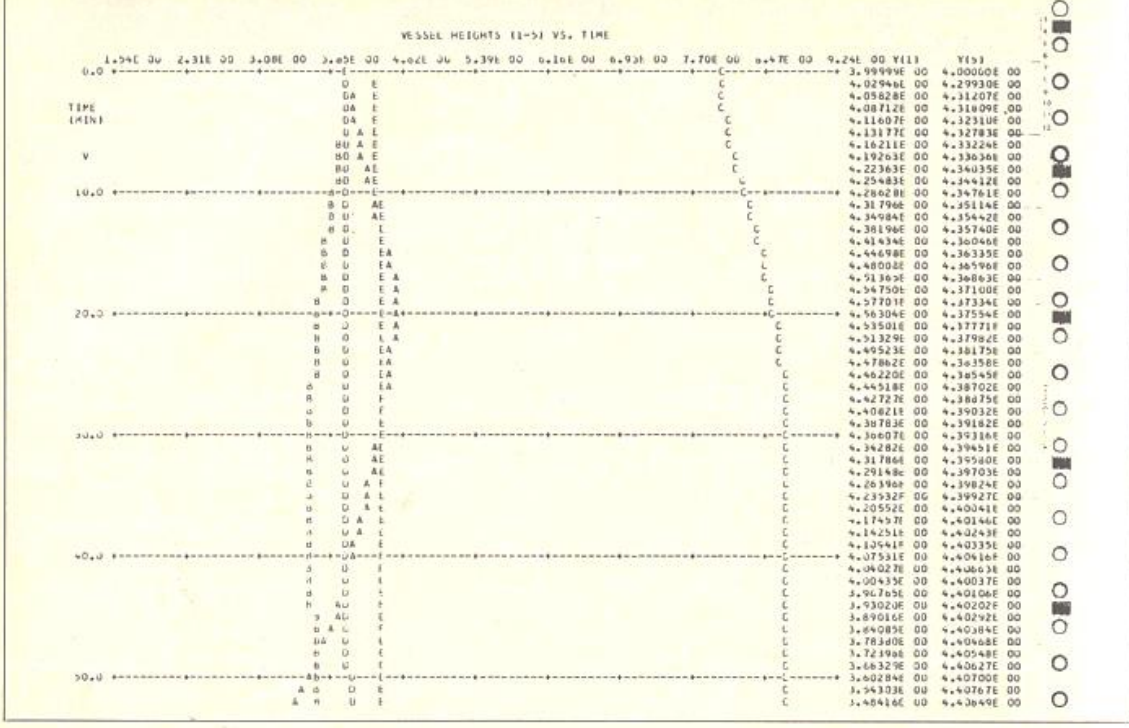


Figure 3. Sample from simulator output (vessel levels).

basis compatible with the steam tables. (*3*) Data from these steam tables for liquid and vapor (saturated and superheated) enthalpies were curve-fitted over a wide range of temperature and pressure and were incorporated into appropriate subroutines.

All these "data oriented" subroutines were continuously employed in the simulator. These data, as well as all other process variables, were incorporated into the program under the general organization suggested by Franks (*4*).

Some details on how the calculations were performed by the simulator are illustrated by Figure 2, which is a flowsheet of a typical subroutine modeling the evaporation system depicted in Figure 1.

At any value of time, the calculation procedure began with integration of all differential variables. Among these variables were the controller signals which fixed the control valve positions and from which equivalent valve resistances to flow were calculated in conjunction with the valve curves. Integrated values of vessel volumes were used for calculation of liquid levels. At this point, the primary steam chest pressures and evaporator operating pressures were assumed. Thus all heat, material and momentum balances could be solved algebraically for the steam generation in each vessel and the flow rates between the vessels. The assumed pressure profile was then checked in a trial and error fashion by comparing the steam generated (corrected for de-superheating) with the steam consumed in the next effect until all pressures were converged. With all the steam and liquid flows into and out of each vessel known, integration of composition, volume, and enthalpy of each body was effected and the procedure was repeated.

Time delays in the steam heater were ignored relative to the large vessel time constants so that all heat and material balances relative to the solution method of Figure 2 were of the "algebraic" type. Furthermore, the calculations for the startup case (in which no steam is being generated initially from each effect) were slightly different from those shown in Figure 2. Also, excess steam de-superheat water was either added to the vessel contents or entrained in the vapor stream depending upon the vapor velocity. Finally, options were available within the program for modeling of 1) "normal," near-steady state operation, 2) startup, or 3) fly-washing of various vessels.

Output from the program was of two types; printed and plotted. The printed portion of the output indicated controller settings, control modes (manual or automatic), evaporator pressures, controller outputs, and detailed information about each stream. This phase of the printed output could be printed at any selected time interval. Another phase of the printed output consisted of various messages from the system: messages from the "operator," messages indicating the occurrences of a sequenced event, and warning and diagnostic messages.

The second type of output was in a plotted format and was performed directly on the line printer by specially designed subroutines. Time histories for variables such as vessel temperatures, pressures and compositions, intervessel flow rates, slurry concentrations, and many others were plotted. This type of output proved invaluable for studying the performance of the system.

Integration techniques available to the simulator were Euler and Runge-Kutta second and fourth order. Of these, the Runge-Kutta fourth order integration was found to give the most satisfactory performance in the present study in terms of both efficiency and accuracy. One measure of this efficiency was the ratio of real time simulated to CPU time used. The simulator was so complex that this ratio usually averaged between 15 and 20.

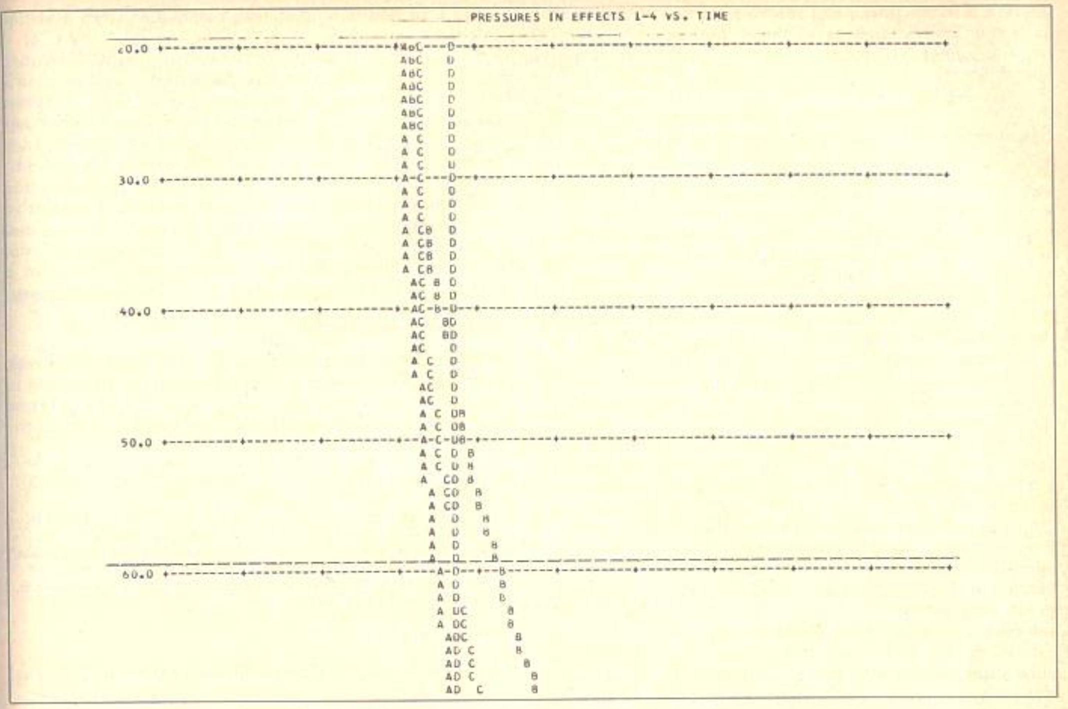


Figure 4. Sample from simulator output (vessel pressures).

Results

The simulator was used to evaluate many operational aspects of the Battleground evaporation area. First, in the near-steady state region, when all controllers were tuned as a first approximation to "reasonable" values, execution of the simulator quickly revealed that one vessel quickly emptied causing a transfer pump to cavitate regardless of the settings on the level controller. An increase in the size of the impeller of the pump feeding this vessel corrected this particular problem. But, since a change in the flow-head relationship was tantamount to a change in the overall loop gain (cf. equation 9), the tuning parameters of the vessel's level controller had to be altered appropriately. Moreover, the increase in flow feeding the vessel tended to empty the upstream vessels and to overflow those downstream. The simulator allowed the resizing of all appropriate pump impellers required to reestablish control of the system at a point prior to completion of construction so that the equipment changes had been completed by the time of startup.

Ultimate tuning of the system for stable operation near steady state was accomplished by trial and error using the simulator with appropriate assistance of open loop methods.

Other applications of the simulator in the near-steady state region included analysis of the effects of potential diurnal variations in vacuum caused by changes in process cooling water temperature, analysis of the effect of composition and temperature changes in the cell liquor feed, location of the optimal control point for product composition, determination of appropriate modes of actions of various controllers (P, PI, or PID) and determination of the effects of changes in feed points for various evaporators. Results from all of these studies were thoroughly discussed with the operations personnel in an effort to maximize the efficiency of the system long before construction was completed and it was placed into service.

Analysis of the most efficient way to start this very complex system was the next and perhaps the most significant contribution of the simulator. Not only were there a host of suggestions from various groups as to startup methods, but at startup the system response is very different from that at near-steady state. Use of the simulator even pointed out quite clearly that the differential pressure transducers measuring the vessel levels gave serious errors in level indication because of gross differences in temperatures and compositions (and, therefore, specific gravity) between initial and steady state conditions.

After some discussion, a preliminary startup method was agreed upon by all parties involved. Initial compositions of each vessel were specified, initial vessel pressures were defined, "manual" or "automatic" modes of operation for all controllers were chosen, and a vessel-by-vessel procedure was agreed upon. One additional stipulation from the operations personnel for startup simulation was that controller settings not be altered from their values previously obtained from near-steady state operation of the simulator. (It was presumed, then, that startup of the evaporation area would have been attempted under all of these conditions had the simulator not been available.)

Use of the simulator quickly pointed out serious deficiencies in the chosen technique. Excess quantities of slurries quickly began to build up in vessels unable to handle such loads. Developing pressure profiles made it impossible to transfer material from body to body effectively. Non-specification product was produced and had to be discharged very early, and vessel levels were impossible to maintain. Careful evaluation and discussion of the results of the initial and subsequent runs with almost daily communication between the authors and the operations personnel eventually resulted in a very efficient and operable startup technique.

Startup not entirely automatic

This technique consisted of the definition of proper initial compositions, temperatures, and feeds for each vessel, and the timing of salt centrifuge startups. One unique aspect of the startup technique resulted from the stipulation of the controller settings. Not only were the controllers tuned to produce satisfactory operation near steady state, but also most control valves were closed initially. The combination of rather sluggish controller response and the peculiarities of the control valve curves rendered a fully "automatic" startup impossible. As a result, many controllers were on "manual" initially, and a sequence was developed for switchover to automatic based upon measurable events.

However, even this manner of startup was not satisfactory. After some controllers were placed on automatic, the tuning parameter-valve curve combination still resulted in an overall sluggish response, and vessels tended to empty or overflow. It became obvious that frequent operator intervention would be essential. The authors and the operations personnel developed criteria for operator intervention in the simulator: a range of values around the set point were established for each vessel within which no intervention would be made and the maximum allowable rate of change of the variable was established. Then a subroutine, which was tantamount to a "proportional-derivative" operator, was written to supervise the control system by assuming "manual" control when necessary to open or close the control valves appropriately.

Typical startup time histories of some vessel levels and pressures are shown in Figures 3 and 4, respectively, which are direct copies of actual output from the simulator. Because of space limitations, both of these figures show only the first 125 min. of the 1,000 min. output. On the level plot the numerical values of the levels in vessels A and E are printed in the two columns at the right hand side, and the values of time (in minutes) are printed along the left hand side. We have noted the simulated operator's manual interruptions by circling the appropriate vessel's indication. An arrow pointing to the circle indicates the onset of manual control, while an arrow pointing away indicates the resumption of automatic control. The pressure plots indicate the manner in which fully developed profiles were obtained.

After a startup technique completely agreeable to all parties had been perfected, copies of the appropriate outputs, as well as a summary of the most important events, were sent to the operations personnel for use during startup. Immediately upon completion of construction, the authors established long-distance telephone communication with the operations personnel once again and directed the sequencing of control system procedures which were required to bring the evaporation area to near-steady state operation and under automatic control. Startup of the first train was extended somewhat over a period of about 48 hr. because of minor difficulties with leaky gaskets and the like. However, startup of the second train required only about 10 hr., and the sequence indicated by the simulator was followed very closely. Thus, the evaporation area was operating at design capacity within a few days.

Between completion of an agreeable startup technique and the actual startup, a procedure for removing salt deposits from the vessels and heat exchangers was developed. This procedure was also difficult to perfect because of the need to keep the evaporation area onstream during the washing sequence. Nevertheless, it was perfected before startup. In addition, shutdown techniques were also developed.

Since the initial startup of the two trains in November and December, 1974, they have been started and shutdown many times. Obviously, the response of the operations personnel during these procedures (as well as fly-washing) is not exactly as indicated schematically in Figure 3 since techniques vary among individuals. Furthermore, additional modifications, some of which were suggested by the simulator prior to startup, have been made to the trains in an attempt to further optimize performance. Nevertheless, it was use of the simulator that "de-bottlenecked" the trains and allowed their initial startup and operation in a manner which has undergone relatively few basic changes.

Acknowledgments

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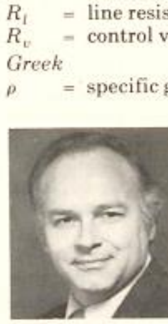
Nomenclature

C_v = valve liquid flow coefficient, gal./min./lb.$^{1/2}$/sq. in.$^{1/2}$
D = pipe diameter, ft.
f = friction factor.
E = electrical voltage.
h_i = height of liquid level in vessel i above datum, ft.
I = electrical current.
L = equivalent length, ft.
P_i = vapor pressure of water in vessel i, lb./sq. in. absolute.
ΔP_f = frictional pressure losses, lb./sq. in.
ΔP_{fl} = pressure drop through equivalent length of pipe, lb./sq. in.
ΔP_{fv} = pressure drop across control valve, lb./sq. in.
ΔP_p = pressure rise through centrifugal pump, lb./sq. in.
Q = volumetric flow rate, gal./min.
R = electrical resistance.
R_l = line resistance, lb./sq. in./gal.^{2}/min.^{2}
R_v = control valve resistance, lb./sq. in./gal.^{2}/min.^{2}

Greek

ρ = specific gravity.



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