

AN APPLICATION OF COMPUTERS FOR THE BEST INTERPRETATION OF CHEMICAL PLANT DATA

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A general feature of modern chemical plant is the provision of instruments for measurement and control. The controllers are indispensable for the proper running of the plant, and are in full-time operation. In the majority of cases, however, the charts from recorders get little careful study, and are usually treated as qualitative records—showing perhaps the input disturbances to the plant, and how well the controllers mitigate such input disturbances, or overcome self-generated variations within the plant itself. Certain plant records will be studied by the Cost Department, and a rate of flow record, for instance, might be integrated using a planimeter to calculate a total flow of raw material or product. Again, when a product is off specification, the relevant plant records might be studied with more care. In general, however, because of the lengthy calculations necessary to reduce the data to a fully comprehensible form, a large proportion of the information contained in the records is lost. In this paper, a description is given of the use of a digital electronic computer to calculate from plant records, a complete heat and mass balance of a continuous process. This work was the precursor of a study to formulate and solve a mathematical model of the process, with a view to improving the control, performance and throughput of the plant.

SIMPLIFIED HEAT BALANCE ON A HEAT EXCHANGER

It is frequently observed that, as far as steady state operation is concerned, the instruments on a plant provide redundant information. A simple example is a heat exchanger (see Fig. 1) where the overall heat transfer coefficient is required. Ignoring losses, the steady state heat balance is

$$F \cdot C_p \cdot \Delta T = F' \cdot C_p' \cdot \Delta T',$$

where F and F' are the fluid flows, C_p and C_p' are the specific heats and ΔT and $\Delta T'$ are the temperature rise and fall respectively. It would be unusual to find that the respective plant readings, when substituted in the equation gave an exact balance. In this situation an engineer undertaking

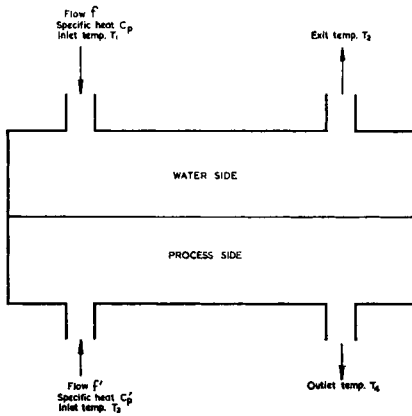


Fig. 1.—Heat balance on a heat exchanger. $T_2 - T_1 = \Delta T$; $T_3 - T_4 = \Delta T'$; $f \cdot C_p \Delta T = f' C'_p \Delta T'$.

such an investigation would have several obvious courses open to him and the calculations are simple.

HYDROGENATION PLANT

The next example is very much more complex, and the solution would have been impracticable without a computer.

In a hydrogenation process (see Fig. 2) re-circulated gas is mixed with fresh make-up hydrogen before being introduced to the converter. The liquid feed is metered, and the flows and compositions of the make-up gas, mixed gas, re-cycled gas and off gas are also recorded.

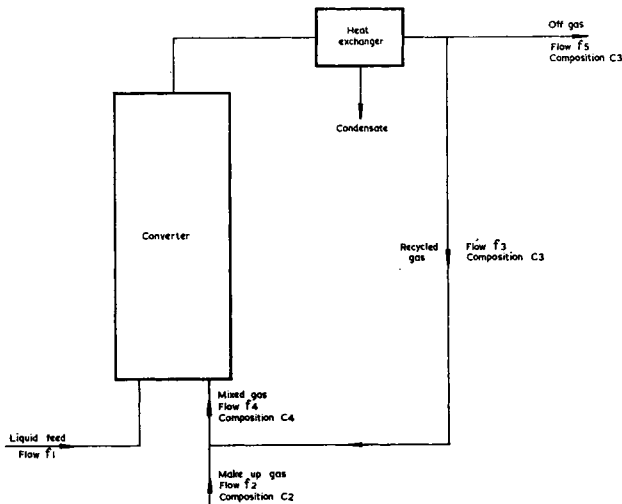


Fig. 2.—Schematic diagram of the gas flow in a hydrogenation plant.

Since the complete system in the steady state can be determined by mass balance from the liquid feed, the make-up flow and composition, and the re-circulation rate, four of the eight instruments are redundant. In the unsteady state, when the instantaneous rate of conversion is unknown, and if additionally, constant gas hold up cannot be assumed, of the six instruments measuring flow and composition of the two gas streams which are blended, two of these instruments are redundant.

Inevitably, if the values of the four parameters are calculated from a mass balance, they will not be in agreement with the measured instrument readings. Since the instruments measuring flows are orifice plates, the indicated flow must be corrected for density, i.e. composition, temperature and pressure, to obtain the true flow. The composition, however, is not precisely known, and little further use can therefore be made of the redundant information, apart from a very rough estimate of the order of magnitude of the possible errors.

MASS BALANCE

In order to obtain a set of consistent values from the plant records the following calculation was programmed for the Mercury computer.

By mass balances: Total flow of mixed gases is the sum of the two separate flows

$$f_2 + f_3 = f_4. \quad (1)$$

The flow of hydrogen in the mixed gas is the sum of the two separate hydrogen flows

$$f_4 C_4 = f_2 C_2 + f_3 C_3. \quad (2)$$

The overall hydrogen balance is given by

$$f_2 C_2 = f_5 C_3 + k f_1, \quad (3)$$

where k is the stoichiometric constant relating hydrogen consumption per unit liquid feed. The overall gas balance is

$$f_2 = f_5 + k f_1. \quad (4)$$

Hence, given f_1 , f_2 , f_3 and C_2 , the remaining quantities can be calculated, thus:

$$f_4 = f_2 + f_3 \quad (5)$$

$$f_5 = f_2 - k f_1 \quad (6)$$

$$C_3 = \frac{f_2 C_2 - k f_1}{f_2 - k f_1} \quad (7)$$

$$C_4 = \frac{f_2^2 C_2 - k f_2 C_2 f_1 + f_2 C_2 f_3 - k f_3 f_1}{(f_2 - k f_1)(f_2 + f_3)} \quad (8)$$

ERROR EQUATIONS

The flow meters measuring f_2, f_3, f_4 and f_5 will give an indicated reading which is a function of the gas compositions C_2, C_3, C_4 and C_3 respectively. Taking the density of pure hydrogen as $d_0 \text{ g/m}^3$ at N.T.P. and the density of the impurities as $d_1 \text{ g/m}^3$ at N.T.P. and the density of the gases at N.T.P. for which the four meters were calibrated as $d_2, d_3, d_4, d_5 \text{ g/m}^3$, respectively, if a gas of composition C_2 flows through the make-up gas flow meter, the "correction factor" to convert the true flow into the expected meter reading will be a function of C_2

$$\sqrt{\{[d_0 C_2 + d_1(1 - C_2)/d_2]\} T_2/P_2 \cdot P_0/T_0} = F(C_2),$$

where P_0 and T_0 are (respectively) the pressure and temperature at which the meter was calibrated, and P_2 and T_2 are the corresponding values at the time of reading the instrument.

Similar "correction factors" can be written for the other three gas flow meters, each being a function of the composition of the measured gas.

Thus a true flow of $f_2 \text{ cu ft/hr}$ should give a meter reading of $f_2 F(C_2)$ if the composition of the gas is C_2 . If the actual reading of the meter were f_2' then the error is

$$f_2 F(C_2) - f_2' = \varepsilon_2.$$

Similarly the error equations for the other flow meters are

$$f_3 F(C_3) - f_3' = \varepsilon_3$$

$$f_4 F(C_4) - f_4' = \varepsilon_4$$

$$f_5 F(C_5) - f_5' = \varepsilon_5$$

$$f_1 - f_1' = \varepsilon_1$$

(f_1 being a liquid flow meter has a negligible correction for density, etc.) and the error equations for the katharometers are

$$C_2 - C_2' = \varepsilon_6$$

$$C_3 - C_3' = \varepsilon_7$$

$$C_4 - C_4' = \varepsilon_8.$$

The object of the calculation is to minimize some function of the errors ε_i .

A suitable function is the sum of the weighted squares of the errors, viz.

$$E = \sum_1^8 (w_i \varepsilon_i)^2.$$

The weighting factors w_1, w_2 , etc., incorporate a factor to reduce all readings to the same numerical magnitude, and an additional factor proportional to the expected reliability of the instrument.

The minimization of E can be done in a number of ways, for example by methods of steepest descent; the way chosen was to solve the normal equations.

FORMULATION OF THE NORMAL EQUATIONS

At the co-ordinates of the minimum in the E dimension of the four dimensional surface formed by f_1, f_2, f_3 and C_2 , the rate of change of the error E with a change of f_1, f_2 etc., is zero. By partial differentiation

$$\partial E / \partial f_1 = \partial E / \partial f_2 = \partial E / \partial f_3 = \partial E / \partial C_2 = 0,$$

i.e.
$$\sum_1^8 w_i^2 \varepsilon_i \frac{\partial \varepsilon_i}{\partial f_p} = 0,$$

where $f_p = f_1, f_2, f_3, C_2$. These are four simultaneous non-linear equations which can be solved by Newton-Raphson's method [1].

SOLUTION OF THE NORMAL EQUATIONS BY NEWTON-RAPHSON'S METHOD

Given a set of non-linear algebraic simultaneous equations

$$f_i(x_j) = 0 \quad i, j = 1, 2, \dots, n$$

consider the Taylor expansions

$$f_i(x_j) = f_i(x'_j) + \sum_k (x_k - x'_k) \frac{\partial f_i}{\partial x_k}(x'_j),$$

where truncation occurs before the second derivatives. Assuming x'_j known and a good approximation to the solution (i.e. $x_k - x'_k$ small), it is reasonable to suppose x_j an improved solution and to equate $f_i(x_j) = 0$. This gives

$$\sum_k (x_k - x'_k) \frac{\partial f_i}{\partial x_k}(x'_j) = -f_i(x'_j),$$

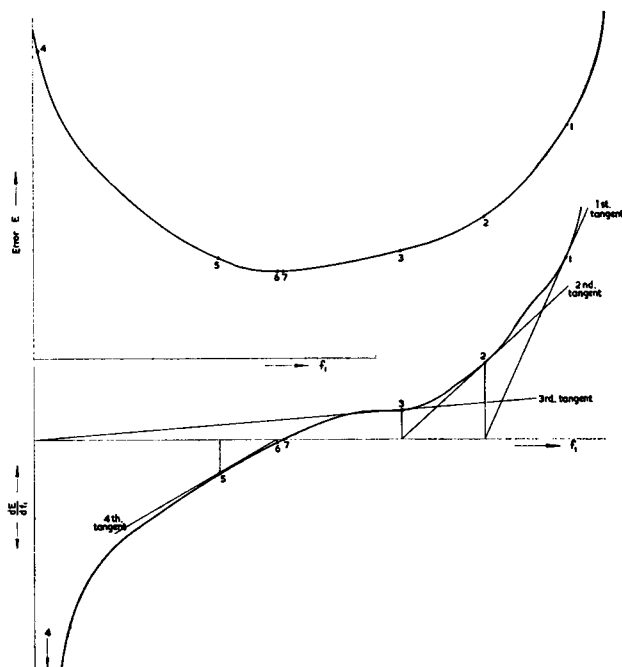


Fig. 3.—Newton-Raphson's method in one dimension.

i.e. n linear simultaneous equations in $(x_k - x'_k)$. The solution added to x'_k gives x_k . And so the iteration proceeds.¹

In one dimension the method is illustrated in Fig. 3.

Starting at any point (1), the slope of the normal equation curve is calculated, and the equation of the tangent is obtained. The value of f_1 where the tangent cuts the X axis is calculated. The error at this point (2) is determined and if less than at point (1) is taken as the new starting point. If the error is greater, as happens when taking the tangent at point (3), the distance along the X axis is repeatedly halved until a point (5) is found where the error E is less than the error at (3). This is continued until the calculated slope is less than a predetermined value.

In a multidimensional problem the direction of movement down the slope in all dimensions simultaneously is determined by the relative magnitudes of the partial differentials and the direction of steepest descent is chosen. The two-dimensional case is illustrated in Fig. 4, where the value of the error E is represented by contours on the surface formed by two of the parameters.

¹ A library programme for the general solution of up to 120 simultaneous non-linear equations was used to solve the normal equations. The library programme was written by Mr. S. E. Stonehewer of the I.C.I. Central Instrument Laboratory Digital Computer Section.

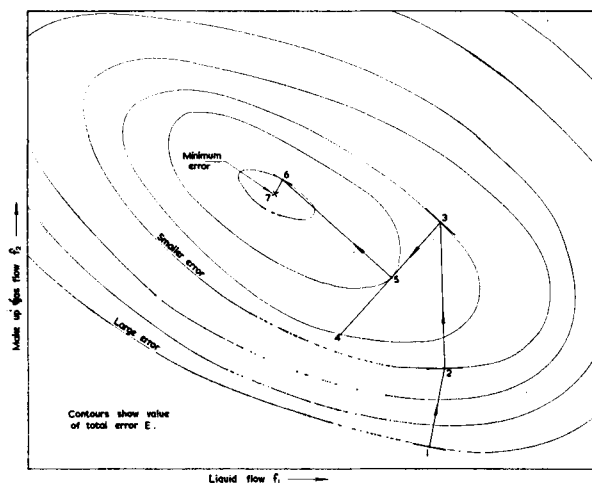


Fig. 4.—A method of steepest descent. Newton-Raphson's method in two dimensions.

In our particular case certain boundary conditions have to be imposed on the permitted values of the parameters. For instance, on practical grounds the gas composition should not exceed 100 per cent hydrogen and the flows must be positive. On mathematical grounds the composition must not exceed about 114 per cent, otherwise the calculated density is zero or negative and an infinite or imaginary flow is required to give a finite and positive meter reading.

In practice the computer arrives at a solution after 4–10 iterations, which takes between 30 and 60 seconds. When one considers that the Mercury computer performs an addition in only $180 \mu\text{sec}$, and a multiplication in $300 \mu\text{sec}$, the magnitude of doing this task by hand is apparent.

COMPUTER RESULTS

A typical set of results is shown in Table I. The first column gives the instrument reading, and the second column gives the flows as obtained by correcting the instrument reading for true composition, temperature and pressure. The third column gives the calculated flows and compositions which are both self-consistent and closest to the original readings. The fourth column gives the instrument error as a percentage of the true flow. As the indicated readings were variously between half- and full-scale reading, the instrument errors as determined are generally within the acceptable tolerance of such meters.

The same programme can be used to calculate the instantaneous rate of

TABLE I. Typical computer print-out of results.
 Plant data, 1250 hrs, 12 Aug. 60, auto h_2 control/3.

| | Instrument reading | Corrected for ptc | Calculated value | % error |
|--------------------|--------------------|-------------------|------------------|---------|
| Make-up hydrogen | 151 000 | 142 100 | 147 205 | - 3.899 |
| Composition % | 94.00 | 94.00 | 93.18 | 0.884 |
| Recycled gas | 50 000 | 46 664 | 48 243 | - 3.274 |
| Composition % | 81.20 | 81.20 | 78.96 | 2.838 |
| h_2 to converter | 232 000 | 206 614 | 195 448 | 6.366 |
| Composition % | 91.50 | 91.50 | 89.96 | 2.044 |
| Off gas flow | 47 500 | 47 262 | 47 739 | - 1.026 |
| Composition % | 81.20 | 81.20 | 78.96 | 2.838 |
| Liquid feed | 7380 | 7159 | 7204 | - 0.625 |

hydrogenation, if the plant records show that the plant is not in a steady state. In this case, the measured rate of liquid feed is treated as being grossly inaccurate, and the weighting factor w_1 is specified accordingly. The rate of hydrogenation is thus determined by the rate of consumption of hydrogen and it is assumed that the hold-up of hydrogen in the vessel is constant.

HEAT BALANCES

Associated with the hydrogenation vessel are seven heat exchangers, and local and overall heat balances can now be computed. By using redundant information of the type described earlier, the best selection of data can be made to satisfy an overall heat and mass balance. Heat transfer coefficients can be calculated and an accurate picture of the state of the catalyst can be obtained. The computed results are presented in a standard form, and any unusual behaviour in the plant can be readily seen. In one particular case, the calculation showed that a liquid flow was in the opposite direction to the expected (and usual) way. This explained the abnormal temperature measured in this flow line, which had earlier been ascribed to a faulty thermocouple.

REFERENCE

1. HILDEBRAND, F. B., Introduction to Numerical Analysis, p. 451. McGraw-Hill, 1956.