

TABLE 1. COMPARISON OF COMPUTATION TIMES BY DIGITAL AND HYBRID COMPUTER TECHNIQUES

	Digital Solution (IBM 360/40)		Hybrid Solution
	Explicit Form	Implicit Form	
Compile time, sec.	130	155	
Program load time, sec. (object form)	22	23	20
Δu increment*	0.0002	0.0002	0.01
Execution times, sec.			
single curve (no output)	0.45	0.48	0.1
single curve (output)	1.45 (print)	1.48 (print)	10.0 (plot)
complete data (Fig. 1)	45,000	48,000	520

* The indicated values of Δu were approximately the maximum usable values for the desired stability and convergence.

putational facilities as well as in computation times. While the problem thus solved was a relatively simple one, and thus required only a nominal outlay for hardware, the computation times show striking differences as illustrated in Table 1. Only if the digital solutions had been obtained on the fastest of current generation computers, whose execution times are one hundred times faster than that of the IBM-360/40 (2), would the solution times be competitive with those on the hybrid machine. As indicated above, in the solution thus presented full advantage was not taken of the speed capabilities of the hybrid machine, nor was the technique fully optimized. The addition of peripheral devices, such as an off-line plotter could further reduce the computation times by a significant factor.

The results represent a demonstration of the capabilities of the hybrid technique by comparison with those obtained by digital means. Hence, this leads to the next step in the progression, the use of the hybrid computer for the solution of more complex mathematical models, where full advantage can be taken of the nonlinear capabilities of the analog machine.

NOTATION

- A = dimensionless coefficient (ρ_B/kf)
 C = normalized gas phase concentration (c/C_o)
 C_o = constant inlet gas phase concentration, moles/volume

- f = void fraction in column, volume void/column volume
 k = mass transfer coefficient, moles/time/volume/concentration
 K = equilibrium coefficient, concentration/solids loading
 n = number of iterations
 q = solids phase loading, moles/weight of solids
 r = dummy variable in Equation (4) for θ
 s = dummy variable in Equations (4) and (6) for v
 u = dimensionless time (kKt/ρ_B)
 v = dimensionless distance (kx/V)
 V = constant superficial gas velocity (distance/time)
 W = normalized solid phase loading, (q/q_s)
 θ = dimensionless time parameter ($u - v/A$)
 ρ_B = bulk density of bed, weight of solid/column volume

LITERATURE CITED

- Hougen, O. A., and K. M. Watson, "Chemical Process Principles," Part III, John Wiley, New York (1947).
- Knight, K. E., *Datamation*, 14, No. 1, 31 (1968).
- Lapidus, Leon, "Digital Computation for Chemical Engineers," McGraw Hill, New York (1962).
- Needham, R. B., J. M. Campbell, and H. O. McLeod, *Ind. Eng. Chem. Process Design Develop.*, 5, 122 (1966).
- Vermeulen, Theodore, in "Advances in Chemical Engineering," T. B. Drew, ed., Vol. 2, pp. 147-208, Academic Press, New York (1958).

Digital Resolution of Residence Time Distributions from Pulse Response Data

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When an input pulse, $f_D(t)$, undergoes mixing in a system of unit response, $f_R(t)$, the output response, $f_{RD}(t)$, is obtained (Figure 1). The relationship is given by

$$f_{RD}(t) = \int_0^t f_D(u) f_R(t-u) du \quad (1)$$

The input and output are measured; the unit response is to be resolved. The problem is to obtain the best numerical solution to the convolution integral, Equation (1).

A hybrid solution for $f_R(t)$ has been described by Cupit

and Moser (1). This solution utilizes a black box (mixed stages in combinations) representation of the unit response. It appears to be more accurate and versatile to solve this system by a purely digital technique. This digital technique is also more readily available to potential users.

DIGITAL SOLUTION OF THE CONVOLUTION INTEGRAL

To solve Equation (1) the distributions are subdivided

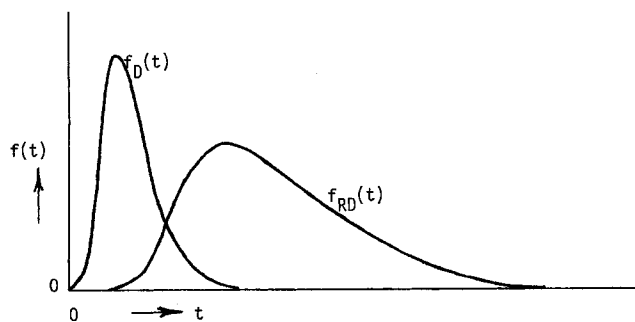


Fig. 1. Input and output frequency distribution curves.

into equal time increments, Δt (Figure 2). There are k increments of the input pulse and n increments of the output pulse. Equation (1) is then written:

$$f_{RD}(t_i) = \sum_{j=1}^i f_D(t_j) f_R(t_{i-j}) \Delta t, \quad 0 < i \leq n \quad (2)$$

The problem is to solve for all possible nonzero values of f_R . There can be $n - k$ of these; but there are n equations to choose from. This gives k degrees of freedom to minimize the errors as follows. Let,

$$\left[\sum_{j=1}^i f_D(t_j) f_R(t_{i-j}) - \frac{f_{RD}(t_i)}{\Delta t} \right] = \epsilon_i \quad (3)$$

and let the best fit be defined as that where:

$$\sum_{i=1}^n \epsilon_i^2 = \text{minimum} \quad (4)$$

This is obtained by setting the partial derivatives with respect to $f_R(t_m)$ equal to zero:

$$\sum_{i=1}^n f_D(t_{i-m}) \left[\sum_{j=1}^i f_D(t_j) f_R(t_{i-j}) - \frac{f_{RD}(t_i)}{\Delta t} \right] = 0 \quad (5)$$

$$0 \leq m \leq n - k$$

It should be noted that $f_D(t_j)$ is zero outside the region of $1 \leq j \leq k$.

This results in an $n - k$ by $n - k$ matrix of coefficients plus the right hand side vector for the linear equations in $f_R(t_i)$.

EXAMPLE SOLUTIONS

A FORTRAN program was written to:

1. Read and convert data into equal time increments.
2. Write the coefficient matrix based on Equation (5).
3. Invert the matrix and solve the linear equations.
4. List and graphically present the results.

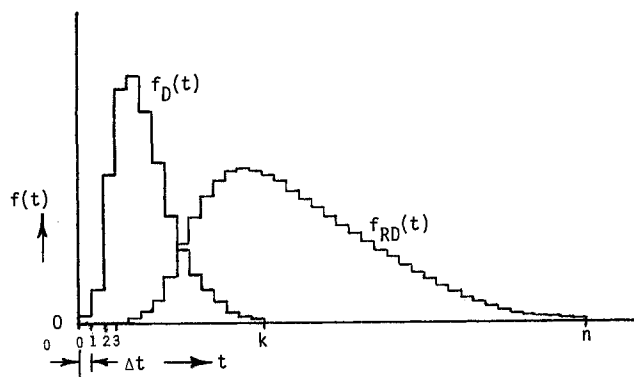


Fig. 2. Incremented curves of Figure 1.

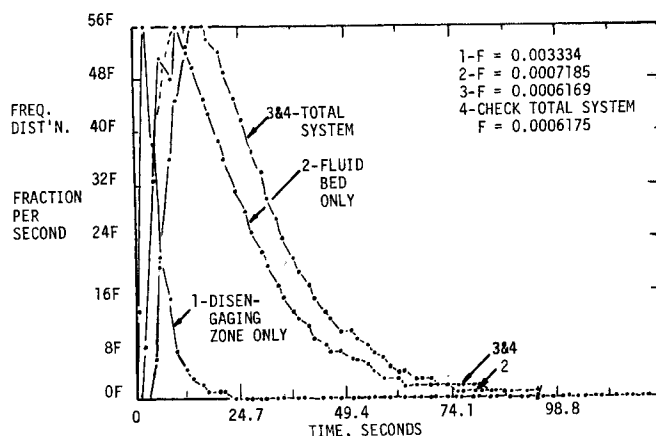


Fig. 3. Pulse response-fluidized bed.

Numerous data sets have been resolved; each required about 0.005 hr. of IBM 7094 time to solve. Typical of these is the resolved curve for a set of fluidized bed data. This is shown along with the input and output curves in Figure 3. Also given on the figure are the mean residence time, MN; relative standard deviations, RSD; and concentration scale factors, F.

To test the goodness of fit, the output move was regenerated from the input and resolved unit response. This is given by points 4 on Figure 3. Except for a single point, they overlay the original measured output curve (point 3).

For exact fits with no noise, the means and variances would be additive. Although not required in the mathematical sense, the additivity is closely approximated in the example as shown on the figure.

The digital technique has not been used previously because of instabilities (wildly fluctuating curves). Hybrid computer experience and the sum of least squares approach helped to overcome these instabilities. Criteria developed are, primarily:

1. The tail of the output is extended far enough to allow the resolved curve to decay naturally to zero. The program used fits for the last fourth of the output curve to an exponential decay and extends the tail 20%.
2. The time increment is changed if excessive oscillations occur (see dashed line in peak region, curve 2, Figure 3). A hundred time increments are normally used; as few as fifty may be required to achieve stability. Sixty-five were used in the example cases.
3. Smoothing the original curves, if necessary, will yield additional smoothing of the resolved curve. Such abnormalities as drifting baselines and negative values should be adjusted for. The program sets negative values to zero. No adjustments were required in the examples.

CONCLUSIONS

The digital technique yields the best resolved curve for the least squares fit.

The response curve is resolved without *a priori* assumptions.

Instabilities are avoided, for the most part, by adjustment now included in the data processing subroutines.

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LITERATURE CITED

1. Cupit, C. R., and Moser, J. H., *Chem. Eng. Prog.*, **62**, 60 (1966).