COMMUNICATIONS TO THE EDITOR

Hybrid Computer Solution of the Simple Fixed Bed Adsorption Model

D. C. ETESON and IMRE ZWIEBEL

Worcester Polytechnic Institute, Worcester, Massachusetts

A simplified version of the mathematical model which describes unsteady state adsorption in fixed beds, and consists of a pair of simultaneous linear partial differential equations, was solved by hybrid computer techniques. This model was deduced from the comprehensive description of the adsorption process by making the overriding assumption that the inlet concentration of the single adsorbate is very low. The dimensionless form of the resulting equations can be written as follows:

$$\frac{\partial C}{\partial v} + \frac{1}{A}\frac{\partial C}{\partial u} + \frac{\partial W}{\partial u} = 0 \qquad (1)$$

$$\frac{\partial W}{\partial u} = C - W \qquad (2)$$

$$C(o,u) = 1 \qquad (3a)$$

$$C(v,o) = 0 \qquad (3b)$$

$$W(v,o) = 0 \qquad (3c)$$

With Laplace transformation techniques Equations (1) to (3) can also be solved to give the semi-analytical solution (*4, 5*)

$$C = 1 - e^{-\theta}\int_o^v e^{-s} I_0(2\sqrt{s\theta})\,ds \qquad (4a)$$

$$W = e^{-v}\int_o^\theta e^{-r} I_0(2\sqrt{vr})\,dr \qquad (4b)$$

where I_0 is the zero order Bessel function of the first kind.

Thus, the proposed hybrid computer solution can be tested by comparing the results with those obtained from Equations (4). The values of C and W presented in Figures 1 and 2 are similar to those of Hougen and Watson (*1*). The accuracy is herewith improved, particularly at lower values of the distance parameter v, and the data are also presented over a wider concentration range. The coordinates on these figures are the same as were used by Hougen and Watson (*1*), the abscissa dimensionless time $\theta = u - v/A$, while the parameter is the dimensionless distance, v.

Also, for comparison, Equations (1) to (3) were solved numerically by using two different finite difference schemes, one explicit and one implicit (*3*). These results are also shown in Figures 1 and 2. While the numerical solution of these equations can be accomplished quite readily by a variety of simple techniques, the finite difference schemes were chosen for comparison of the time economy. Normally, when the simplified techniques cannot be applied, for example in the case of nonlinear equations, the finite difference schemes are still applicable, and

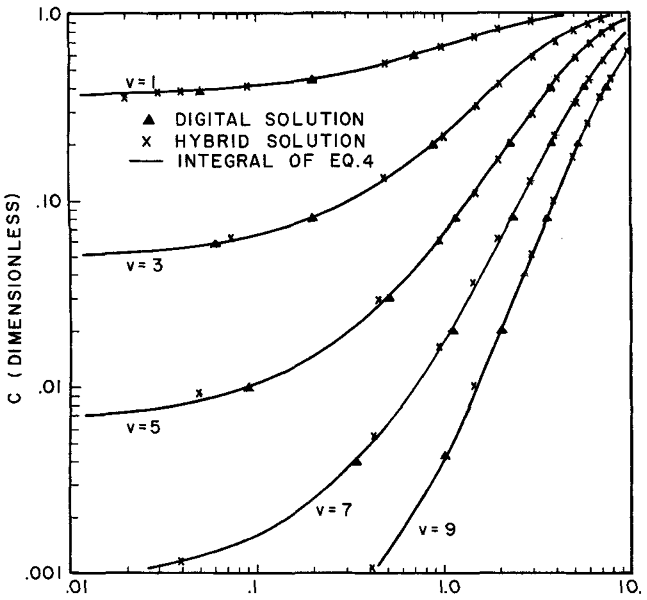

Fig. 1. Comparison of the adsorbate concentration results calculated by the indicated techniques.

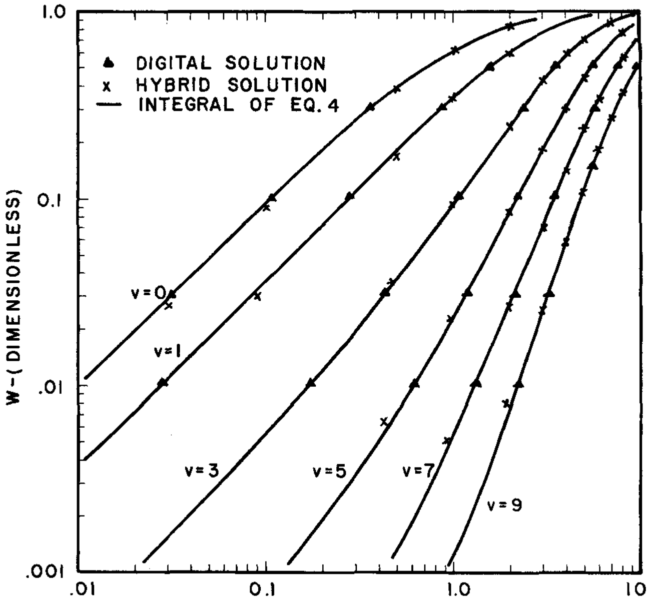

Fig. 2. Comparison of the adsorbent loading results calculated by the indicated techniques.

as a rule are the last and only resorts to the solution.

The hybrid solution was accomplished by using an analog computer program for the solution of the ordinary differential equation:

$$\frac{dC_2(v)}{dv} + \left[\frac{1}{A\Delta u} + \frac{1}{1 + \Delta u} \right] C_2(v) = Z_1(v) \quad (5)$$

where

$$Z_1(v) = \frac{1}{A\Delta u} C_1(v) + \frac{1}{\Delta u} W_1(v)$$

Equation (5) is the combination of the relationships obtained by writing the backward difference forms of the time derivatives of Equations (1) and (2). The subscript 2 represents the functions evaluated at the new time level, $u_2 = u_1 + \Delta u$, and the subscript 1 represents the functions at the old time level, u_1. The closed form integration of Equation (5), at least in principle, may be accomplished provided the function on the right hand side, $Z_1(v)$, is known. Lapidus (3) proposed such a scheme of solution by digital means. However, such technique provides only a slight improvement in computer time consumption over the finite difference methods previously mentioned.

Equation (5) involves the various functions at two consecutive time levels, and the solution at the higher level, $u_2 = u_1 + \Delta u$, requires that the solutions obtained at the lower level, u_1, be available continuously. It should be noted that in this case Equation (5) is linear, and it can be solved readily with the aid of the integrating factor

$$I(v) = \exp\left\{ \left[\frac{1}{A\Delta u} + \frac{1}{1 + \Delta u} \right] v \right\}$$

to give

$$C_2(v) = (I(v))^{-1} \left[(C_2)_o + \int_o^v I(s) Z_1(s) ds \right] \quad (6)$$

which, after sufficient repetitions will give a convergent power series solution. The solution of such recursive equations is a tedious task, since after as few as four integrations the coefficients of the terms in the series are complicated compendia of the constants A and Δu. For practical solutions as many as a thousand repetitions may be necessary, since the total operating time $U = n(\Delta u)$, where n is the number of increments taken, or the number of repetitive integrations required. Of course, n depends upon the magnitude of Δu, and if the solution is to converge into the exact solution, that is Equations (4), these increments must be small. Hence, one is inevitably led to a computer solution, with a need for some sort of memory for the preservation of the $Z_1(v)$, the solutions at the lower time levels.

Analog computer memory usually consists of storage elements capable of holding a single value of a continuous variable for a somewhat limited time. Although there are devices for storing a selected interval of a continuous function, their limited accuracy and high cost tend to force a preference toward digital memory combined with appropriate digital to analog (D-A) and analog to digital (A-D) converters. Where large numbers of values are to be stored, an analog memory to perform the same function would be one to two orders of magnitude more expensive.

Hence, the solution of Equation (5) by hybrid computer technique is proposed, provided the values of $Z_1(v)$ can be synchronously retrieved from the digital computer and supplied to the operating circuitry as the new time level integration is proceeding. This is the task of the hybrid interfacing between the two computers. Since the data from the digital computer are available at discrete values of v, they enter the analog machine as a staircase function. As the frequency of sampling is increased, the continuous function is most closely approximated. This, however, runs into hardware (D-A Converter) limitations and may greatly affect the computation times. Thus, the matching of the converted function to analog integration domain is one of the major tasks in programming the hybrid machine.

The calculations were carried out on a hybrid computer consisting of a model 680 analog computer, a PDP-7 digital computer, and an interface designed and constructed by members of the Electrical Engineering Department of Worcester Polytechnic Institute. The digital computer has 4,000 words of 18-bit memory and hardware multiply-divide. Neither machine, by itself, could have efficiently handled the problem at hand, if only because of the small memory capacity available.

The analog solution of the differential equation was standard with the single exception that the maximum output of the integrator representing $C_2(v)$ was limited by hardware to the initial value. This was necessitated by the fact that the D-A converters were calibrated so that the small, systematic roundoff error was positive; and hence it was determined that the effect of long-time accumulated error occasionally made $C_2(v)$ larger than its initial value, which is a physical impossibility. The solution of this systematic error problem was accomplished with the use of a feedback limiter on the integrator generating $C_2(v)$. It should be noted that one advantage of the hybrid solution may lie in the representation by analog signals of real variables so that a person familiar with the physical system can exert this knowledge in improving the solution.

To utilize the available time effectively, digital programs have been written to set all potentiometers, initialize the D-A converters, and log the output of selected amplifiers. The choices of potentiometer values, amplifiers, and other constants can be output on paper tape.

The programming was done in PDP-7 assembly language. All subroutines were written by the staff of the Hybrid Computer Center. Though FORTRAN could have been used for the initial condition (IC) state arithmetic, the sections run in real time would have been slowed by its use.

The output was plotted on a low speed X-Y plotter. During the analog operational (OP) cycles for which plots were desired, the digital program slowed the analog running time by a factor of 100 (to 10 sec. OP time), and appropriately adjusted its own timing and interpolation rate to the new time scale.

It is evident from Figures 1 and 2 that the solutions to Equations (1) to (3) obtained by the various methods agree with each other very well. The greatest deviations from the theoretical results, that is, the values of the integrals in Equations (4), are at the low values of C or W.

However, even under the most adverse conditions, the error is never greater than 5%. As the values of C increase these deviations decrease to less than 0.5% at $C = 0.5$ and less than 0.1% at $C = 0.9$. All these errors represent a systematic error of about 0.002 normalized concentration units resulting from the reading of the data. All data were read from the plots obtained from the X-Y plotter; increased accuracy could have been attained by providing for digital output or direct voltmeter readings from the analog circuitry. No doubt, these techniques would have considerably slowed down the computation times.

In obtaining these solutions, the hybrid computer technique was demonstrated to give satisfactory results, at considerable savings. These savings occur in both com-

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

	Digital Solution (IBM 360/40) Explicit Form	Implicit Form	Hybrid Solution
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_*)
θ = dimensionless time parameter ($u - v/A$)
ρ_B = bulk density of bed, weight of solid/column volume

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Digital Resolution of Residence Time Distributions from Pulse Response Data

J. E. GWYN

Shell Oil Company, Houston Research Laboratory, Deer Park, Texas

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

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

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