ChE curriculum

COMPUTERS AND APPLIED MATH IN THE ENGINEERING CURRICULUM

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THE INSTRUCTIONAL USE of analog and digital computers in today's engineering curriculum is assuming an ever increasing role. This situation has apparently arisen out of necessity, mainly because we tend to emphasize more sophisticated mathematical techniques as the basic key to comprehension and learning. Whereas in the b.c. era (i.e., before computers) undergraduates lived primarily in the "steady-state world", the contemporary student investigates the dynamics of processes in which the "steady-state" assumes its proper perspective as a limiting condition. Therefore the introduction of computers into the curriculum has been a major factor in fostering the evolution of engineering instruction from the art into the science stage.

In developing the full potential of computers and associated mathematics to meet the challenge of present day curricula, the possibility can exist that too much time is devoted to the tools and not enough to the subject matter. Therefore our purpose in this article is to indicate how we at LSU are attempting to bridge such a gap. Toward this end we require fundamental courses in analog and digital computation at the sophomore level, followed by advanced (hybrid) computation and applied mathematics for qualified students. We not only provide instruction on the use of these tools, but encourage such usage throughout the educational program with suitable applications in other coursework.

Employing practical demonstration examples in these advanced courses which submit readily to analysis by a variety of methods from classical mathematics to computer implemented numerical techniques, we stress the problem solving approach in each case. Thus a student's academic training provides the following two-fold methodology to support his professional capabilities:

- He must develop the ability to study a situation, evaluate facts and formulate the problem to be solved based upon sound and fundamental engineering principles.
- Once the problem has been defined quantitatively in engineering terms he must know, and be able to apply the tools with which to effect a reasonable solution.

Obviously one without the other is less than satisfactory.

In order to stimulate our students and to gage their progress in adapting to new situations it is instructive to challenge them with a "realistic" problem of a normally non-academic origin. The following example is of this type, having been culled from an article in the literature. We first describe the problem, develop the mathematical model subject to reasonable assumptions, and then outline several solutions applying analytical methods as well as various computer techniques.

STATEMENT OF THE EXAMPLE PROBLEM[1]

In a continuing effort to improve both the quality and performance characteristics of its packaging, a soft-drink corporation desired to consumer field test a newly designed returnable bottle for one of its products. Specifically, it wished to ascertain whether or not the new bottles would have a significantly longer service life than the bottles presently in use.

During the field test new bottles were inserted into the filling line at a specific daily rate over a period of several days. The filled containers (both new type and old bottles interspersed) were displayed for sale as usual in the marketplace. The "empties", returned by the consumer to the market after a reasonable delay period,

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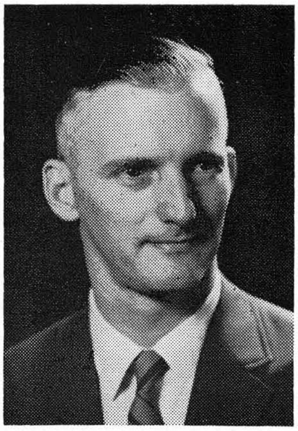

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were then sent to the plant for refilling. Data collected consisted of a daily count of the new type bottles as they passed the capping station during the bottling process. At this monitoring point both newly inserted bottles as well as bottles that had completed one or more field cycles were included in the count.

In order to obtain a quantitative evaluation of the test results it is necessary to model mathematically the complete cycle, then define and evaluate the performance parameters. To facilitate the development of a mathematical model the following simplifying assumptions are made:

a. The rate of purchase of test containers is directly proportional to the number of these bottles in the marketplace at any time.
b. The losses at the plant and market are negligible compared to the losses sustained in the home by the consumer.
c. There is a constant (average) time delay between purchase and re-insertion of the bottle in the market. This delay accounts for consumption of the product by the purchaser.
d. Time delays in the bottling plant are negligible compared to that by the consumer described in (c) above.

With these assumptions the modified process cycle is described by Figure 1 from which the model is to be derived.

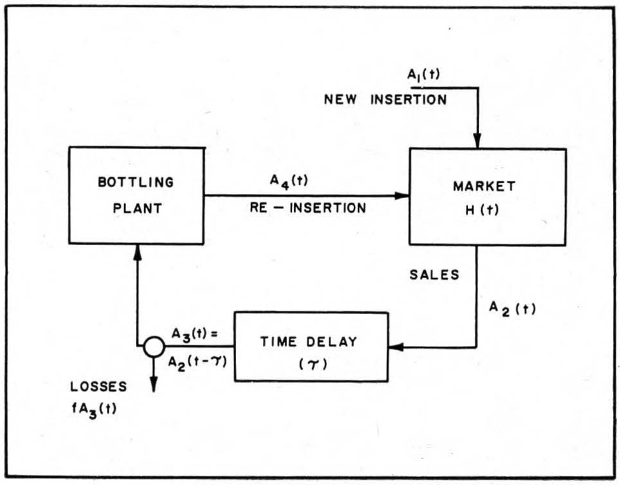

Figure 1. Flow Diagram for the Mathematical Model

DERIVATION OF THE MATHEMATICAL MODEL

An overall material balance for new type bottles on the market yields:

Rate of market accumulation		Rate of sale		Rate of re-insertion		Rate of new insertion
$\frac{dH(t)}{dt}$	$= -$	$A_2(t)$	$+$	$A_4(t)$	$+$	$A_1(t)$

$$\frac{dH(t)}{dt} = - A_2(t) + A_4(t) + A_1(t) \quad (1)$$

Focusing on the right hand side of Equation (1) the functions are evaluated as:

Rate of sale. If H(t) represents the number of bottles in the market at any time t, then by assumption (a) above

$$A_2(t) = kH(t) \quad (2)$$

where k is the constant of proportionality.

Rate of new insertion. For purposes of the field test, bottles will be inserted at a constant rate C (bottles per unit time) over a given period θ, thus

$$A_1(t) = C \text{ for } 0 \leq t \leq \Theta \quad (3a)$$

and,

$$A_1(t) = 0 \text{ for } t \geq \Theta \quad (3b)$$

Rate of re-insertion. If f is the fraction of bottles lost per cycle, the input to the bottling plant becomes the product of the fraction returned (1-f) and the number of empty bottles returned by the consumer, or

$$A_4(t) = (1\text{-}f)\ A_3(t) \quad (4)$$

But noting that A_3 is evivalent to the rate of sales A_2 displaced in time by the delay period τ, we have

$$A_4(t) = (1\text{-}f)\ A_2(t\text{-}\tau) = (1\text{-}f)\ kH(t\text{-}\tau) \qquad (5)$$

The substitution of these terms into Equation 1 yields:

$$\frac{dH}{dt} = -kH(t) + (1\text{-}f)\ kH(t\text{-}\tau) + A_1(t) \qquad (6)$$

Equation 6 is the mathematical model describing the process and is characterized by the three parameters k, f, and τ which must be evaluated by field test data. Clearly from the model it is obvious that k is a first order rate constant and the term 1/f represents the average number of cycles a bottle makes in the field before becoming lost. This latter term becomes, therefore, the criterion for comparison between old and new type bottles.

Data (Field test data is given in Table 1)

1/f (old type bottles) $\cong$ 3-4 cycles.

C = 200 new bottles/day inserted into cycle.

θ = 5 days (at a rate of 200/day for 5 days, a total of 1000 new type bottles are put into circulation for the test).

τ = 7 days (this represents the normal time between shopping trips for the average family).

Table 1. Field Test Data

Time (days)	Carrier Count Rate (per week)	(cumulative)
7	0	0
12	56	56
19	164	220
26	183	403
33	178	581
40	140	721
47	145	866

ANALYTICAL SOLUTION

Because of the transport delay term, $H(t\text{-}\tau)$, the solution can be most readily handled by Laplace transform methods. It should also be noted that Equation 6 lends itself to solution by finite difference methods on the digital computer by which the authors of the original article obtained their results. We define the Laplace transform of each term and make appropriate substitutions in Equation 6 to obtain the following algebraic expression:

$$sh(s) = -kh(s) + \alpha e^{-s\tau}h(s) + \frac{C}{s}(1-e^{-s\theta}) \qquad (7)$$

where $\alpha = (1\text{-}f)k$, and $H(0) = 0$ for this situation

Equation 7 when solved for the transformed dependent variable h(s) becomes:

$$h(s) = \frac{\frac{C}{s}(1-e^{-s\theta})}{(s+k-\alpha e^{-s\tau})} \qquad (8)$$

The analytical solution follows by first rearranging, then expanding Equation 6 using the binomial theorem, and inverting term-by-term to give:

$$H(t)=\frac{C}{k}\sum_{n=0}^{\infty}(1\text{-}f)^n e^{-k(t-n\tau)}\left\{e^{k\theta}\sum_{J=0}^{n}\frac{k^J(t-n\tau-\theta)^J}{J!}u(t-n\tau-\theta)-\sum_{J=0}^{n}\frac{k^J(t-n\tau)^J}{J!}u(t-n\tau)\right\} \qquad (9)$$

where $u(t-n\tau-\theta) = \begin{cases}0 \text{ for } t \leq n\tau-\theta \\ 1 \text{ for } t > n\tau-\theta\end{cases}$ is the Heaviside unit function.

The complete solution to this problem requires that parameter 1/f, the average number of cycles per bottle, be evaluated. To obtain this term we must first compute both $H\tau = H(t\text{-}\tau)$, the time displaced bottle concentration in the market, and $Hc(t\text{-}\tau)$ the cumulative total of bottles progressing through the bottling plant. By calculating the absolute value of the difference between $Hc(t\text{-}\tau)$ and He the cumulative field test data, an error function E(t) can be obtained. The correct values of k and f are therefore determined by varying these parameters systematically so as to minimize the criterion E(t) over the entire test period. With Equation 9 as a starting point it is evident that such a task can be quite formidable in terms of time even for the digital computer. A more reasonable approach using statistical-numerical methods follows:

DIGITAL COMPUTER SOLUTION

We first define an expression for the cumulative total of bottles in the bottling plant in terms of the bottle concentration $H(t\text{-}\tau)$

$$Hc_i = \sum_{j=1}^{i}(1\text{-}f)\ kH(t_j-\tau) \qquad (10)$$

where the summation ranges over daily values of concentration up to time t_i. As before the error function is calculated as the difference between Hc, the analytical, and He, the cumulative field test data. We require values of k and f to minimize E(t) summed over all data points.

$$E(t) = \sum_{i=1}^{m}(He_i - Hc_i)^2 \qquad (11)$$

where the index m represents the total number of data points collected in the field test and E(t) is a function of f and k. By the method of least squares a pair of equations may be derived by differentiating E(t) with respect to both f and k and setting the results to zero. Before differentiation Equation 11 is expanded by Taylor's series about some point z. We then differentiate

E(t) with respect to each parameter, equate the resulting partials to zero, and obtain the following linear equations:

$$\sum_{i=1}^{m}\left(He_i-g_{i,z}\right)\frac{\partial g_{i,z}}{\partial f} = \Delta f \sum_{i=1}^{m}\left(\frac{\partial g_{i,z}}{\partial f}\right)^2 + \Delta k \sum_{i=1}^{m}\left(\frac{\partial g_{i,z}}{\partial f}\right)\left(\frac{\partial g_{i,z}}{\partial k}\right) \quad (12a)$$

$$\sum_{i=1}^{m}\left(He_i-g_{i,z}\right)\frac{\partial g_{i,z}}{\partial k} = \Delta f \sum_{i-1}^{m}\left(\frac{\partial g_{i,z}}{\partial f}\right)\left(\frac{\partial g_{i,z}}{\partial k}\right) + \Delta k \sum_{i=1}^{m}\left(\frac{\partial g_{i,z}}{\partial k}\right)^2 \quad (12b)$$

where $\triangle f = f - f_z$ and $\triangle k = k - k_z$.

Initial estimates f_z and k_z of the unknowns f and k at some arbitrary point z, but sufficiently close that convergence will occur, are used to evaluate all sums in Equations 12, from which Δf and Δk are computed. Application of these incremental changes results in estimates f_{z+1} and k_{z+1} which should converge eventually to f and k.

By taking derivatives of Equation 10 with respect to the parameters f and k we obtain the following expressions:

$$\frac{\partial g_{i,z}}{\partial f} = \frac{\partial Hc_i}{\partial f} = -C\sum_{j=1}^{i}\left[\sum_{n=0}^{\infty}(n+1)(1-f)^n\left\{u_j - v_j + e^{-ka_j}\left(e^{k\dot{\theta}}v_j\alpha_j - u_j\beta_j\right)\right\}\right] \quad (13a)$$

$$\frac{\partial g_{i,z}}{\partial k} = \frac{\partial Hc_i}{\partial k} = C\sum_{j=1}^{i}\left[\sum_{n=0}^{\infty}(1-f)^{n+1}e^{-ka_j}\left\{v_j e^{k\theta}\left[\sum_{r=1}^{n}\frac{k^{r-1}b_j}{(r-1)!} + \alpha_j(\theta - a_j)\right] - u_j\left(\sum_{r=1}^{n}\frac{k^{r-1}a_j^{\,r}}{(r-1)!} - a_j\beta_j\right)\right\}\right] \quad (13b)$$

where $\alpha_j = \sum_{r=0}^{n}\frac{k^r(t_j - n\tau - \theta)^r}{r!}$; $\beta_j = \sum_{r=0}^{n}\frac{k^r(t_j - n\tau)^r}{r!}$

$a_j = t_j - n\tau$; $b_j = t_j - n\tau - \theta$

Heaviside unit functions:

$u_j = u(t_j - n\tau)$; $v_j = u(t_j - n\tau - \theta)$

Equations 12 and 13 are in a form which permits a digital computer solution. Given m cumulative field test data points and reasonable initial estimates for f_z and k_z, the partials in Equations 13 may be calculated for each point. Cross products of these partials at each point are accumulated according to Equation 12.

In order to test the convergence of this method, initial values f_z and k_z were taken at values given in Table 2 following. This Table also shows the final approximations f and k and the number of iterations required to achieve 3-place accuracy. The time required on an IBM 7040 computer for each case is given.

Table 2. Convergence Values, Digital Solution

Initial Estimates		Iterations Required	Time Required	Final Approximation	
f_z	k_z		sec	f	k
.058	.0293	22	61	.1636	.03701
.239	.043	21	59	.1643	.03704
.1	.01	26	72	.1636	.03701

Today's engineer must have a solid foundation in applied math to avoid absolescence in the light of advances in science and engineering . . .

In all cases above the computing time to converge to a satisfactory result was on the order of one minute. Certain steps could be taken to speed up convergence, but unless the problem is one which would be used frequently, there is little incentive for the extra programming effort. (Program documentation and sample problems are available from the authors for interested readers).

ANALOG COMPUTER SOLUTION[2]

From the student's point of view analog solution methods are often the most interesting, for the system model is programmed directly on the computer which responds (hopefully) to perturbation as does the real physical system. Furthermore, in this case there is considerable man-machine interaction, because the student forms an integral part of the information feedback loop.

In programming this problem for the analog the basic equations to be considered are Equations 6, 10, and 11. We perform the task of magnitude and time scaling and rewrite them in integral form below.

$$[.01H] = -\int_0^t\left\{10^{-1}(10k)[.01H] + 10^{-1}\langle 10k(1-f)\rangle[-.01H\tau] + (10^{-3}A_1)[-10]\right\}dt \quad (14)$$

$$[.01Hc] = -\int_0^t 10^{-1}\langle 10k(1-f)\rangle[-.01H\tau]\,dt \quad (15)$$

$$[e] = -\left\{[-.01Hc] + [.01He]\right\} \quad (16)$$

$$[E] = -\int_0^t\left[-\frac{e^2}{10}\right]dt \quad (17)$$

The parameter [e] represents the instantaneous difference between model and experimental value of the cumulative total of bottles, and [E], the criterion function, is proportional to the accumulated total error between these terms.

In the mechanization of these equations an electronic switch, triggered by the polarity change of a ramp function signal, was used to generate the discontinuous function $A_1(t)$. A variable diode function generator provided an approximation to the experimental field test data, He, and the transport delay was simulated by a fourth order modified Padé circuit. As indicated by the output curve, $H(t-\tau)$ of Figure 2, this approximation is quite adequate for the low fre-

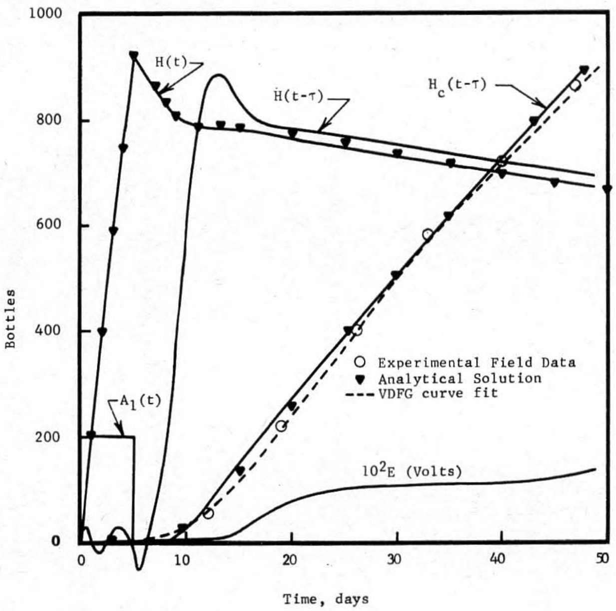

Figure 2. Output Curves, Final Run

quencies involved here (time scale for this example was chosen as 1.0 seconds of compute time per day of problem time).

The analog procedure, a global search technique, is relatively straight forward. Computing in the repetitive operation mode, the parameters k and f, each isolated on a potentiometer, are varied in alternative fashion, one discretely and the other continuously and E(t) values are obtained visually on the oscilloscope. When an approximate absolute minimum has been established, a few real time computer runs can be made to obtain a more accurate value of the criterion function. Three place accuracy in the answer is readily attainable with a digital voltmeter.

DISCUSSION OF RESULTS

The analog output for the final real-time run is presented in Figure 2. For purposes of comparison the analytical solution which was evaluated on the digital computer has also been included. As the figure shows both results predict accurately the peak of the H(t) curve and the slight dip beyond that point. In general, the agreement between these two results is excellent.

It is also apparent that the analog and analytical solutions for the cumulative field data, $Hc(t-\tau)$ curve, also show close agreement. In comparing these results with the analogous experimental data points also plotted in Figure 2, we observe that for these final k and f values the mathematical model provides a reasonable curve fit except initially where the rate of slope change is greatest. The difference here is due in part to the imperfect nature of the transport delay simulation circuit employed; the initial transients of which are clearly evidenced on the curve of Figure 2.

A comparison of the final parameter values is given in Table 3. The approximately 7% lower value of the parameter f obtained from the analog solution arises from the fact that experimental field data points were fit by a series of 10 straight line segments with the VDFG. On the other hand an almost exact fit using a 7th degree polynomial was employed to fit the data for the analytical solution. Despite these differences the final result in all cases suggests that the new type containers have a service life of more than 50-75% longer than the original carriers.

Table 3. Comparisons of Final Parameter Values

Parameter	Analog	Digital	Analytical
k	0.036	0.037	0.037
f	0.152	0.164	0.163
1/f	6.0	6.1	6.1

SUMMARY

In this article we have attempted to show by a specific example how digital and analog computers are being used in the undergraduate engineering curriculum at LSU to enhance instruction in applied mathematical methods. This particular problem, although relatively elementary from a mathematical point of view, has been useful in developing and exercising student proficiency in the following areas:

- The use of Laplace Transform techniques to obtain an analytical solution.
- The use of a statistical numerical method (least squares) to effect a digital solution.
- Finite difference methods (presented in the original publication) for the digital computer.
- Digital programming logic for the analytical as well as the two numerical methods.
- Analog programming techniques: the use of analog logic, switching, and other non-linear equipment, the development of a method of transport delay simulation.
- The use of a simple optimization method.

Analog and digital computers are needed in today's curriculum because we emphasize more sophisticated math techniques as the key to comprehension and learning.

Of equal importance from an instructional standpoint in the fact that this exercise, of an interdisciplinary nature, is a very practical industrial problem that any professional engineer might encounter. It follows therefore that the problem is completed when an interpretation of the mathematical solution invokes a practical engineering decision. We have found with this problem as with others which we have developed, that this "practical flavor" or realistic aspect has been an important factor in eliciting a most favorable response from among our students. As a follow-up to the problem presented here it was interesting for our students to discover that similar mathematics were reported by T. Wood[3], who investigated first order irreversible chemical kinetics in a series connected well-mixed and tubular reactor system.

REFERENCES

1. Barnes, B. G., R. E. Fuchs, and R. A. Somsen, TAPPI, **50**, 72A (1967).
2. The analog computer solution: Simulation, **Vol. X**, No. 4, 157 (April 1968).
3. Wood, T., Nature, **191**, 589 (1961).

KING: CASE PROBLEMS

(Continued from page 125)

CP-3. **Removal of Water Vapor in Freeze-Drying.** Process Synthesis (Kumar and King). 89 pages ($2.75).

This problem requires that the student generate and give a rough, evaluative screening to different approaches to the removal of water vapor which is being continually generated in a vacuum chamber, in this case a freeze-drying process. Initial attention is given to the conception of various techniques for removing water vapor. Then preliminary analyses are made of the proposed schemes to check the feasibility of each process, to gauge its requirements in terms of materials and energy, and to determine the merits and drawbacks of the proposal.

CP-4 **Desalination by Reverse Osmosis.** Process Synthesis and Optimization (Thompson and King). 60 pages ($2.00).

The student is presented with the basic physical concepts underlying reverse osmosis and is given some indication of the difficulties which may arise and the factors to be compromised in a reverse osmosis desalination process. The principal problem is to determine the best configuration of a reverse osmosis unit so as to achieve minimum energy consumption. The student must recognize the mechanisms by which design parameters influence pressure drop and water flux. He must ascertain which decisions can be made on the basis of qualitative or common sense thinking rather than through the optimization of formal mathematical equations. Finally, he can determine optimum values of the remaining decision variables through either mapping or a formal optimization procedure.

CP-5. **Sulfate Removal from Brackish Water.** Process Synthesis (Forrester and Lynn). 50 pages ($1.50).

This problem concerns the synthesis of a process which removes sulfate from a brackish water supply and which permits the recovery of both the potable water and its previous mineral content. The student is given several existing processes with which to work and is asked to combine them in the best way. Several different elements of process engineering are involved, including development of process flow sheets and mass balances, consideration of the heat requirements of different processing sequences, thermodynamics of reactions in aqueous solution, and consideration of pollution potentials during a process design.

CP-6. **An Evolutionary Problem in Process Simulation.** Process Simulation (Grens). about 55 pages ($1.75).

In this problem a number of basic aspects of process simulation are incorporated in a series of computer implemented projects, which evolve from basic equilibrium vaporization calculations to simulation of a process with material and enthalpy recycle loops. The problem is based upon a hydrocarbon absorber-stripper system, with absorber and stripper each having only one stage. First the student is asked to develop efficient procedures for equilibrium flash computations. Then he must develop simulations for the absorber-stripper system, with alternative convergence techniques being used and compared. Finally interstream heat exchange is added to the problem, and simulations of the dual loop system (material and thermal recycle loops) using both direct substitution and convergence accelerating techniques are sought. Development of efficient modular simulation programs is stressed throughout.

CP-7. **Removal of Inerts from Ammonia Synthesis Gas.** Process Synthesis and Analysis (Alesandrini, Sherwood and Lynn). about 60 pages ($1.75).

The purge of methane and argon from ammonia synthesis recycle gases causes a substantial simultaneous loss of hydrogen and nitrogen. This problem pursues the question of somehow obtaining a partial or complete separation of methane and argon from the other gases, by taking advantage of the unusual vapor-liquid equilibrium behavior of the system of these gases mixed with ammonia. Successively better process modifications are developed and are explored through energy and mass balances, followed by preliminary equipment sizing and economic evaluation. A computer calculation of the behavior of an absorber-stripper may be included at the discretion of the instructor.