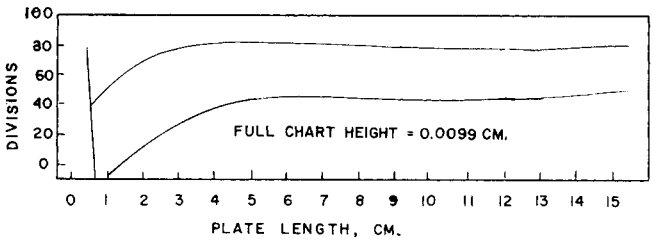

Fig. 3. Typical chart reading from profilometer.

is the surface of a naphthalene plate prior to its exposure to warm air. After sublimation for a period of time the surface was again measured and is shown as the lower trace. Thus, the difference between the two lines can be used as a direct measure of the amount of naphthalene that has sublimed.

The reproducibility achieved with this extremely sensitive profilometer was excellent. This profilometer lends itself nicely to continuous measurement of surface contours and should be quite useful for certain types of mass transfer studies as well as studies which require a record of changing surfaces.

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Examples of the Use of the Initial Value Method to Solve Nonlinear Boundary Value Problems

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Nonlinear ordinary differential equations of boundary value type occur rather frequently in various fields of chemical engineering. Different methods have been suggested to solve the governing equations. Runge-Kutta method is the most generally used numerical integration scheme. Due to the nature of boundary conditions, it is necessary to guess appropriate missing initial conditions and to match the computed result with the known final condition. This is always done by the trial-and-error method. This method takes considerable computer time to obtain accurate missing initial conditions. The purpose of this note is to illustrate the initial value method as a quite different approach to attack this kind of problem. Initiated by Topfer, Goldstein (1957) and extended by Klamkin (1962) and Na (1967, 1968), the method provides a very convenient alternative. By this method the original boundary value problem is transformed into an initial value problem which in turn is easily solved by any numerical integration scheme. Two problems previously appeared in literatures are solved to illustrate the application of this method.

POWER-LAW FLUIDS FLOW PAST A SEMI-INFINITE FLAT PLATE

Hsu (1969) recently examined the steady two-dimensional boundary layer flow of power law fluids past a flat plate, using the methods of series expansion and steepest descent to solve the governing equation. The present study solves this problem by the initial value method in an exact way.

Following Hsu, the resulting equation and the boundary conditions after similarity transform are given by

$$f''' + f(f'')^{2-n} = 0 \tag{1}$$

and

$$f(0) = 0, \quad f'(0) = 0, \quad \text{and} \quad f'(\infty) = 1 \tag{2}$$

where the prime denotes differentiation with respect to η. Now we define the following new variables

$$f = A^{\alpha_1} \bar{f} \tag{3}$$

$$\eta = A^{\alpha_2} \bar{\eta} \tag{4}$$

where A, α_1, and α_2 are constants to be determined. Substituting Equations (3) and (4) into Equation (1) we obtain

$$\bar{f}''' + \bar{f}(\bar{f}'')^{2-n} A^{\alpha_1(2-n)+\alpha_2(2n-1)} = 0 \tag{5}$$

For Equation (5) to be independent on A we let

$$\alpha_1(2-n) + \alpha_2(2n-1) = 0 \tag{6}$$

Thus Equation (5) becomes

$$\bar{f}''' + \bar{f}(\bar{f}'')^{2-n} = 0 \tag{7}$$

The first two boundary conditions then become

$$\bar{f}(0) = 0, \quad \bar{f}'(0) = 0 \tag{8}$$

To obtain the missing initial condition we let

$$f''(0) = A \tag{9}$$

Expressing in new variables, Equation (9) becomes

$$A^{\alpha_1 - 2\alpha_2}\bar{f}''(0) = A \tag{10}$$

By letting

$$\alpha_1 - 2\alpha_2 = 1 \tag{11}$$

we obtain

$$\bar{f}''(0) = 1 \tag{12}$$

Solving Equations (6) and (11) for α_1 and α_2 gives

$$\alpha_1 = \frac{2n-1}{3} \quad \text{and} \quad \alpha_2 = \frac{n-2}{3} \tag{13}$$

Now the original boundary value problem is already transformed into initial value problem of Equation (7) subject to the conditions of Equations (8) and (12). To determine the constant A we use the final condition of Equation (2). Introducing the new variables we obtain

$$A^{\alpha_1 - \alpha_2}\bar{f}'(\infty) = 1 \tag{14}$$

Inserting Equation (13) we finally obtain

$$A = [\bar{f}'(\infty)]^{-\frac{n+1}{3}} \tag{15}$$

The procedures to solve the transformed problem are as follows:

1. Choose a value of n.
2. Integrate Equation (7) with the conditions given by Equations (8) and (12) by the fourth-order Runge-Kutta method for $\bar{f}$ and $\bar{f}'$ until $\bar{f}'$ becomes a constant value which is equivalent to $\bar{f}'(\infty)$.
3. Calculate A from Equation (15) which is $f''(0)$ by definition as given by Equation (9).
4. Repeat steps 1 through 3 as we desire.

The computed results are tabulated in Table 1 for various n. The drag coefficient C_d is calculated from the following equation

$$C_d = [n(n+1)]^{-\frac{n}{n+1}}[f''(0)]^n \tag{16}$$

It is seen from Table 1 that Hsu's results agree quite well with the present exact solution. However, the present method is much easier to use. The whole computations took less than one and one-half minutes of computer time on an IBM 360/model 50 digital computer.

AXIAL DIFFUSION IN ISOTHERMAL TUBULAR FLOW REACTORS

For the second illustration we consider the steady isothermal flow tubular reactor, a topic of extensive investigation. Wehner and Wilhelm (1956) obtained an analytical solution for the first-order reaction. Fan and Bailie (1960) numerically solved the problem for reaction other than first order by finite difference method. For the present illustration we consider general order reaction. The governing material balance and its boundary conditions are given by

$$\frac{1}{P_e}\frac{d^2Y}{dX^2} - \frac{dY}{dX} - RY^n = 0 \tag{17}$$

with

$$X = 0; \quad \frac{1}{P_e}\frac{dY}{dX} = Y - 1 \tag{18}$$

$$X = 1; \quad \frac{dY}{dX} = 0 \tag{19}$$

where $Y = C/C_0$, $X = x/L$, $P_e = uL/E$, and $R = kLC_0^{n-1}/u$.

By the initial value method we define the new independent variable by

$$Y = A\bar{Y} \tag{20}$$

where A is constant to be determined. Introducing the new variable, Equation (17) becomes

$$\frac{1}{P_e}\frac{d^2\bar{Y}}{dX^2} - \frac{d\bar{Y}}{dX} - RA^{n-1}\bar{Y}^n \tag{21}$$

For Equation (21) to be independent on A we define a new dimensionless reaction rate parameter by

$$R^* = RA^{n-1} \tag{22}$$

Then we have

$$\frac{1}{P_e}\frac{d^2\bar{Y}}{dX^2} - \frac{d\bar{Y}}{dX} - R^*\bar{Y}^n = 0 \tag{23}$$

Its final condition is given by

$$\frac{d\bar{Y}}{dX}(1) = 0 \tag{24}$$

To obtain the missing final condition we let

$$Y(1) = A \tag{25}$$

Then we have

$$\bar{Y}(1) = 1 \tag{26}$$

Thus Equation (23) can be readily integrated by the fourth-order Runge-Kutta method with the two final conditions given by Equations (24) and (26). Calculation proceeds from $X = 1$ until $X = 0$. Then A is ob-

TABLE 1. COMPARISON OF HSU'S RESULTS WITH PRESENT STUDY FOR BOUNDARY LAYER FLOW OF POWER-LAW FLUIDS

	Present study		Hsu	
n	$f''(0)$	C_d	$f''(0)$	C_d
0.1	0.11711	0.98629	0.1160	0.9853
0.2	0.15483	0.87352	0.1528	0.8712
0.3	0.19487	0.76074	0.1922	0.7577
0.4	0.23612	0.66252	0.2332	0.6592
0.5	0.27790	0.58021	0.2748	0.5770
0.6	0.31901	0.51160	0.3163	0.5090
0.7	0.35913	0.45453	0.3569	0.4526
0.8	0.39779	0.40676	0.3963	0.4055
0.9	0.43502	0.36669	0.4339	0.3659
1.0	0.47032	0.33256	0.4696	0.3321
1.1	0.50511	0.30427	0.5033	0.3030
1.2	0.53533	0.27821	0.5347	0.2778
1.3	0.56556	0.25666	0.5640	0.2558
1.4	0.59629	0.23710	0.5912	0.2363
1.5	0.61885	0.22027	0.6164	0.2190
1.6	0.64319	0.20529	0.6398	0.2046
1.7	0.66606	0.19199	0.6614	0.1897
1.8	0.68575	0.18014	0.6815	0.1773
1.9	0.70781	0.16593	0.7003	0.1661
2.0	0.72757	0.16032	0.7180	0.1561

TABLE. 2. COMPARISON OF ANALYTICAL AND COMPUTED INLET AND OUTLET CONCENTRATIONS

$P_e = 0.01$						
		Computed			Analytical	
R	0.5	1.0	5.0	0.5	1.0	5.0
Inlet concentration	0.6681422	0.5020777	0.1696589	0.6681417	0.5020772	0.1696591
Outlet concentration	0.6664966	0.4995871	0.1655181	0.6664810	0.4995859	0.1655178
$P_e = 5.0$						
		Computed			Analytical	
R	0.5	1.0	5.0	0.5	1.0	5.0
Inlet concentration	0.9163044	0.8542762	0.6180384	0.9163044	0.8542765	0.6180390
Outlet concentration	0.6280848	0.4166188	0.0388571	0.6280797	0.4166156	0.0388568

TABLE 3. CONCENTRATION PROFILES FOR HALF-ORDER REACTION

	$P_e = 0.01$			$P_e = 5.0$		
$X \backslash R$	0.75011	1.48392	19.1057	0.66474	1.11443	33.4150
0.0	0.66823	0.45197	0.12195	0.85312	0.84253	0.72871
0.1	0.66792	0.45145	0.12111	0.78145	0.76586	0.60037
0.2	0.66764	0.45098	0.12037	0.71335	0.69334	0.48612
0.3	0.66739	0.45057	0.11917	0.64893	0.62505	0.38647
0.4	0.66718	0.45021	0.11914	0.58835	0.56115	0.30009
0.5	0.66699	0.44991	0.11866	0.53194	0.50194	0.22682
0.6	0.66685	0.44966	0.11826	0.48025	0.44796	0.16616
0.7	0.66673	0.44947	0.11796	0.43431	0.40022	0.11768
0.8	0.66665	0.44934	0.11774	0.39593	0.36048	0.08117
0.9	0.66660	0.44925	0.11761	0.36830	0.33198	0.05714
1.0	0.66658	0.44923	0.11756	0.35717	0.32052	0.04796

TABLE 4. CONCENTRATION PROFILES FOR SECOND-ORDER REACTION

	$P_e = 0.01$			$P_e = 5.0$		
$X \backslash R$	0.75041	1.11133	12.0761	0.14093	2.55472	26.8962
0.0	0.66796	0.60159	0.25198	0.97463	0.78648	0.49736
0.1	0.66765	0.60121	0.25127	0.96213	0.69125	0.32097
0.2	0.66737	0.60087	0.25064	0.94998	0.61480	0.22846
0.3	0.66712	0.60057	0.25008	0.93822	0.55235	0.17334
0.4	0.66690	0.60031	0.24959	0.92689	0.50065	0.13757
0.5	0.66672	0.60010	0.24918	0.91607	0.45745	0.11290
0.6	0.66645	0.59992	0.24885	0.90592	0.42129	0.09517
0.7	0.66638	0.59978	0.24859	0.89668	0.39139	0.08214
0.8	0.66633	0.59968	0.24840	0.88881	0.36771	0.07268
0.9	0.66631	0.59962	0.24829	0.88307	0.35126	0.06649
1.0	0.66629	0.59960	0.24825	0.88074	0.34474	0.06410

tained from Equation (18) as

$$A = \left[\bar{Y}(0) - \frac{1}{P_e} \frac{d\bar{Y}}{dX}(0) \right]^{-1} \qquad (27)$$

and R is obtained from Equation (22). Finally Y is calculated from Equation (20).

A step size of 0.02 is used for numerical integration. In Table 2, the computed results for first-order reaction are compared with that calculated from the analytical solution. It is seen that the error is less than 10^{-5} which ascertains the accuracy of the fourth-order Runge-Kutta method. Other sample results are shown in Tables 3 and 4 for half and second-order reactions, respectively.

It is apparent from the above two illustrations that the initial value method provides a very useful tool for solving the nonlinear boundary value problems. It saves computer time in addition to its easy application. However, it should be noted that not all the problems of boundary value type can be solved by this method. Its applicability depends on finding the appropriate transformation of variables. Otherwise this method fails. Fortunately, a wide spectrum of problems of fluid mechanics, heat and mass transfer, reactor design, and reactor stability fall into the realm where the initial value method is applicable.

NOTATION

A = constant
B = constant
C = concentration
C_0 = inlet concentration
C_d = drag coefficient
E = axial dispersion coefficient
f = dimensionless stream function
k = reaction rate constant
n = parameter in power-law model
L = reactor length
u = velocity
x = axial coordinate
Y = dimensionless concentration

Greek Letters

α_i = constant
η = stretched dimensionless coordinate

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