PRINCIPLE OF ENVIRONMENTAL MATHEMATICS

Shooting Methods

We now take the approach of attempting to convert a boundary value problem into an equivalent initial value problem. This would permit the use of the powerful and accurate techniques developed in preceding sections for initial value problems.

To illustrate the approach, we turn again to the example used earlier:

$$\frac{d^2y}{dx^2} + Ay = B \tag{1}$$

$$y(0) = 0, y(L) = 0$$

This problem can be recast as the following initial value problem:

$$\frac{d^2y}{dx^2} + Ay = B \tag{2}$$

$$y(0) = 0, \; \frac{dy}{dx}(0) = U$$

where U is unknown, and must be chosen such that $y(L)$ and thus the boundary value problem (1) is reproduced, if we arbitrarily choose a value for U, and solve the initial value problem (2) by any standard numerical method, the solution might appear graphically as shown in Fig.1. (We will assume that the step size is sufficiently small that truncation error is negligible, and we will neglect round off error. Since $y(L)$ is not zero, we have not reproduced the boundary value problem (1). (Since $y(L)$ is clearly a function of U. we have denoted $y(L)$ as $y,(U)$.) In order to bring y_L (U) closer to zero the strategy should apparently be lo reduce U. (The similarity to a ballistics problem is of course the motivation for the term "shooting method.") Seeking the appropriate value of U in order to satisfy the boundary condition at $x = L$ can be stated as searching for U such that

$$y_L(U) = y(L) = 0 \tag{3}$$

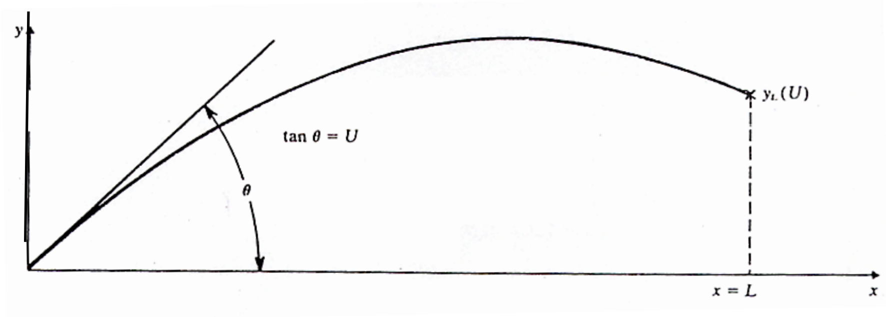


Figure 1

This is a root solving problem, and we can employ any of the standard methods which do not utilize explicitly [lie derivative of the function. Thus bisection or the secant method is likely candidates in this situation. Since the secant method is more rapidly convergent for well-behaved functions with simple roots, it will usually be the first choice for the present application.

We have only to provide two estimates of the root of (3); call them U_∞ and U_0. Now two solutions of the initial value problem (2) are carried out, yielding $y_L(U_\infty)$ and $y_L(U_0)$. A new estimate of U can then be obtained, given by

$$U_1 = U_0 + \frac{y(L) - y_L(U_0)}{[y_L(U_0) - y_L(U_\infty)]/(U_0 - U_\infty)} \qquad (4)$$

The process is continued to convergence, with each functional evaluation of $y_L(U)$ requiring a numerical solution of the initial value problem (2). Examples are given in Problems 1.

Since iteration to convergence may require from three to ten or more iterations, depending on many factors, it makes good economic sense in many cases to use a reasonably efficient method to solve the initial value problem. One of the predictor-corrector schemes such as the fourth-order Adams method or Hamming's method would seem suitable. However, since the solution must be obtained precisely at $x = L$, the use of a method winch makes automated slop size changes is probably not desirable. Instead, it may be best to use a fixed step size or a series of predetermined step sizes which together arrive exactly al $x = L$. (If the end point is not hit exactly, the value of y at this point can be found by interpolation, but this is just another complicating factor and adds to the possibility of error.)

Example 1:

By using the shooting method described above, solve the boundary value problem. We first transform the boundary value problem to an equivalent initial value problem:

$$\begin{cases} \dfrac{dy}{dx} = z & y(0) = 0 \\ \dfrac{dz}{dx} = 8 - \dfrac{1}{4}y & z(0) = U \end{cases}$$

where U is unknown and must be determined such that $y(10)=0$, We choose $U = 10$ for our first attempt. (From the preceding problem a reasonable estimate can be obtained for this slope; in many cases the initial guess will be farther off, but the method will usually still work unless the initial estimate is *very* far the correct value.) Using a fourth-order Rung-Kutta method with $\triangle x = 0.1$, we find $y(10) = 3.74517$. A second solution must be obtained before the root solving approach discussed above can be employed. If $U = 11$ is used, then the numerical solution of the initial value problem yields $y(10)= 1.82730$. This is (perhaps surprisingly) closer to the desired value of zero than the solution for $U = 10$. (One would be tempted to reduce the slope if $y(10)$ is too high for the first estimate of U. However, this is by no means always the proper approach. The secant method will eventually converge to the correct value in any case.) Enough information is now available to determine the next estimate of U based on the secant method given by (4). We let $U_\infty = 10$ and $U_0 = 11$. Then $y_L(U_\infty)=3.74517$ and $y_L(U_0)=1.82730$. Equation (4) then yields

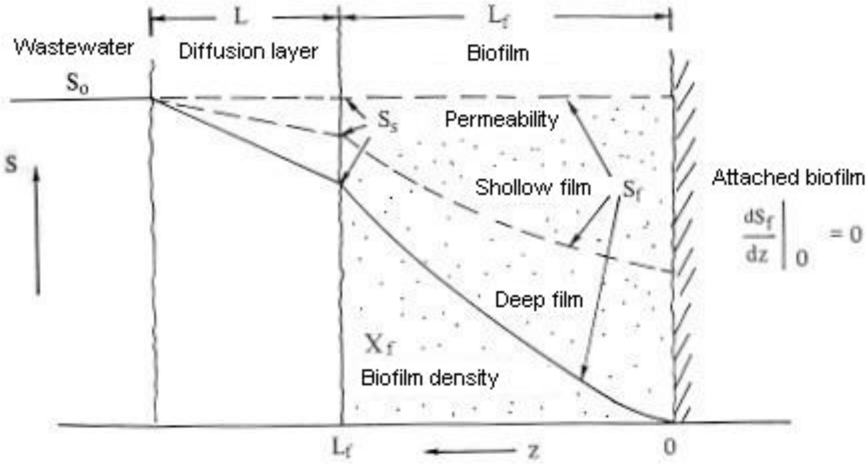
$$U_1 = 11 - \frac{1.82730}{(1.82730 - 3.74517)} = 11.95227$$

The solution to the initial value problem with this as z(0) gives $y(10) = 5.72205\times10^{-5}$. This is remarkably small, and we will accept this solution, which is

$y(0) = 0$	$y(6) = 67.0530$
$y(1) = 15.3783$	$y(7) = 53.5809$
$y(2) = 34.8260$	$y(8) = 34.8250$
$y(3) = 53.5817$	$y(9) = 15.3776$
$y(4) = 67.0535$	$y(10) = 0.000057$
$y(5) = 71.9429$	

Comparison with Table 9.7 shows that these values differ from the exact solution by less than 1 digit in the third decimal place. Only three solutions of the initial value problem were necessary to obtain this solution. More iterations would be required if poorer initial estimates of U were made.

Example 2:



Simulate the removal of phenol from wastewater by biofilm. The governing equation can be formulated by Haldane equation at steady state is given by:

$$D_f \frac{d^2 S_f}{dz^2} = \frac{k X_f S_f}{K_s + S_f + \frac{S_f^2}{K_I}}$$

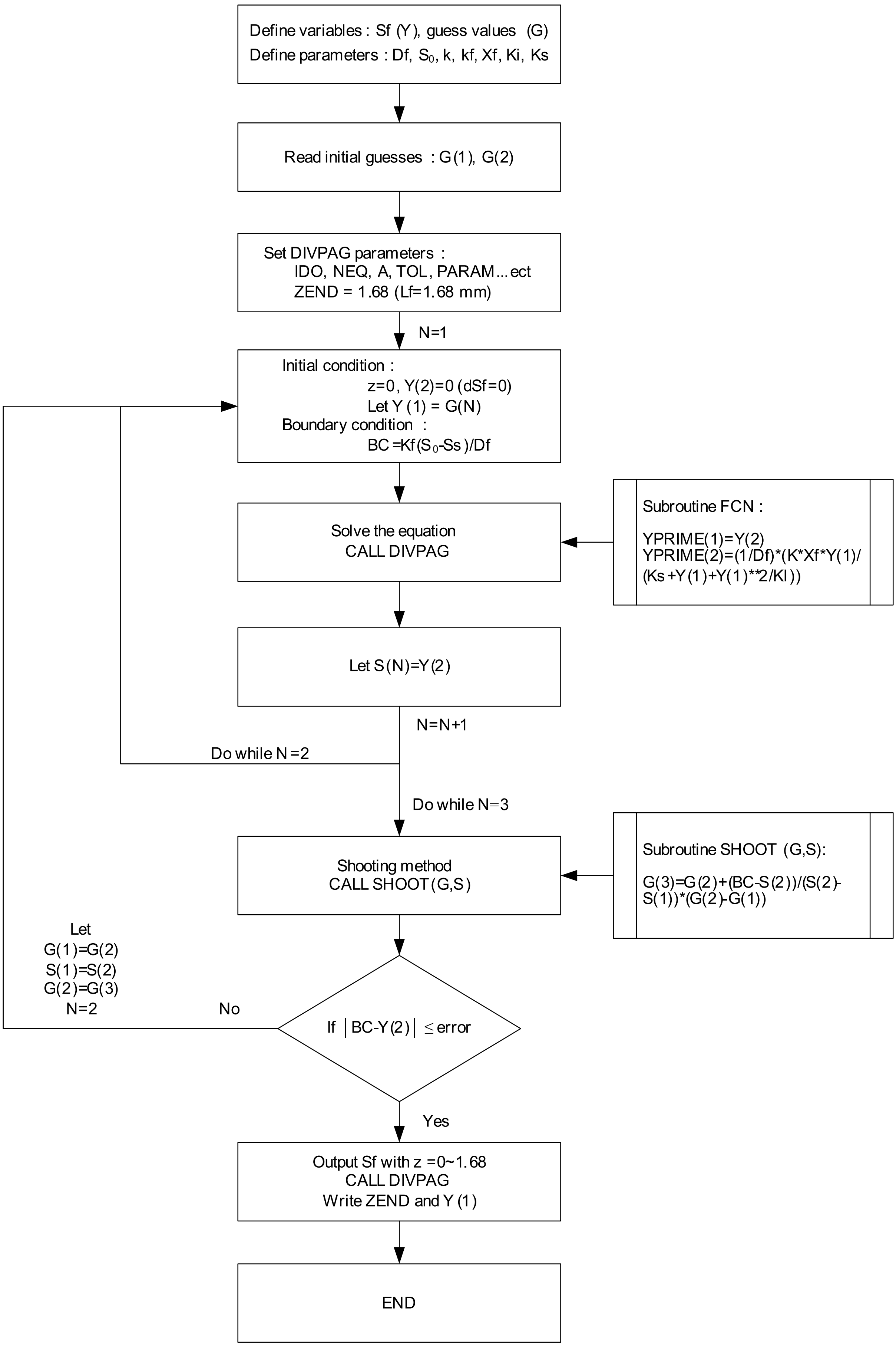
Boundary conditions:
$$\begin{cases} \dfrac{dS_f}{dz} = 0 & at \quad z = 0 \\ D_f \dfrac{dS_f}{dz} = k_f (S_0 - S_s) & at \quad z = L_f \end{cases}$$

D_f = diffusion coefficient of phenol in biofilm
S_0= Conc. of phenol in wastewater
k = maximum specific rate of the substrate utilization
S_f = Conc. of phenol in biofilm
k_f= mass transport factor of liquid–solid interface
X_f = biofilm density
K_I = resistant factor
K_S = semisaturation coefficient

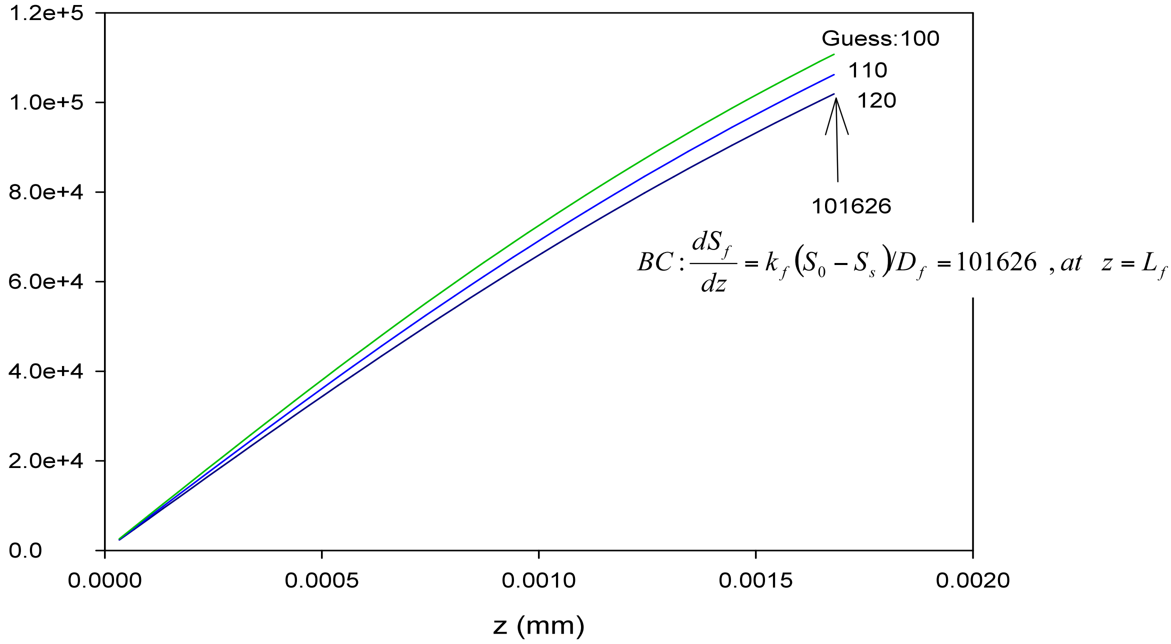
k = 0.51day^{-1}; K_s = 40 mg/L; K_I = 40.4 mg/l; X_f = 50000 mg/l; D_f = 0.85 cm^2/day; k_f = 2 × 10^{-7} m/sec; L_f = 1.68 mm; S_0 = 5000 mg/l; S_s≈0.9 S_0 .

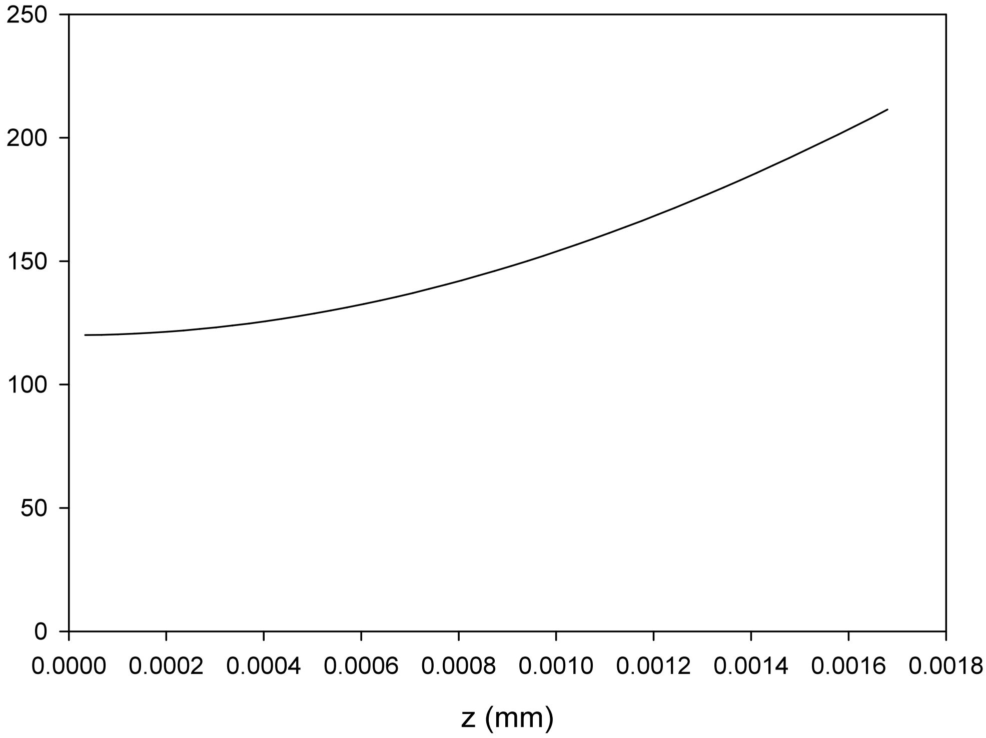
Please plot the concentration of phenol as function of Z-direction ($S_f(Z)$).

Flowchart for example 2



Solution:


1.2e+5
1.0e+5
8.0e+4
6.0e+4
4.0e+4
2.0e+4
0.0
Guess:100
110
120
101626
$BC: \frac{dS_f}{dz} = k_f (S_0 - S_s)/D_f = 101626 \;, at \;\; z = L_f$
0.0000
0.0005
0.0010
0.0015
0.0020
z (mm)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200
150
100
50
0
0.0000
0.0002
0.0004
0.0006
0.0008
0.0010
0.0012
0.0014
0.0016
0.0018
z (mm)