CHAPTER 6
NUMERICAL METHODS I: AN INTRODUCTION TO NUMERICAL METHODS FOR SOLUTION OF THE ONE-DIMENSIONAL FLOW-BOILING EQUATIONS

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ABSTRACT

Simple finite-difference methods are introduced for solution of the one-dimensional flow-boiling equations. Upwind difference methods are described, and the topic of numerical diffusion is discussed. Explicit and implicit integration methods are presented.

6.1 Introduction

Computer codes such as FIREBIRD, SOPHT and RAMA are used to study the transient behaviour of nuclear reactor transport systems. These codes consist of mathematical models for flow in pipes, through pumps, headers, steam generator, valves, and so on, which have been written in an algebraic form suitable for digital computation. In this session we will concentrate on models for flow in pipes, and we will look at various ways of constructing the algebraic equations using finite difference approximations.

Finite difference approximations are based on use of Taylor's series:

$$f(x+\Delta x) = f(x) + \Delta x \frac{\partial f(x)}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 f(x)}{\partial x^2} + + \qquad 6.1$$

with first order approximations to the derivative $\partial f/\partial x$ being given, forwards and backwards, respectively, by

$$\frac{\partial f(x)}{\partial x}_+ \simeq \frac{f(x+\Delta x) - f(x)}{\Delta x} \; ; \quad \frac{\partial f(x)}{\partial x}_- \simeq \frac{f(x) - f(x-\Delta x)}{\Delta x} \qquad 6.2$$

Another definition clearly comes from averaging equations (6.2)

$$\frac{\partial f(x)}{\partial x} \simeq \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \qquad 6.3$$

A common approximation for the second derivative in equation (6.1) is obtained by using (6.3):

$$\frac{\partial^2 f(x)}{\partial x^2} \simeq \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} \quad . \qquad 6.4$$

With these definitions in mind we will proceed to look at the conservative laws for one-dimensional boiling flow. These laws may be written conveniently using the simple expression

$$\frac{\partial}{\partial t} \bar{\Psi}(x,t) + \frac{\partial}{\partial x} \bar{\theta}(x,t) = \bar{b}(x,t) \qquad 6.5$$

Here $\bar{\Psi}$ is a vector of the conserved quantities (e.g. mass, momentum and energy), $\bar{\theta}$ is a vector of their fluxes and $\bar{b}$, a vector of source terms (e.g. friction and heat). The reader is referred to reference [1] by Hancox and McDonald for further explanation, and, in fact, for a more in-depth analysis of the whole business of one-dimensional flow-boiling methodology.

6.2 A Simple Beginning

The conservation equations (6.5) are in partial differential equation form. An integral form is readily obtained by integrating equation (6.5) from point $x-\Delta x$ to point $x+\Delta x$ along the duct:

$$\frac{d}{dt} \int_{x-\Delta x}^{x+\Delta x} \bar{\psi}(x,t)dx = \bar{\theta}(x-\Delta x,t) - \bar{\theta}(x+\Delta x,t) + \int_{x-\Delta x}^{x+\Delta x} \bar{b}(x,t)dx \qquad 6.6$$

This expression is perhaps more common as a statement of conservation: the rate of accumulation of a conserved quantity is given by the net influx to the control volume.

Applying the approximation:

$$\int_{x-\Delta x}^{x+\Delta x} f(x)dx \doteq 2\Delta x f(x) \qquad 6.7$$

to the integrals in (6.6) we obtain

$$\frac{d}{dt} \bar{\psi}(x,t) = \frac{\bar{\theta}(x-\Delta x,t) - \bar{\theta}(x+\Delta x,t)}{2\Delta x} + \bar{b}(x,t) \quad . \qquad 6.8$$

Note in passing that the first term on the right could have been obtained directly by applying (6.3) to (6.5): the same algebraic equations can result from processing either form of the conservation laws. Equation (6.8) is an ordinary differential equation in time and could be integrated by any one of a number of existing packages for that purpose. The technique involves dividing the duct into N-1 equally spaced segments, yielding N points x_i

$$\frac{d}{dt}\bar{\psi}_i = \frac{\bar{\theta}_{i-1} - \bar{\theta}_{i+1}}{2\Delta x} + \bar{b}_i \;;\quad i=1,N \qquad 6.9$$

and performing the integrations in parallel.

6.3 A Closer Look

While the simple algorithm (6.9) could be applied directly, it is not very efficient. A closer look at the equations and their nature will help in designing better methods. We note that both $\bar{\psi}$ and $\bar{\theta}$ variables appear, and it is often desirable to reduce the set to a common variable $\bar{U}$. This is accomplished by applying chain-rule differentiation to (6.5):

$$\left[\frac{\partial\bar{\psi}}{\partial\bar{U}}\right]\frac{\partial\bar{U}(x,t)}{\partial t} + \left[\frac{\partial\bar{\theta}}{\partial\bar{U}}\right]\frac{\partial\bar{U}(x,t)}{\partial x} = \bar{b}(x,t) \qquad 6.10$$

The coefficient matrices are called Jacobians and the system at (6.10), often called a primitive system, is usually written as

$$\frac{\partial\bar{U}}{\partial t} + [A]\frac{\partial\bar{U}}{\partial x} = \bar{c} \;;\; [A] = \left[\frac{\partial\bar{\psi}}{\partial\bar{U}}\right]^{-1}\left[\frac{\partial\bar{\theta}}{\partial\bar{U}}\right] \;;\; \bar{c} = \left[\frac{\partial\bar{\psi}}{\partial\bar{U}}\right]^{-1}\bar{b} \qquad 6.11$$

We note that the equation of state for the fluid gets into the picture, and that $\bar{U}$ could be any appropriate set of variables, including $\bar{\psi}$ or $\bar{\theta}$, for example. If the eigenvalues, or characteristic velocities of the system are real, it is convenient to write the characteristic form

$$[B]\frac{\partial\bar{U}}{\partial t} + [\Lambda][B]\frac{\partial\bar{U}}{\partial x} = \bar{d} \;;\; [\Lambda] = [B]^{-1}[A][B] \;,\; \bar{d} = [B]\bar{c} \;. \qquad 6.12$$

The matrix $[\Lambda]$ is a diagonal matrix containing the eigenvalues and the columns of $[B]^{-1}$ are the eigenvectors of $[A]$. For homogeneous flow, the eigenvalues are u, the fluid velocity and u ± a, where a is the local fluid sound speed.

Now, we are going to apply the one-sided spatial difference operators, equation (6.2) in a special way to (6.12). Consider two diagonal matrices [L] and [R] with the only constraint being [L] + [R] = [I], the unit matrix (i.e. $l_i + r_i = 1$, i = 1,2,3 for the homogeneous model). We will identify the forward (or positive x) operator [R] with forward differencing

$$[R][B]\frac{\partial\bar{U}}{\partial t} + [R][\Lambda][B]\frac{\partial\bar{U}}{\partial x+} = [R]\bar{d} \qquad 6.13$$

and [L] with backward differencing:

$$[L]\,[B]\,\frac{\partial \bar{U}}{\partial t} + [L]\,[\Lambda]\,[B]\,\frac{\partial \bar{U}}{\partial x}^{-} = [L]\,\bar{d} \qquad 6.14$$

Now, adding (6.13) and (6.14), we get

$$[B]\,\frac{\partial \bar{U}}{\partial t} + [R]\,[\Lambda]\,[B]\,\frac{\partial \bar{U}}{\partial x}^{+} + [L]\,[\Lambda]\,[B]\,\frac{\partial \bar{U}}{\partial x}^{-} = \bar{d} \qquad 6.15$$

Expansion using (6.2) produces, at point x_i

$$[B]\,\frac{d\bar{U}_i}{dt} + \frac{1}{\Delta x}\,[L-R]\,[\Lambda]\,[B]\,\bar{U}_i = d_i + \frac{1}{\Delta x}\left\{[L]\,[\Lambda]\,[B]\,\bar{U}_{i-1} - [R]\,[\Lambda][B]\,\bar{U}_{i+1}\right\} \qquad 6.16$$

(Note that i subscripts are implied for all matrices).

Equation (6.16) may be integrated analytically assuming constant coefficients and a constant source term:

$$[B]\,U_i(t+\Delta t) = \left\{e^{-\frac{\Delta t}{\Delta x}[L-R]\,[\Lambda]}\right\}[B]\left\{\bar{U}_i(t) - \bar{U}_i(\infty)\right\} + [B]\,\bar{U}_i(\infty) \qquad 6.17$$

An expression for $\bar{U}_i(\infty)$ can be obtained from (6.16) by setting the time derivative to zero.

Equation (6.17) deserves special consideration. The exponential matrix is diagonal, and in fact, for the homogeneous case, can be written as

$$\begin{bmatrix} e^{-\frac{\Delta t}{\Delta x}(l_1-r_1)(u+a)} & o & o \\ o & e^{-\frac{\Delta t}{\Delta x}(l_2-r_2)\,u} & o \\ o & o & e^{-\frac{\Delta t}{\Delta x}(l_3-r_3)(u-a)} \end{bmatrix}$$

For the particle velocity, as an example, we can say that exponential decay will occur if

$$(l_2-r_2)\ u > o \qquad 6.18$$

and exponential growth will occur if

$$(l_2-r_2)\ u < o \qquad 6.19$$

Equation (6.18) describes a system which is inherently stable, whereas equation (6.19) defines a system which is inherently unstable. Since the velocity u is a function of the solution, and could be either positive or negative, clearly the sign of l_2-r_2 must change with a change in sign of the velocity to preserve inherent stability. Recalling the definition of [L] and [R], this implies that backwards differencing (-x direction) must dominate when the velocity is positive, and forward differencing (+x direction) when the velocity is negative. This is the idea of upwind differencing: difference in the direction from which the information comes. The same argument quite clearly applies for the other terms in the exponential matrix as well. In any scheme, some upwind differencing is necessary to preserve inherent stability. Note that when central differencing is used (i.e. [L] = [R], or the definition at equation (6.3)) a fine line between inherent stability and inherent instability is prescribed, and often can lead to computing difficulties.

Another interesting observation can be made by replacing the directional derivatives in (6.15) by the averaged spatial difference, equation (6.3), and employing (6.4): the system actually solved by (6.15) is

$$[B]\frac{\partial \bar{U}}{\partial t} + [\Lambda]\,[B]\frac{\partial \bar{U}}{\partial x} + \frac{\Delta x}{2}\,[R-L]\,[\Lambda]\,[B]\frac{\partial^2 \bar{U}}{\partial x^2} = \bar{d}\ . \qquad 6.20$$

The presence of the second derivative, caused by upwind differencing, indicates that a diffusion equation is the one actually solved. This diffusion can be controlled by reducing Δx but is none the less present. Dynamic grid spacing is discussed in the references.

The characteristic form has been used as an example because it illustrates quite clearly the presence of diffusion, and as well its effect. Experience has shown that for practical applications, all methods will contain some upwind differencing, directly, as described here, or implied (e.g. donor cell methods), and, therefore, will suffer diffusion.

6.4 Time Integration

Nothing yet has been said about performing the time integration of the ordinary differential equations, except that some existing packages could be used. Here we will consider some particular, simple approaches, and we will use the characteristic form as the example.

Returning to equation (6.16), we will specify the characteristic finite difference scheme, wherein the [L] and [R] matrices are specified by $l_i = 1$ if $\lambda_i > 0$ and $l_i = 0$ if $\lambda_i < 0$. Defining $|\Lambda|$ as the diagonal matrix of the absolute values of the characteristics, equation (6.16) becomes.

$$[B]\frac{d\bar{U}_i}{dt} = -\frac{1}{\Delta x}|\Lambda|\,[B]\,U_i + \bar{d} + \frac{1}{\Delta x}\left\{[L]\,[\Lambda]\,[B]\,\bar{U}_{i-1} - [R]\,[\Lambda]\,[B]\,\bar{U}_{i+1}\right\} \qquad 6.21$$

and the analytical solution, assuming constant coefficients and source term, may be written as

$$[B]\,\bar{U}_i(t+\Delta t) = [B]\,U_i(t) + \Delta x\left\{[I] - e^{-\frac{\Delta t}{\Delta x}|\Lambda|}\right\}|\Lambda|^{-1}\,[B]\,\frac{d\bar{U}_i}{dt}(t) \qquad 6.22$$

This is obtained similarly to (6.17), but employing (6.21) (which vanishes at $t=\infty$) to produce the substitution

$$[B]\frac{d\bar{U}_i(t)}{dt} = \frac{1}{\Delta x}\,|\Lambda|\,[B]\left\{\bar{U}_i(t) - \bar{U}_i(\infty)\right\}.$$

We now consider approximations to the exponential matrix. First of all, the simplest approximation is

$$[I] - e^{-\frac{\Delta t}{\Delta x}|\Lambda|} \simeq \frac{\Delta t}{\Delta x}|\Lambda| \qquad 6.23$$

which produces the form

$$[B]\,\bar{U}_i(t+\Delta t) = [B]\,\bar{U}_i(t) + \Delta t\,[B]\,\frac{d\bar{U}_i(t)}{dt} \qquad 6.24$$

This can be identified as forward Euler integration and is often referred to as explicit integration, as each $\bar{U}_i$ at the new time can be calculated directly from old time information. Various numerical stability studies can be performed for explicit methods, and the general result is that for stability

$$\frac{\Delta t}{\Delta x}|\Lambda| \leq [I] \qquad 6.25$$

which implies a maximum timestep:

$$\Delta t \leq \frac{\Delta x}{\max |\lambda_i|} \quad . \qquad 6.26$$

One can make the observation that while explicit schemes are simple, they suffer from inefficiency due to the timestep restriction. This restriction is referred to as the CFL (Courant, Friedrichs, Levy) limit. (One may observe that evaluating the exponentials in (6.22) directly overcomes this).

Another simple approach is derived by writing equation (6.22) backwards in time.

$$[B]\, \bar{U}_i(t-\Delta t) = [B]\, U_i(t) + \Delta x \left\{ [I] - e^{+\frac{\Delta t}{\Delta x}|\Lambda|} \right\} |\Lambda|^{-1} [B] \frac{d\bar{U}_i}{dt}(t) \qquad 6.27$$

Applying the same approximation as before we get

$$[B]\, \bar{U}_i(t-\Delta t) = [B]\, \bar{U}_i(t) - \Delta t\, [B] \frac{d\bar{U}_i}{dt}(t) \qquad 6.28$$

This algorithm is used to determine the solution at time t given the solution at time t-Δt. One may observe that the time derivative at each point x_i needs to be evaluated at time t, and from (6.21) is seen to involve linear combinations of the solution values at point x_i as well as its neighbours. The method is thus said to be implicit, and a set of simultaneous equations needs to be solved at each step. We note as well that the coefficient matrices and source terms are required at the new time, time t. A simple approach is to assume the values they had at the old time, t-Δt. This is called a one-step implicit, or semi-implicit form. Alternatively, one can iterate, at each iteration updating the coefficient matrices and source terms to time t. It is clear that implicit methods require more work per time step than do explicit methods. However, they are (from linear analysis) usually unconditionally stable, with no timestep restriction. Timestep is thus determined strictly from accuracy considerations, and the net result is usually a large reduction in overall computing costs.

6.5 Conclusion

In this session various simple numerical methods for solution of the flow-boiling equations have been introduced. The main points are that some upwind differencing is necessary to ensure essential stability of the basic system, at the expense of diffusion, and that implicit time-integration methods, although more work per timestep are preferable to explicit methods because they are not timestep restricted. Several other interesting topics are covered in references [1] and [2].

6.6 References

[1] W.T. Hancox and B.H. McDonald, "Finite Difference Algorithms to Solve the One-Dimensional Flow-Boiling Equations", ANS/ASME International Topical Meeting on Reactor Thermalhydraulics, Saratoga Springs, New York, 1980.

[2] B.H. McDonald, D.J. Richards and P.J. Mills, "Application of Dynamic Grid Control in the RAMA Code", Simulation Symposium on Reactor Dynamics and Plant Control", Sheridan Park, 1982.