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Numerical Solution of the Thermalhydraulic Conservation Equations from Fundamental Concepts to Multidimensional Two-Fluid Analysis

Solution numérique des équations de conservation thermohydraulique des concepts fondamentaux à l'analyse multidimensionnelle de deux fluides

M.B. Carver

This version of the report, AECL 11387 Revision 1, is an addendum that includes some additional text and figures that were used in the presentation of this work at McMaster University in 1995. To incorporate these addenda the point of insertion is flagged in the original text. The small amount of additional text to be inserted and the figures it relates to are inserted as separate sheet(s) between the page having the insertion flag and the page immediately following.

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NUMERICAL SOLUTION OF THE THERMALHYDRAULIC CONSERVATION EQUATIONS FROM FUNDAMENTAL CONCEPTS TO MULTIDIMENSIONAL TWO-FLUID ANALYSIS

by

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SOLUTION NUMÉRIQUE DES ÉQUATIONS DE CONSERVATION THERMOHYDRAULIQUE DES CONCEPTS FONDAMENTAUX À L'ANALYSE MULTIDIMENSIONNELLE DE DEUX FLUIDES

par

M.B. Carver

RÉSUMÉ

Ces données ont été présentées dans le cadre d'un cours de courte durée sur l'écoulement diphasique et le transfert de chaleur à l'université McMaster et elles ont été consignées sous forme de rapport aux fins de consultation ultérieure.

L'exposé établit brièvement certains concepts nécessaires de la théorie des équations différentielles, et les applique pour décrire les méthodes de solution numérique des équations de conservation thermohydraulique sous leurs diverses formes. L'objectif est d'aborder la méthodologie générale sans obscurcir les principes par des détails. Pour donner une vue d'ensemble du calcul thermohydraulique, le document donne les fondements d'introduction, de façon que ceux qui travaillent à la mise en application des codes thermohydrauliques peuvent commencer à comprendre les multiples éléments des codes et leurs relations sans avoir à rechercher et à lire les références données. Ceux qui ont l'intention de travailler à l'élaboration des codes devront lire et comprendre toutes les références.

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NUMERICAL SOLUTION OF THE THERMALHYDRAULIC CONSERVATION EQUATIONS FROM FUNDAMENTAL CONCEPTS TO MULTIDIMENSIONAL TWO-FLUID ANALYSIS

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Summary

This material was presented as part of a short course in Two-Phase Flow and Heat Transfer at McMaster University and is documented in report form for further reference.

The discussion briefly establishes some requisite concepts of differential equation theory, and applies these to describe methods for numerical solution of the thermalhydraulic conservation equations in their various forms. The intent is to cover the general methodology without obscuring the principles with details. As a short overview of computational thermalhydraulics, the material provides an introductory foundation, so that those working on the application of thermalhydraulic codes can begin to understand the many intricacies involved without having to locate and read the references given. Those intending to work in code development will need to read and understand all the references.

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1. INTRODUCTION

The numerical solution of the thermalhydraulic conservation equations is complex, and a successful numerical solution requires painstaking attention to many details; however, only such details required for context and continuity of the discussion are included here. The intent is to cover the general methodology without obscuring the principles with details, hence matrix notation is used, when feasible, to condense the mathematical representation. The discussion first briefly establishes some requisite concepts of differential equation theory, and then applies these to describe methods for numerical solution of the thermalhydraulic conservation equations in their various forms.

2. ORDINARY DIFFERENTIAL EQUATIONS

The literature on **ordinary differential equations (ODE's) and partial differential equations (PDE's)** is immense. The fundamental theory required to understand the solution of the conservation equations is given in references [1-4], and has been condensed in the following nine pages.

The conservation equations are a set of coupled PDE's; however, they are normally converted to ODE form for solution, and a number of the requisite concepts can be addressed much more simply with respect to ODE's, so the discussion starts with basic ODE concepts.

An ordinary differential equation contains a single independent variable and a single dependent variable. Below these are designated x and y, respectively. The simplest form, a first-order ODE, may be expressed in full generality as

$$y'=dy/dx=f(x,y) \tag{1}$$

and its general solution is given by

$$y=\int f(x,y)dx+C \tag{2}$$

If f(x,y) is a simple function, an analytical solution can be found. In practice, one normally requires specific solutions, which can be found if a solution point is known (i.e., y is known for a particular x). For **initial value problems**, that point is given as

$$y(x_0)=y_0 \tag{3}$$

and solutions are sought from x_0 to x_m.

The order of an ODE refers to the highest power of derivative present. Hence a general higher-order ODE can be written:

$$d^n y/dx^n + a_1(x,y)(d^{n-1}y/dx^{n-1}) + .. + a_n(x,y)dy/dx = f(x,y) \quad (4)$$

It is more difficult to find analytical solutions of higher-order ODE's, although for some classes the solutions are well known. The general solution of an n'th-order ODE contains n arbitrary constants; specific solutions require n boundary constraints; these may involve values of y or derivatives up to the order of n-1. The statement of such an ODE is referred to as a **boundary value problem** if any constraints exist at x_m.

A particular phenomenon may be described fully by a single ODE; however, when modelling physical systems it is more common to encounter systems of ODE's. Most engineering systems can be modelled by sets of first- or second-order ODE's. ODE's of order n can often be reduced to n-coupled first-order ODE's.

This discussion will focus on first-order ODE's. A set of such ODE's can be written in full generality as

$$\bar{y} = [y_1, y_2, \ldots, y_n]^T, \quad \bar{f} = [f_1, f_2 \ldots, f_n]^T \quad (5)$$

$$\bar{A}\bar{dy}/dx = \bar{f}(\bar{y}, x) \quad (6)$$

$\bar{A}$ is defined as a square matrix, but commonly is merely the identity matrix $\bar{I}$, and can therefore be omitted.

For **initial value problems**, the equation set (5) is accompanied by an initial condition matrix

$$\bar{y_0} = [y_1(x_0), y_2(x_0), \ldots, y_n(x_0)]^T \quad (7)$$

and the solution must merely integrate the equation set from the initial conditions (7) at $x=x_0$, through various values of x to some end value x_m.

The initial condition can be regarded as a **boundary constraint**. The number of boundary constraints required for full definition of an ODE is equal to the order of the ODE, and hence for an ODE set is equal to the number of first-order ODE's in the set.

The additional constraints of a higher-order ODE may be in the form of values of derivatives at x_0 or at x_m. The solution must integrate the equations in a manner that satisfies all boundary constraints.

2.1 Implicit and Explicit Forms of Solution

The task of numerically solving the initial value problem posed by the first-order set of ODE's (5-7) is, given the values of the functions y at $x=x_0$, to generate the values y(x) at a series set of grid points $x = x_1$,$x=x_2$, ...$x=x_n$... $x=x_m$ using some sort of numerical scheme. This will be discussed in terms of the single first-order ODE problem (1,3).

If the increment in x between successive grid points is

$$h=x_{n+1}-x_n \tag{8}$$

then the **Taylor series expansion** allows the function y to be expanded in terms of derivatives

$$y(x+h)=y(x)+hy'(x)+(h^2/2)y''(x)+.....+(h^k/k!)y^{(k)}(x)+... \tag{9}$$

Normally, h<<1 is required for convergence of this series. Since we don't have higher-order derivatives, the simplest approach is to truncate the series at the first derivative. This gives **Euler's single-step explicit formula**

$$y_{n+1}=y_n+hy'_n \tag{10}$$

The formula arrives at y_{n+1} by evaluating the derivative from

$$y'_n=f(x_n,y_n) \tag{11}$$

As this uses only information from the previous integration step, this method is classified as explicit, and, as the other terms in the Taylor series have been omitted, a truncation error at least of order h^2y'' is expected.

Any number of alternate integration formulae can be obtained by forming approximations of the second and higher derivatives in the Taylor series, in terms of the first derivative. These can produce various new coefficients for y_{n+1}, and y_n, and even introduce terms involving y_{n+2}, y_{n-1}, etc.

The simplest, single-step formulae, merely introduce an approximation to the second derivative; that results in some form of averaging of y' over the interval h, and decreases the associated truncation error to order h^3.

A family of such formulae can be expressed as:

$$y_{n+1}=y_n+h\ [\theta f(x_{n+1},y_{n+1})+(1-\theta)f(x_n,y_n)] \quad , \quad 0\le\theta\le1 \tag{12}$$

This is a general **partially implicit** formulation, generally rather loosely referred to as semi-implicit. It ranges from:

fully explicit at $\theta=0$, through
truly semi-implicit (trapezoidal rule) at $\theta=0.5$ to
fully implicit Euler form at $\theta=1$.

Introducing a formula analogous to (10) for the second derivative gives $\theta=0.5$.

Any implicit form requires the value $f(x_{n+1},y_{n+1})$, which is difficult, since the problem would already be solved if y_{n+1} was known. If f(x,y) is linear, Equation (12) can easily be solved in implicit form by collecting terms at each time level. This is not possible for the general non-linear case. The implicit requirement leads to **predictor-corrector** (PC) methods, where Equation (10) is used to get a first estimate of y_{n+1}, and this is then used in Equation (12) to improve the value. For two-step PC methods, this second estimate is taken as sufficiently implicit; a further improvement in implicitness is provided in iterated PC methods, in which Equation (12) is then iterated to obtain a specified level of convergence.

Introducing various approximations to higher-level derivatives leads to classic families of variable-order integration methods, such as the Adams-Bashforth multi-step formulae, and the Runge-Kutta single-step (multi-substep) formulae. A general multi-step method of order m can be written:

$$y_{n+1}=\Sigma_{i=1}^{m}[\alpha_i y_{n+1-i}+h\beta_{i-1}y'_{n+2-i}] \tag{13}$$

2.2 Error Control and Accuracy

As noted, the **truncation error** of any integration formula is related to the power of h in the first neglected term in the Taylor series. Hence the explicit Euler integration scheme can be expressed

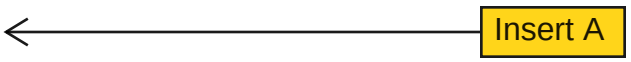
$$y_{n+1}=y_n+hf(x_n,y_n)+E_{trunc} \tag{14}$$

The truncation error E generates a deviant or spurious part of the solution that must be controlled. However, except for equations with analytical solutions, there is no formula for the magnitude of error. Hence an estimate must be made of the error associated with using a particular step size, h.

This can be done in a number of ways, the two most common being (a) to estimate the difference in y_{n+1} as computed by one step of h and two steps of h/2, or (b) to use the difference between estimates of different orders.

The latter is most effective for predictor-corrector methods, as it is already built-in; the difference provides a criterion for the acceptability of the current h, and the convergence rate of the predictor-corrector iteration can be used to control the integration step h, by indicating the amount by which h should be decreased or increased.

Standard error control such as the above can ensure that a required **local accuracy** is maintained over each individual integration step. Clearly, the **global accuracy** of the final result at x_m depends strongly on the local accuracy of each step, but cannot be predetermined for use in error control.



2.3 Stability, Stiffness and the Jacobian Matrix

The explicit Euler method has been shown to be first-order accurate, and the semi-implicit Euler method to be second-order accurate. In dealing with more than one ODE, the question of stability must be addressed. A stable solution follows the expected evolution without generating spurious oscillations or becoming unbounded.

The implicit form of the general ODE set (5) with A=I can be expanded, using Taylor series, into another very useful variant, the semi-implicit Jacobian form:

$$(\bar{dy}/dx)_{n+1}=\bar{f}(\bar{y}_{n+1},x_{n+1})=\bar{f}(\bar{y}_n,x_n)+(\bar{y}_{n+1}-\bar{y}_n)(\bar{J})_n \quad +..$$
$$\bar{J}=\overline{df/dy} \qquad (15)$$

The matrix **J** is the **Jacobian** matrix and the individual terms of the Jacobian are

$$j_{i,j}=\partial f_i/\partial y_j \qquad (16)$$

The stability of the numerical solution is governed by the **eigenvalues** λ_i of the Jacobian matrix; it can be shown that for the explicit Euler method, the stability criterion is:

$$h<2/\lambda_{max} \qquad (17)$$

By contrast, the fully implicit Euler formula is unconditionally stable. However, any semi-implicit multi-step formulation of order greater than two has some associated step-size limit.

Insert A

An example of the pitfalls of taking a too large a step size in calculating a very simple two ODE set is illustrated by solving the Lotka-Volterra or predator-prey equations; the results are in Figure 1.

If an error controlled step size is used, the correct limit cycle behaviour is obtained, as in the results from FORSIM [4]. For uncontrolled step size, the result is the wildly incorrect spiral solution also shown. This false solution appeared in the Hewlett-Packard journal, 1975, where the (incorrect) results were discussed at length. The thermalhydraulics system codes discussed later (Section 8) use fixed time steps related to transit time but not related to truncation error. They are thus always haunted by numerical instabilities.

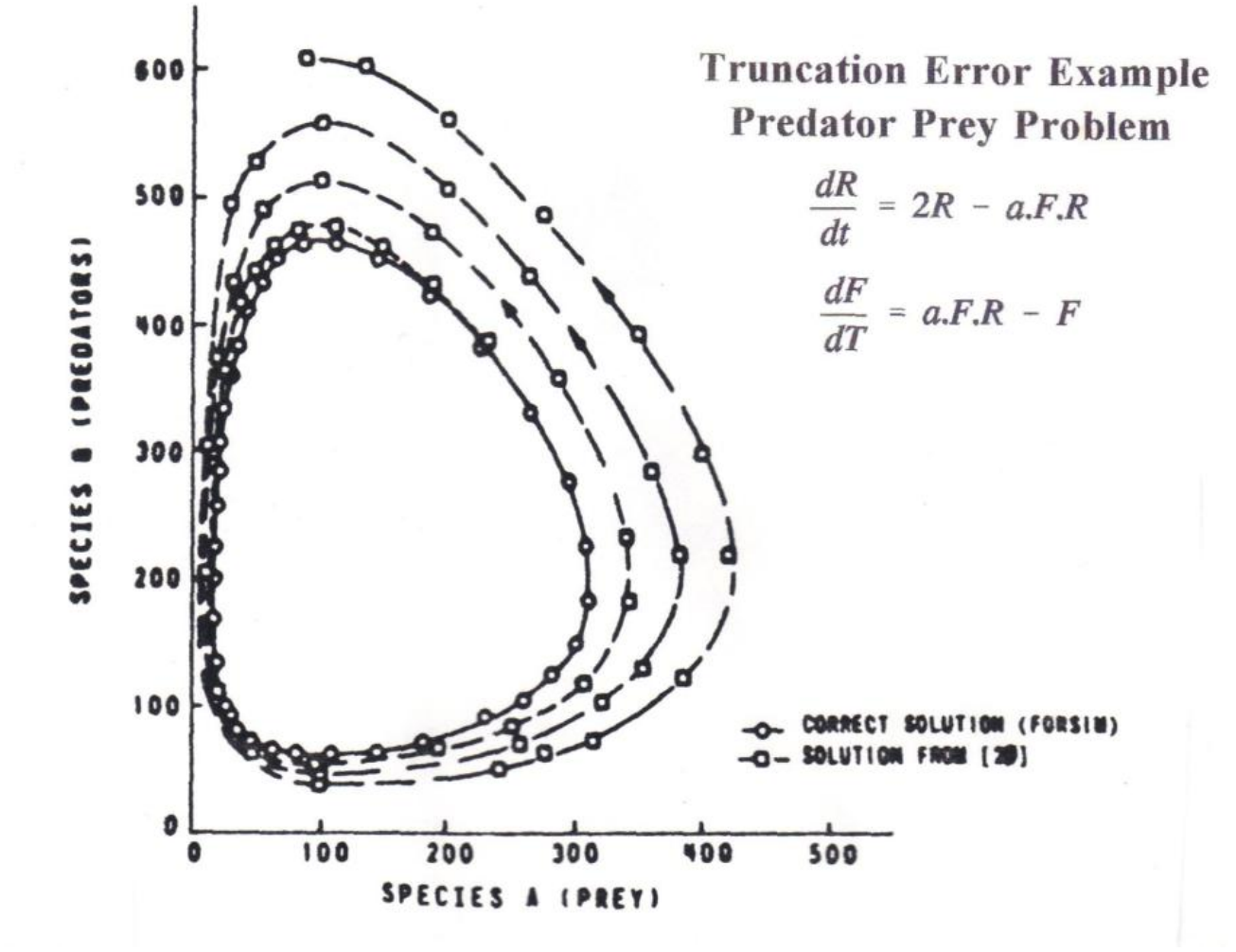


Figure 1 The Predator-Prey Equations, a Limit Cycle

A simple approach is to solve Equation (15) in matrix form:

$$(\bar{I}/h-\bar{J}_n)(\overline{y_{n+1}}-\overline{y_n})=\bar{f}_n \tag{18}$$

This form is semi-implicit and will have stability restrictions that depend on how complete the estimation of the Jacobian matrix can be made.

The range of magnitudes among the eigenvalues governs the **stiffness** of the equation set. This is best explained in terms of time constants; i.e., replacing x by t as the independent variable. The decay constants of the problem can be related to the inverse of the eigenvalues. In general, the solution scale of the problem can be related to the inverse of the smallest eigenvalue, while the stability of the method is governed by the inverse of the largest eigenvalue. Hence for an eigenvalue range of $1<\lambda_i<10^6$, the solution would normally be required for a time span of one second, but steps would be restricted to 10^{-6}. This severely restricted the performance of most multi-step integration algorithms, until the development of stiff integration algorithms overcame the problem.

Most stiff ODE algorithms utilize a particular class of multi-step formulae, termed backward difference formulae (BDF)[5], that are stiffly stable; that is, they maintain stability for large step sizes once the fast-decaying components have decreased below the level of significance. This permits a calculation to start with very small step sizes, as above, but to increase step size once the short-life terms have decayed.

The BDF formulae are cast in the form of Equation (14), with only one implicit derivative:

$$y_{n+1}=\Sigma_{i=1}^{m}\alpha_i y_{n-i}+h\beta_0 y'_{n+1} \tag{19}$$

The simplest of these, m=1, is again the implicit Euler method. This can be written in terms of the residual error $\mathscr{E}$, arising from using an estimate of y_{n+1} in the Euler formula:

$$\mathscr{E}(y_{n+1})=(y_{n+1}-y_n)-hf(y_{n+1},x_{n+1}) \tag{20}$$

the predictor-corrector is written in Newton iteration form to drive $\mathscr{E}$ to zero, thus for iteration k+1:

$$y_{n+1}^{k+1}=y_{n+1}^{k}-\frac{\mathscr{E}(y_{n+1}^{k})}{(d\mathscr{E}/dy)_{n+1}^{k}} \quad , \quad (d\mathscr{E}/dy)_{n+1}^{k}=1-h\,(df/dy)_{n+1}^{k} \tag{21}$$

For the case of an ODE set, Equation (21) becomes:

$$\bar{y}_{n+1}^{k+1}=\bar{y}_{n+1}^{k}-\frac{\bar{\mathscr{E}}(y_{n+1}^{k})}{\overline{d\mathscr{E}/dy}_{n+1}^{k}} \quad , \quad \overline{d\mathscr{E}/dy}_{n+1}^{k}=\bar{I}-h\,\bar{J}_{n+1}^{k} \tag{22}$$

The Jacobian can be regarded as an accelerator in the predictor-corrector iteration. The versatility of this method is that because J is used merely as an accelerator, it does not have to be precise, hence the Jacobian from a previous k or even a previous n can be used [5], providing the iteration is taken to convergence.

Systems that include equations that can be put into groups having either fast or slow time constants are often partitioned on physical considerations, and solved by different algorithms for each group. However, since the magnitude of the Jacobian terms is also a measure of the coupling between equations, and the strength of coupling can also vary during the evolution of the solution, it is more effective to have a dynamic partitioning within the solution algorithm. This can be accomplished by using a sparse approximation to the Jacobian in (22), that includes only terms that exceed a certain significance value in J [6], thus reducing the size of the sparse matrix without affecting efficiency.

3. PARTIAL DIFFERENTIAL EQUATIONS

Differential equations with more than one independent variable are expressed in terms of partial derivatives.

3.1 Classification and its Implications

A fairly general second-order two-dimensional PDE may be written in terms of a dependent variable v and independent variables x and y, as:

$$A\frac{\partial^2 v}{\partial x^2}+B\frac{\partial^2 v}{\partial x\partial y}+C\frac{\partial^2 v}{\partial y^2}+D\frac{\partial v}{\partial x}+E\frac{\partial v}{\partial y}+Fv=G(x,y) \tag{23}$$

The behaviour of this equation is often characterised by the relationship of the coefficients:

If B^2 - 4AC	< 0	the system is elliptic
	$= 0$	it is parabolic
	> 0	it is hyperbolic.

The **Laplace equation** is retrieved from (23) by setting A=C, B=D=E=F=0, and is an **elliptic**

boundary value problem. The **wave equation** is retrieved by setting x=t, $C/A=-c^2$, B,D,E,F=0, and is **hyperbolic.** The **diffusion equation** is retrieved by A=1, B=C=E=F=0, and is **parabolic.** In general, the coefficients A to E may be functions themselves, and this may lead to the equation characteristics changing from one classification to another as the solution evolves.

As ODE'S have only one independent variable, it is not important whether this is designated x or t. However, PDE's have two or more independent variables, and, as often one of these is time and others involve space, it can be constructive to distinguish between them. This leads to a less general but more useful classification [2].

Consider a system of PDE's that has a matrix $\bar{v}$ of dependent variables and is first-order in time and second-order in space, with up to three space dimensions $\bar{x}$:

$$\frac{\partial \bar{v}}{\partial t} = \bar{f}(t, \bar{x}, \bar{v}, \frac{\partial \bar{v}}{\partial \bar{x}}, \frac{\partial^2 \bar{v}}{\partial \bar{x}^2}, ...) \qquad \textbf{(24)}$$

This equation is **elliptic** if it has only second-order derivatives in space, **parabolic** if it has only first-order derivatives in time and second-order in space, and **hyperbolic** if it has first-order derivatives in time and first-order in space. Equation (24) also leads to a wide classification of equations that may contain all the above terms, and have been termed **semi-parabolic** or **hyperbolic/parabolic**. These are the notorious **convective-diffusion** equations that have also been referred to as the **defective confusion equations** [7], and this wide classification includes the conservation equations of thermalhydraulics.

3.2 Numerical Solution

Certain types of PDE's can be solved analytically, but often, numerical solution is the only recourse. In general, PDE's are solved numerically by spatial discretisation; that is, introducing a spatial coordinate grid, i.e., a system that divides the geometry to be considered into a number of connected control volumes or nodes having a finite size. Numerical approximations to the spatial derivatives are obtained by applying the Taylor series to each element of that grid in each coordinate direction.

Spatial discretisation essentially converts the PDE's into a coupled set of ODE's, that can then be solved in the time domain. Explicit time algorithms, such as Euler's (10), may be used with appropriate discretion to solve the ODE set; however, a number of implicit and semi-implicit methods have evolved, each with its own stability restraints. Such methods are known as Finite Difference Methods if the equations are solved in differential form, and Finite Control Volume Methods if the equations are first integrated over the control volumes.

For example, the **Crank-Nicholson** method is a finite difference formulation of the 1-D heat

equation for temperature T at point x_i at time t_{n+1}:

$$\frac{\partial T}{\partial t}=\kappa\frac{\partial^2 T}{\partial x^2} \quad , \quad \frac{T_i^{n+1}-T_i^n}{\Delta t}=\kappa\frac{<\partial^2 T>_i^n+<\partial^2 T>_i^{n+1}}{2(\Delta x)^2} \quad , \quad <\partial^2 T>_i=T_{i+1}-2T_i+T_{i-1} \tag{25}$$

Equation (25) is semi-implicit in T, but, as it is also linear, can be solved by a matrix inversion at each time step.

A large variety of PDE's can be solved simply by applying a standard implicit ODE solver package to the coupled ODE set that is generated by the discretisation. This powerful approach has been referred to generically as differential quadrature, or more commonly as the method of lines, and a number of computer packages exist that automate the solution of arbitrarily defined PDE's in this manner [3,4]. Unfortunately, the conservation equations cannot be solved successfully in this manner without special treatment [8]. This will be discussed below.

3.3 Numerical Diffusion

The truncation error is an important consideration in ODE's, and the truncation error associated with spatial discretisation influences the PDE solution in a more insidious manner.

Consider the simple advection equation with dependent variable v:

$$\frac{\partial v}{\partial t}+c\frac{\partial v}{\partial x}=0 \tag{26}$$

Use of the first-order Taylor series approximation to dv/dx over n spatial increments, dx, yields a set of n ODE's:

$$\left[\frac{dv_i}{dt}=-c\frac{(v_i-v_{i-1})}{dx_i}+E_{trunc}\right]_{i=1,n} \tag{27}$$

The truncation error is similar to that in Equation (14):

$$E_{trunc}=\Theta\left(\frac{dx}{2}\frac{\partial^2 v}{\partial x^2}\right) \tag{28}$$

Assume that the truncation error in time is taken care of by an error-controlled integration algorithm, and consider the spatial error alone. A simplistic interpretation of (28) is that the term E adds a second derivative to the original equation, hence the numerical solution is simulating the convection diffusion equation, rather than the simple advection equation. The proper solution of the hyperbolic equation (26) will propagate a wave form at speed c without distortion. Application of (27) will introduce significant diffusion, such that an initial step function becomes a diffuse 's' curve in a very short time, or an initial triangular wave becomes a bell curve that also substantially decreases in amplitude as it propagates.

Insert B

Numerical diffusion can be reduced in a number of ways, the three most common options being to take smaller step size, to use a higher order formula, or to add a compensatory second derivative correction term, usually referred to as an artificial viscosity term.

Since the conservation equations are convection-diffusion equations, it is clear that numerical diffusion must be minimised if numerical results are to be at all realistic. As in ODE solution, this error may be reduced by using a smaller dx, or by using a higher-order approximation. As noted above, the truncation error associated with time step of the ODE set can be controlled by adjusting the time step size as the solution evolves. Attempts applying a similar logic to control spatial increments have been reported, but have not met widespread use [2].

4. EQUATIONS OF THERMALHYDRAULICS

4.1 Conservation Equations

The three-dimensional equations of thermalhydraulics consist of equations expressing the **conservation of mass, momentum and energy**:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \bar{V}) = 0 \tag{29}$$

$$\frac{\partial (\rho \bar{V})}{\partial t} + \nabla.(\rho \bar{V}\bar{V}) = \bar{F} + \nabla.\bar{\sigma} = -\nabla P + \bar{F} + \nabla.\bar{\tau} \tag{30}$$

$$\frac{\partial (\rho e_t)}{\partial t} + \nabla.(\rho e_t \bar{V}) = \frac{\partial Q}{\partial t} - \nabla.q - \nabla.P\bar{V} + \bar{F}.\bar{V} - \nabla.(\bar{\tau}.\bar{V}) \tag{31}$$

$$e_t = e_i + e_{ke}$$

Insert B

This deterioration of a triangular wave in the advective equation is shown clearly in Figure 2. The first part shows this attenuation for first order upwind differencing in space and the second shows how higher-order upwind differencing can ameliorate this considerably. Figure 3 shows the propagation of a step wave with similar problems. In each case the method of characteristics provides the exact solution. Consider again the thermalhydraulics conservation equations. All the big system codes, discussed in Section 8, use first order upwind differencing with quite large spatial nodes, and any pressure waves, such as shock waves, will be significantly attenuated, leading to the forward edge of a wave arriving far too soon, and the rear edge arriving far too late as in figure 3. See reference [8].

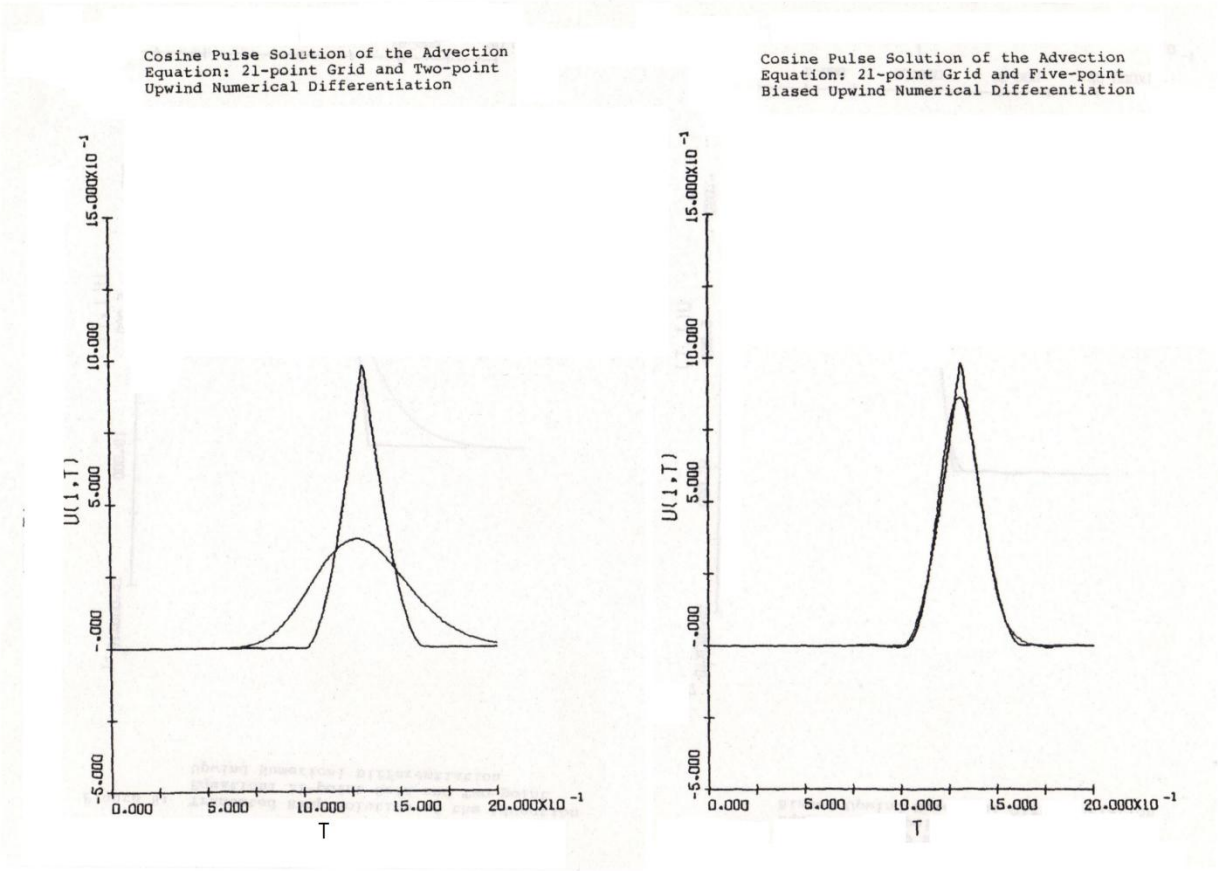


Figure 2 Numerical Diffusion Attenuating Triangle Signal in Advective Equation

Insert B continued

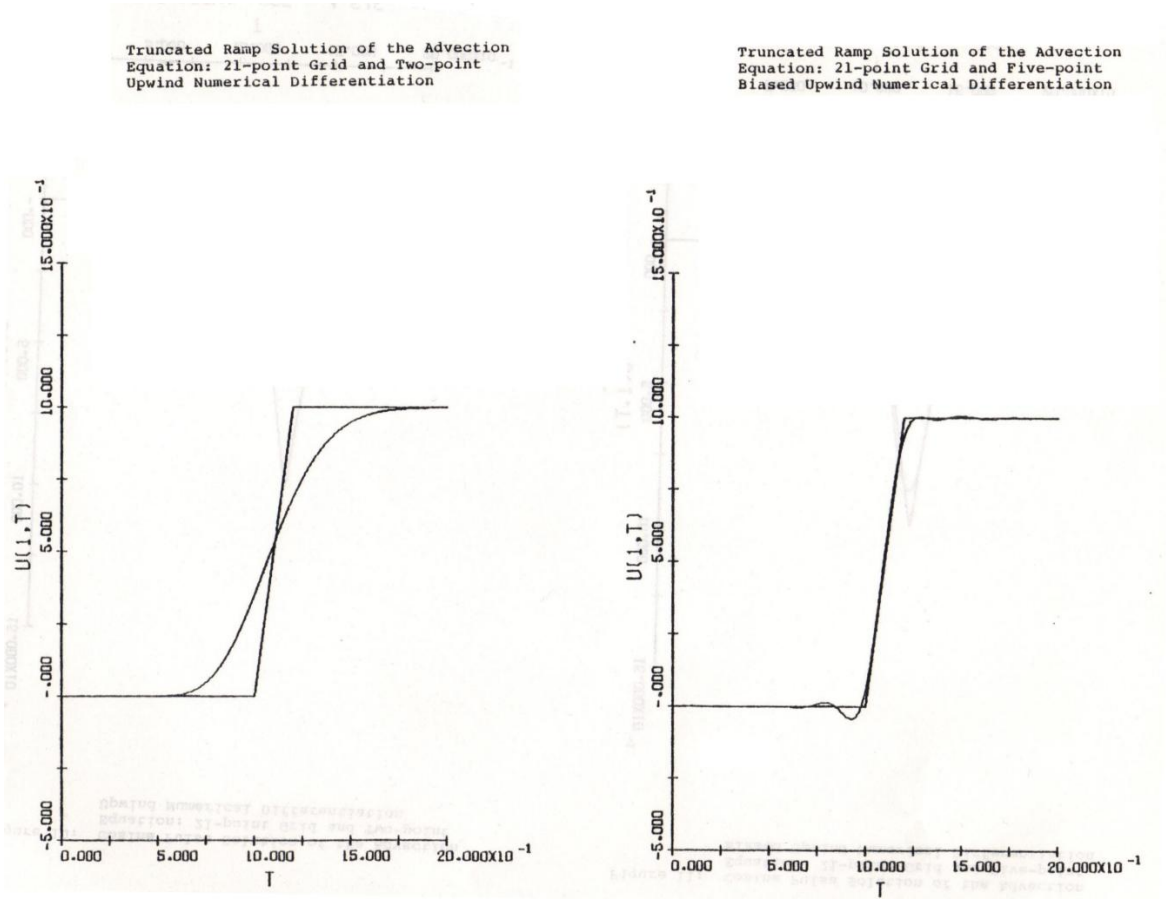


Figure 3 Numerical Diffusion Spreading Shock Wave in Advection Equation

In the second form of the momentum equation (30), the pressure term has here been extracted from the stress tensor so that the modified stress tensor now has only viscous terms.

The right side of the energy equation (31) contains terms addressing energy input from, respectively, external heating, internal conduction, pressure work, gravitational work, and viscous dissipation work.

The rhythm of equations is better revealed by using cartesian tensor notation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho v_i)}{\partial x_i}=0 \tag{32}$$

$$\frac{\partial(\rho v_i)}{\partial t}+\frac{\partial(\rho v_i v_j)}{\partial x_j}=-\frac{\partial \overline{P}}{\partial x_i}+\overline{F_i}+\frac{\partial \tau_{ij}}{\partial x_j} \tag{33}$$

$$\frac{\partial(\rho e_t)}{\partial t}+\frac{\partial(\rho v_i e_t)}{\partial x_i}=RHS_{(31)} \tag{34}$$

4.2 The Viscous Stress Terms

The most general form of the momentum equation is for the case of a compressible fluid with variable viscosity. For the simpler case of an incompressible fluid, the modified stress tensor becomes:

$$\nabla.\overline{\tau}=\nabla\times[\mu(\nabla\times\overline{V})] \quad , \quad \frac{\partial \tau_{ij}}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)\right] \tag{35}$$

It is clear that
- for most applications the momentum field will be strongly influenced by the stress terms; and,
- these terms are quite complicated.

In computational fluid dynamics (CFD) of three-dimensional laminar flow, it is sufficient to include the molecular viscosity in the above terms. For successful simulation of turbulent flows the molecular viscosity is insufficient; instead, an effective turbulent viscosity is often introduced, defined by

$$\mu=\mu_{mol}+\mu_{turb} \tag{36}$$

A major part of the field of CFD consists of formulating turbulent models that use auxiliary PDE's to describe the generation, transport and dissipation of turbulent kinetic energy, and hence provide a characterization of turbulence effects within an effective turbulent viscosity. An introduction to turbulence modelling is given in [9].

The equations of aerodynamics are inviscid, and thus avoid this particular problem. One-dimensional systems neatly circumvent this problem by replacing the viscous terms with a single term involving the friction factor. This has some implication on the classification of the equations, and will be discussed later.

4.3 Conservative and Transportive Forms

The conservation equations stated above are in **conservative form.** The **transportive form** of the momentum or energy equation is obtained by subtracting the continuity equation. The general transportive form of the three-dimensional momentum equations is often referred to as the Navier-Stokes Equations:

$$\rho\frac{D\overline{V}}{Dt}=\rho\left[\frac{\partial\overline{V}}{\partial t}+(\overline{V}.\nabla)\overline{V}\right]=\overline{F}+\nabla.\overline{\sigma}=-\nabla P+\overline{F}+\nabla.\overline{\tau} \qquad (37)$$

The transportive forms and the conservative forms of the equations are equivalent, providing all equations are satisfied. This remains true for equations that have been discretised properly; however, the transportive form is not valid if mass continuity is not precisely maintained during the evolution of a solution. This subtlety is exploited in some numerical schemes by incorporating the mass equation in the momentum and energy equations only when it leads to better convergence properties [10].

4.4 Equation of State and Physical Properties

The conservation equations above have four primary variables, and can be expressed in matrix ODE form as

$$\overline{A}\ \overline{(d\Phi/dt)}=\overline{B} \quad , \quad \overline{\Phi}=[\overline{V},\rho,e_t,P]^T \quad , \quad \overline{V}=[u,v,w]^T \qquad (38)$$

where the B matrix contains all external sources.

For n dimensions, n≤3, there are n momentum equations, and hence n+2 equations for n+3 unknowns. The remaining fluid equation is the **equation of state.** This relates the thermodynamic properties of the fluid and may be in the form of an equation (e.g., for an ideal gas) or in the form of a correlation or tables (e.g., steam tables).

Unlike the conservation equations, the equation of state is particular to the fluid involved; the general form may be written in terms of internal energy or enthalpy:

$$e_i = e_t - v^2/2 = \eta(P,\rho)$$
$$h = e_i + p/\rho = \eta'(P,\rho) \tag{39}$$

4.5 Alternative Forms of the Energy Equation

The energy equation may also be expressed using e_i or h as the primary variable. The derivation involves both the mass and momentum Equation [9], but results in similar forms:

$$\frac{\partial(\rho e_i)}{\partial t} + \nabla.(\rho e_i \bar{V}) = \frac{\partial Q}{\partial t} - \nabla.q - \nabla.P\bar{V} - \nabla.(\bar{\tau}.\bar{V}) \tag{40}$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla.(\rho h \bar{V}) = \frac{\partial P}{\partial t} + \frac{\partial Q}{\partial t} - \nabla.q - \nabla.(\bar{\tau}.\bar{V}) \tag{41}$$

The appearance of the additional time derivative of P in (41) leads to further numerical complications, as it introduces a fourth time derivative in the three differential equations.

4.6 Constitutive Relationships

If the **B** matrix in (38) contains m additional auxiliary variables, then m constitutive relationships are required for closure of the equation set; i.e., to provide a set of n+3+m definitive equations for the n+3+m variables. The constitutive relationships describe the various processes through which the fluid exchanges momentum and energy with its container and beyond. These are usually algebraic equations, as in the case of friction and heat transfer, but also additional PDE's may be coupled to the conservation equations, as in the case of modelling heat transfer to and through structures, modelling the neutron kinetics equations, and modelling effective turbulent viscosity.

Most constitutive relationships have some form of nonlinearity in the primary variables, and this exerts a strong influence on the convergence of any solution method.

5. ONE-DIMENSIONAL METHODS

Most of the system thermalhydraulics codes used for safety analysis solve the transient one-dimensional equations. This represents the variables by their cross-sectional average values,

and their interaction with the surroundings are based on correlations involving bulk values.

5.1 Method of Characteristics

The method of characteristics is very useful, as it was established particularly to address the peculiar feature of hyperbolic equations - the fact that waves are propagated along characteristic directions. As noted above, the one-dimensional advective equation

$$\frac{\partial u}{\partial t}+c\frac{\partial u}{\partial x}=0 \tag{42}$$

merely propagates an initial condition along the x-axis at speed c. The method of characteristics reveals the characteristic vectors of the conservation equations, and how to utilize these in a numerical solution.

Replacing the viscous terms by a friction correlation as discussed above, the one-dimensional Eulerian equations (29-31) can be expressed [11] in general conservation law form as:

$$\frac{\partial}{\partial t}\overline{\phi}+\frac{\partial}{\partial x}\overline{B}(\overline{\phi})=\overline{C}(\overline{\phi}) \tag{43}$$

$$\overline{\phi}=[\rho,\rho u,\rho e_t]^T=[\rho,G,E_t]^T \quad , \quad \overline{B}=u\overline{\phi}+[0,p,pu]^T \quad , \quad \overline{C}=[0,-\rho(f+g_x),Q]^T \tag{44}$$

It is convenient to introduce the local speed of sound:

$$c^2=(dp/d\rho)_s \tag{45}$$

This leads to the primitive form of the Eulerian equations:

$$\frac{\partial}{\partial t}\overline{\psi}+\overline{D}(\psi)\frac{\partial}{\partial x}(\overline{\psi})=\overline{E} \tag{46}$$

where:

$$\overline{\psi}=\begin{bmatrix}u\\ \rho\\ p\end{bmatrix} \quad , \quad \overline{D}=\begin{bmatrix}u & 0 & 1/\rho\\ \rho & u & 0\\ \rho c^2 & 0 & u\end{bmatrix} \tag{47}$$

Finally, the matrix A can be reduced to diagonal form Λ by *similarity transformation*, where Λ is the matrix of eigenvalues:

$$\overline{B'}\frac{\partial}{\partial t}\psi+\overline{\Lambda}\ \overline{B'}\frac{\partial}{\partial x}\psi=\overline{E'}(\psi) \tag{48}$$

$$\overline{\psi}=\begin{bmatrix}u\\ \rho\\ p\end{bmatrix}\quad,\quad \overline{\Lambda}=\begin{bmatrix}u+c & 0 & 0\\ 0 & u & 0\\ 0 & 0 & u-c\end{bmatrix}\quad,\quad \overline{B'}=\begin{bmatrix}\rho c & 0 & 1\\ 0 & c^2 & -1\\ -\rho c & 0 & 1\end{bmatrix} \tag{49}$$

Equation (47) defines three characteristics, each having one equality that is to be maintained along each characteristic, for example:

$$\frac{dx}{dt}=u+c\quad:\quad \rho c\frac{\partial u}{\partial t}+\frac{\partial p}{\partial t}+(u+c)(\rho c\frac{\partial u}{\partial x}+\frac{\partial p}{\partial x})=0 \tag{50}$$

Combining the two equations (50) leads to an ODE to be solved along the u+c characteristic:

$$\frac{dp}{du}+\rho c=0 \tag{51}$$

The method of characteristics computes value from finite-difference approximations to the three compatibility equations thus obtained, and establishes the solution on a grid that evolves with the solution (wave tracing). Unlike fixed-grid methods, this allows waves to propagate without diffusion, hence the method is regarded as attaining the best attainable accuracy. The method is primarily used in gas dynamics, but has also been adapted for two-phase flow [12].

Obtaining numerical solutions from the method consumes too much time for general use, and it becomes increasingly difficult as the flow model increases in complexity, so alternatives that combine the characteristic approach with more general integration methods have been sought [8,13,14].

5.2 Characteristic Differencing and Boundary Conditions

The classic method establishes the characteristic nature of hyperbolic equations and defines a pragmatic method of properly choosing differencing algorithms and of assigning boundary conditions for alternate numerical methods.

For positive flow, the above set has two forward characteristics, u,u+c, and one backward characteristic, u-c. Hence, the equations require two inlet boundary conditions, normally u

and ρ, and one outlet condition, normally P. Also, should u change sign, the method confirms the fact that a boundary condition on inflow at the exit is then required.

Further, the method establishes that directional differencing formulae, rather than central differences, are most appropriate for hyperbolic equations; hence most alternative methods use some form of upwind differencing that takes account of the fact that signals are propagated in the characteristic directions. First-order upwind (donor-cell) differencing of the advective equation (42) results in:

$$c\frac{\partial u}{\partial x} = \begin{pmatrix} c(u_i - u_{i-1})/dx) & ,c>0 \\ c(u_{i+1} - u_i)/dx) & ,c<0 \end{pmatrix} \tag{52}$$

Numerical diffusion can be reduced by using higher-order formulae, by adding artificial viscosity terms [10], or by using very small dx.

5.3 Explicit and Implicit Finite-Difference Methods

The equation set (43) can be solved explicitly by applying (10); however, the explicit solution is restricted by its largest eigenvalue to the **Courant stability limit**:

$$(u+c)<\Delta x/\Delta t \quad : \quad \Delta t<\Delta x/(u+c) \tag{53}$$

The Courant limit can be relieved by using semi-implicit methods, and it is something of an art to choose which terms are to be assigned to the new time level n+1. As noted in section 2.3, the choice depends on the strength of coupling. A useful choice is to recognize the coupling between pressure, continuity and momentum, such that the mass equation is solved in fully implicit form and only the pressure term in the momentum equation is semi-implicit.

This relieves the Courant time step limit to the fluid transit time; i.e., removes the acoustic restriction, c, from (53) to give the so-called **Material Courant limit:**

$$u<\Delta x/\Delta t \quad : \quad \Delta t<\Delta x/u \tag{54}$$

Returning to the general ODE methodology, the conservation equations (43) can be written in ODE form, and the solution may be obtained from (18):

$$[\bar{I}/\Delta t - \bar{J}](\overline{\phi^{n+1}} - \overline{\phi^n}) = \bar{F}(\overline{\phi^n}, t^n) \tag{55}$$

This is the basis of the **Porsching method** [15], which is used in many thermalhydraulic

codes. The method is almost fully implicit and has no stability limit on time step if the full Jacobian **J** is used. Recall from section 2.3 that the Jacobian is a linear representation of the coupling between variables, and an approximation to **J** can be used to employ (55) as a predictor corrector iteration. If **J** is neglected entirely, (55) reduces to the Euler explicit method and is subject to the Courant limit (53). Including only the derivatives associated with the mass equation and pressure in J relieves this restriction to (54). It is impossible to include all coupling in **J**, as the partial derivative linearises non-linear terms.

It is also difficult to include even a linearised form of the coupling inherent in the heat transfer equations appearing in the constitutive relationships, so normally either some iteration is required, or some penalty applies in the form of a time step restriction.

It is useful to express the conservation equations (43) in ODE form, to illustrate the coupling:

$$\frac{d\bar{\phi}}{dt}=\bar{F}(\bar{\phi},t) \quad , \quad \bar{\phi}=[\bar{\rho},\bar{G},\bar{E}]^T \quad , \quad \bar{F}=[\bar{F_C},\bar{F_M},\bar{F_E}]^T \quad , \quad \bar{G}=\overline{\rho u} \quad , \quad \bar{E}=\overline{\rho e_t} \qquad (56)$$

Equations (56) can be put in the Jacobian form (55) as follows:

$$\begin{bmatrix} i-\frac{\partial F_C}{\partial \rho} & -\frac{\partial F_C}{\partial G} & -\frac{\partial F_C}{\partial E} \\ -\frac{\partial F_M}{\partial \rho} & i-\frac{\partial F_M}{\partial G} & -\frac{\partial F_M}{\partial E} \\ -\frac{\partial F_E}{\partial \rho} & -\frac{\partial F_E}{\partial G} & i-\frac{\partial F_E}{\partial E} \end{bmatrix} \begin{bmatrix} \delta\rho \\ \delta G \\ \delta E \end{bmatrix} = \begin{bmatrix} F_C \\ F_M \\ F_E \end{bmatrix} \quad , \; i=I/\Delta t \qquad (57)$$

Utilising the equation of state, $\delta\rho=(\partial\rho/\partial \mathbf{P})\delta\,\mathbf{P}$, gives:

$$\begin{bmatrix} (i-\frac{\partial F_C}{\partial \rho})\frac{\partial \rho}{\partial P} & -\frac{\partial F_C}{\partial G} & -\frac{\partial F_C}{\partial E} \\ -\frac{\partial F_M}{\partial P} & i-\frac{\partial F_M}{\partial G} & -\frac{\partial F_M}{\partial E} \\ -\frac{\partial F_E}{\partial P} & -\frac{\partial F_E}{\partial G} & i-\frac{\partial F_E}{\partial E} \end{bmatrix} \begin{bmatrix} \delta P \\ \delta G \\ \delta E \end{bmatrix} = \begin{bmatrix} F_C \\ F_M \\ F_E \end{bmatrix} \qquad (58)$$

This is an almost implicit set that can be integrated in time using P, G and E as state variables. The inclusion of P is a practical choice, as it enables pressure-boundary conditions to be properly introduced as characteristic theory dictates.

It is also instructive to express (56) in residual form (20) and use Newton-Raphson to derive the equivalent matrix equation to (58):

$$\overline{\delta F}=\frac{d\overline{\phi}}{dt}-\overline{F}(\overline{\phi},t) \quad , \quad \overline{\phi}=[\overline{\rho},\overline{G},\overline{E}]^T \quad , \quad \overline{\delta F}=[\overline{\delta F_C},\overline{\delta F_M},\overline{\delta F_E}]^T \quad , \quad \overline{G}=\overline{\rho u} \tag{60}$$

$$\begin{bmatrix} \frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial P} & \frac{\partial \delta F_C}{\partial G} & \frac{\partial \delta F_C}{\partial E} \\ \frac{\partial \delta F_M}{\partial P} & \frac{\partial \delta F_M}{\partial G} & \frac{\partial \delta F_M}{\partial e} \\ \frac{\partial \delta F_E}{\partial P} & \frac{\partial \delta F_E}{\partial G} & \frac{\partial \delta F_E}{\partial E} \end{bmatrix} \begin{bmatrix} \delta P \\ \delta G \\ \delta E \end{bmatrix} = - \begin{bmatrix} \delta F_C \\ \delta F_M \\ \delta F_E \end{bmatrix} \quad , \quad \delta\phi=\phi_{n+1}^{k+1}-\phi_{n+1}^{k} \tag{59}$$

This is equivalent to (58), for the first iteration, as $\phi^0_{n+1}=\phi_n$, but the residuals can be used as acceptance criteria for convergence. Further, if sufficient terms are included in the Jacobian derivatives, (60) can also be used for steady-state calculations.

A number of approximate forms can be used to reduce the size of the matrix solution to one involving only one variable, usually pressure or flow. Examples of these methods are discussed below.

5.4 Flow-Based Solution

The approach of reducing the matrix solution can be applied to equation set (57). In this case, the coupling to be considered is:

$$\begin{bmatrix} i-\frac{\partial F_C}{\partial \rho} & -\frac{\partial F_C}{\partial G} & 0 \\ -\frac{\partial F_M}{\partial \rho} & i-\frac{\partial F_M}{\partial G} & -\frac{\partial F_M}{\partial E} \\ 0 & -\frac{\partial F_E}{\partial G} & i-\frac{\partial F_E}{\partial E} \end{bmatrix} \begin{bmatrix} \delta \rho \\ \delta G \\ \delta E \end{bmatrix} = \begin{bmatrix} F_C \\ F_M \\ F_E \end{bmatrix} \quad , \; i=I/\Delta t \tag{61}$$

In this case, Porsching et al. [15] noted that the mass and energy equations can be solved

algebraically in terms of the flow matrix:

$$[\delta\rho] = \Delta t([F_C]+[\frac{\partial F_C}{\partial G}][\delta G])$$
$$[\delta E] = \Delta t([F_E]+[\frac{\partial F_E}{\partial G}][\delta G]) \quad (62)$$

Equations (62) may now be substituted in (61) to give a single matrix equation for δG:

$$-[\frac{\partial F_M}{\partial \rho}]\ [F_C+[\frac{\partial F_C}{\partial G}][\delta G]]\Delta t + [i-\frac{\partial F_M}{\partial G}][\delta G] - [\frac{\partial F_M}{\partial E}]\ [F_E+[\frac{\partial F_E}{\partial G}][\delta G]]\Delta t = F_M \quad (63)$$

The final form is more complex as the pressure terms enter (63) through the derivative terms:

$$\frac{\partial F_M}{\partial G}=\frac{\partial F_M}{\partial G}+\frac{\partial F_M}{\partial P}\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial G}+\frac{\partial F_M}{\partial P}\frac{\partial P}{\partial E}\frac{\partial E}{\partial G} \quad (64)$$

Any constitutive relationships can also be linked via Jacobian terms. Porsching developed a rigorous definition of the above methodology for piping networks, using a node-link grid in which scalars are defined at nodes, and velocities are defined in links joining the nodes.

5.5 Pressure-Velocity Solution

The large group of numerical methods generally classified as **pressure-velocity (PV)** methods were originally developed for multi-dimensional analysis, but are also widely used for the one-dimensional equations. The well-known ICE [16] and SIMPLE [17] methods are the earliest variants of the PV theme, and use a staggered grid, in which scalars are defined at control volume centres, and velocities are placed on the boundaries. Although expressed differently, the methods are much the same [18]. In one dimension, the staggered grid is identical in concept to the node-link approach used in the flow-based solutions.

The PV methods were developed to recognize the fact that although the conservation equations in conservation-law form have four primary variables, they are governed by three

differential equations (56) and the equation of state (39). Although pressure is the driving variable, it is not computed from the differential equations, but enters the equations in a secondary manner through the equation of state.

This can lead to difficulties in handling boundary conditions if the equations are posed as a standard ODE set. The PV methodology circumvents this problem by re-establishing pressure as the driving influence. The simplest form can be illustrated by restating (60), and assuming weak coupling between the energy and the mass/momentum set:

$$\begin{bmatrix} \frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial P} & \frac{\partial \delta F_C}{\partial G} & 0 \\ \frac{\partial \delta F_M}{\partial P} & \frac{\partial \delta F_M}{\partial G} & 0 \\ 0 & 0 & \frac{\partial \delta F_E}{\partial E} \end{bmatrix} \begin{bmatrix} \delta P \\ \delta G \\ \delta E \end{bmatrix} = - \begin{bmatrix} \delta F_C \\ \delta F_M \\ \delta F_E \end{bmatrix} \tag{65}$$

Starting with an assumed pressure field, first estimates of G, and the relationship between δG and δP can be obtained by solving the momentum equation alone with $\delta F_M=0$:

$$\frac{\partial \delta F_M}{\partial P}\delta P + \frac{\partial \delta F_M}{\partial G}\delta G = 0 \tag{66}$$

Then, solving the mass and momentum equations together, as above, gives an equation in pressure correction alone:

$$\left[\frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial P} - \frac{\partial \delta F_C}{\partial G}\frac{\partial \delta F_M}{\partial P} \Big/ \frac{\partial \delta F_M}{\partial G} \right] [\delta P] = -\delta F_C \tag{67}$$

Having solved (67), mass flows are now corrected using (66) and the energy equation is then solved using the updated values of G and P; finally, density is computed from the state equation. The sequence is iterated to re-establish the coupling to the energy equation.

If the Jacobian terms are applied to (44) in a simple manner that ignores second-order terms, Equation (67) becomes:

$$\left[\frac{1}{\Delta t}\frac{\partial \rho}{\partial P} - \varsigma \frac{\partial}{\partial x}\ \frac{\partial}{\partial x} \right] [\delta P] = -[\delta F_C] \quad , \quad \varsigma = \frac{1}{\Delta t} + \frac{u}{\Delta x} \tag{68}$$

This is a wave equation for propagation of pressure at sonic velocity. For incompressible flow, or steady state, it is a Poisson equation.

For two-phase flows, the energy coupling is often strong enough to require coupling to the pressure correction equation. This can be done in a similar manner, defining additional coupling in (65) through the equation of state:

$$\begin{bmatrix} \frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial P} & \frac{\partial \delta F_C}{\partial G} & \frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial E} \\ \frac{\partial \delta F_M}{\partial P} & \frac{\partial \delta F_M}{\partial G} & 0 \\ 0 & \frac{\partial \delta F_E}{\partial G} & \frac{\partial \delta F_E}{\partial E} \end{bmatrix} \begin{bmatrix} \delta P \\ \delta G \\ \delta E \end{bmatrix} = - \begin{bmatrix} \delta F_C \\ \delta F_M \\ \delta F_E \end{bmatrix} \qquad (69)$$

Then solve the energy equation for E, with $\delta F_E=0$, and derive the relation between δE and δG, and substitute this along with (66) into the mass equation, to get the pressure correction equation:

$$\left[\frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial P}+\left(\frac{\partial \delta F_C}{\partial G}+\frac{\partial \delta F_C}{\partial \rho}\frac{\partial \rho}{\partial E}\frac{\partial E}{\partial G}\right)\frac{\partial G}{\partial P}\right][\delta P]= -\delta F_C \qquad (70)$$

Equation (70) is then used to update P,G,E and ρ. Some iteration is still required.

5.6 The Control Volume Equations

Equations (32-34) can be integrated over the control volumes, using Green's theorem, to give the finite control volume statement of the equations; e.g., for the mass equation (32):

$$\begin{gathered} d(\rho V)/dt=(\rho uA)_{inl}-(\rho uA)_{out} \quad , \quad V=\int A\ dx \\ i.e. \\ dM/dt=W_{inl}-W_{out} \quad , \quad M=\rho V \quad , \quad W=\rho uA \end{gathered} \qquad (71)$$

The finite control volume method is basically the simplest form of finite-element method, as it uses a unit weighting function in the integration.

6. THREE-DIMENSIONAL METHODS

The one-dimensional equations can be solved as a set of simultaneous ODE's by some of the above methods, but this is not always practical, and for multidimensional problems the matrices become unwieldy. It is more practical to use **segmented** methods that, like the latter methods discussed, seek solutions by setting up matrix methods that solve one conservation equation at a time, and then incorporate the inter-equation coupling by iteration.

6.1 Pressure-Velocity Methods

Most multidimensional algorithms are based on some form of P-V algorithm. Multi-dimensional P-V algorithms are intricate and precise; however, the general approach is equivalent to Equations (65-67) and may be expressed [19] as follows.

The 3-D momentum equations with source terms, S, may each be discretised for coordinate direction, i, at the point, x_i, with respect to the other coordinates, j, and a previous time, t^0:

$$\frac{(\rho v-(\rho v)^0)_i}{\Delta t}+\Sigma_j\frac{(\rho v_i v_j)_D-(\rho v_i v_j)_U}{(\Delta x)_j}+\frac{P_D-P_U}{(\Delta x)_j}=S_i \qquad (72)$$

$$D=i_{downstream} \quad , \quad U=i_{upstream}$$

If an initial pressure field, P, is assumed, each component of (72) may be linearised and integrated over the control volume, to give

$$a_i(\rho v)_i=\Sigma_n b_n(\rho v)_n+c_i(P_D-P_U)_i+<R>_i \quad , \quad <R>_i=\int S dV=\iiint S_i dxdydz \qquad (73)$$

where n is an index of each neighbouring control volume in each coordinate direction. This may be solved as a linear matrix equation for a new estimate of the mass flux matrix, [ρv].

Integrating the mass equation and solving, using the [ρv] matrix, resulting from (73) will in general leave a non-zero residual D_i, such that:

$$V_i\frac{(\rho-\rho^0)_i}{\Delta t}+\Sigma_j((A\rho v)_D-(A\rho v)_U)_j=D_i \qquad (74)$$

The change in the pressure field to drive **D** to zero may be determined by Newton Raphson:

$$\overline{\delta D}=\overline{\left[\frac{dD}{dP}\right]}\overline{\delta P}=-\overline{D} \tag{75}$$

An expression for δD_i is obtained by differentiating (74) and (73):

$$\delta D_i=V_i\ \frac{\delta \rho_i}{\delta t}+\Sigma_j(A(\delta(\rho v)_D-\delta(\rho v)_U))_j=-D_i \tag{76}$$

and

$$\delta(\rho v)_i=1/a_i[\Sigma_n\ b_n(\rho v)_n+c_i(\delta P_D-\delta P_U)] \tag{77}$$

Equations (75-77) can be arranged into a matrix equation for the pressure correction field in a form that is the three-dimensional equivalent to Equation (68):

$$\overline{A}\ \overline{\delta P}\ =\ -\overline{D} \tag{78}$$

Once (78) is solved, the resulting pressure correction matrix can be used to adjust the mass flux matrix by applying (77), and the procedure iterated to convergence for the time step. The method can be used as defined for homogeneous two-phase flow, and can be generalised to two-fluid flow [19].

For heated systems, the usual practice is to solve the energy equation subsequent to the PV iteration; however, the strong coupling between energy and momentum requires that the interaction be catered for by also iterating around the PV-Energy sequence. Extensions equivalent to the sequence (69-70) can also be derived.

6.2 Under Relaxation

Because segmented methods seek solutions to one conservation equation at a time, the outer iteration to address the inter-equation coupling may not converge. It is normally necessary to incorporate some form of relaxation. For example, the two coupled equations:

$$\overline{A}\ \overline{X}=\overline{B}(\overline{X},\overline{Y})\quad ,\quad \overline{C}\ \overline{Y}=\overline{D}(\overline{X},\overline{Y}) \tag{79}$$

should be solved simultaneously, but could possibly be solved first for X, then for Y and repeating the sequence; the fact that Y changes with X and vice-versa is neglected, and this

may inhibit or destroy convergence.

Convergence can be improved by introducing relaxation factors. For example if the vector X^m is returned from the m^{th} iteration of the first equation, then a relaxed vector X^{mr} is sent to the second equation:

$$\overline{X^{mr}}=\gamma_x\overline{X^m}+(1-\gamma_x)\overline{X^{m-1}} \qquad \textbf{(80)}$$

The second equation is similarly relaxed using a λ_y. Judicious choice of λ_x and λ_y will improve convergence. In applying (79), however, some of the coupling in X inherent to the first equation may now have been destroyed. It is more efficient [10] to modify the matrix equation to return a pre-relaxed value by building (80) into the matrix equation and solving:

$$\overline{A'}\,\overline{X^{mr}}=\overline{B}(X,Y)-\overline{A''} \quad , \quad \overline{A'}=\overline{A}/\gamma \quad , \quad \overline{A''}=-\overline{A}(1-\gamma)\overline{X^{m-1}}/\gamma \qquad \textbf{(81)}$$

6.3 Numerical Diffusion

Numerical diffusion is omnipresent in three-dimensional computation, and is harder to control, because it no longer suffices to just take higher-order differences in the coordinate directions. It is necessary to "upwind" the differentiation in the characteristic direction of the flow, a method that has come to be known as "skew upwinding" [20].

6.4 Alternate Coordinate Systems and Porous Medium Representation

Only rarely does the geometry of a physical system fit a standard coordinate system; hence a need for more general methods arises.

Insert C

Nuclear systems are often characterised by cylindrical vessels containing an array of tubes. Alternate ways of modelling such vessels are reviewed in [21] and [22], and include:

Insert D

Subchannel Coordinate System - in which the equations are written for subchannels inside a fuel bundle defined by imaginary lines joining fuel-element centres. This reduces a cylindrical (z,r,6) coordinate system into a (z,ζ) system, where ζ is a coordinate defining the immediate neighbours to each subchannel. Since only first derivatives in the ζ direction can be taken, correlations must be used for diffusion terms.

Insert E

Porous Medium Representation - in which the equations are written in full 3-D form, but the internal hardware is catered for by using a matrix of known porosity fractions, β, that represent the fraction of each control volume available to the fluid (i.e., not occupied by the hardware). The porosity β is included in the equations simply by replacing ρ by βρ.

Insert F

Insert C

Figure 4 shows a simplified (quarter-circuit) diagram of a representative CANDU Reactor system.

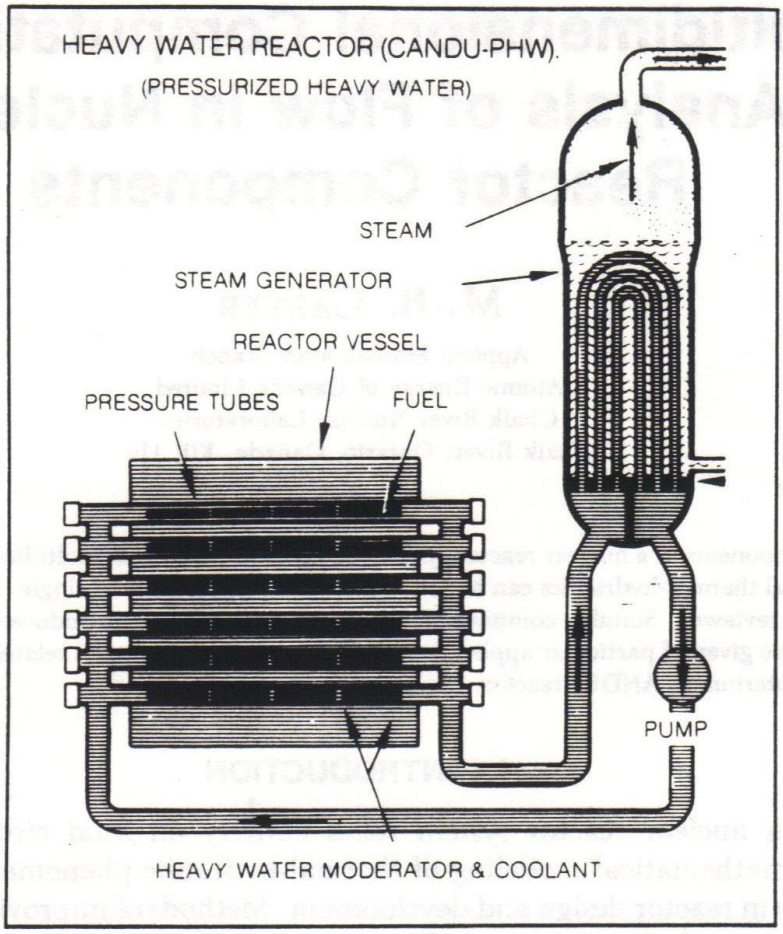


Figure 4 Simplified (quarter circuit) Diagram of CANDU Reactor Components

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In Figure 4. these include the fuel coolant channels, the Steam Generator and the Calandria Vessel.

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Figure 5 shows how a CANDU fuel channel can be modelled using subchannels.

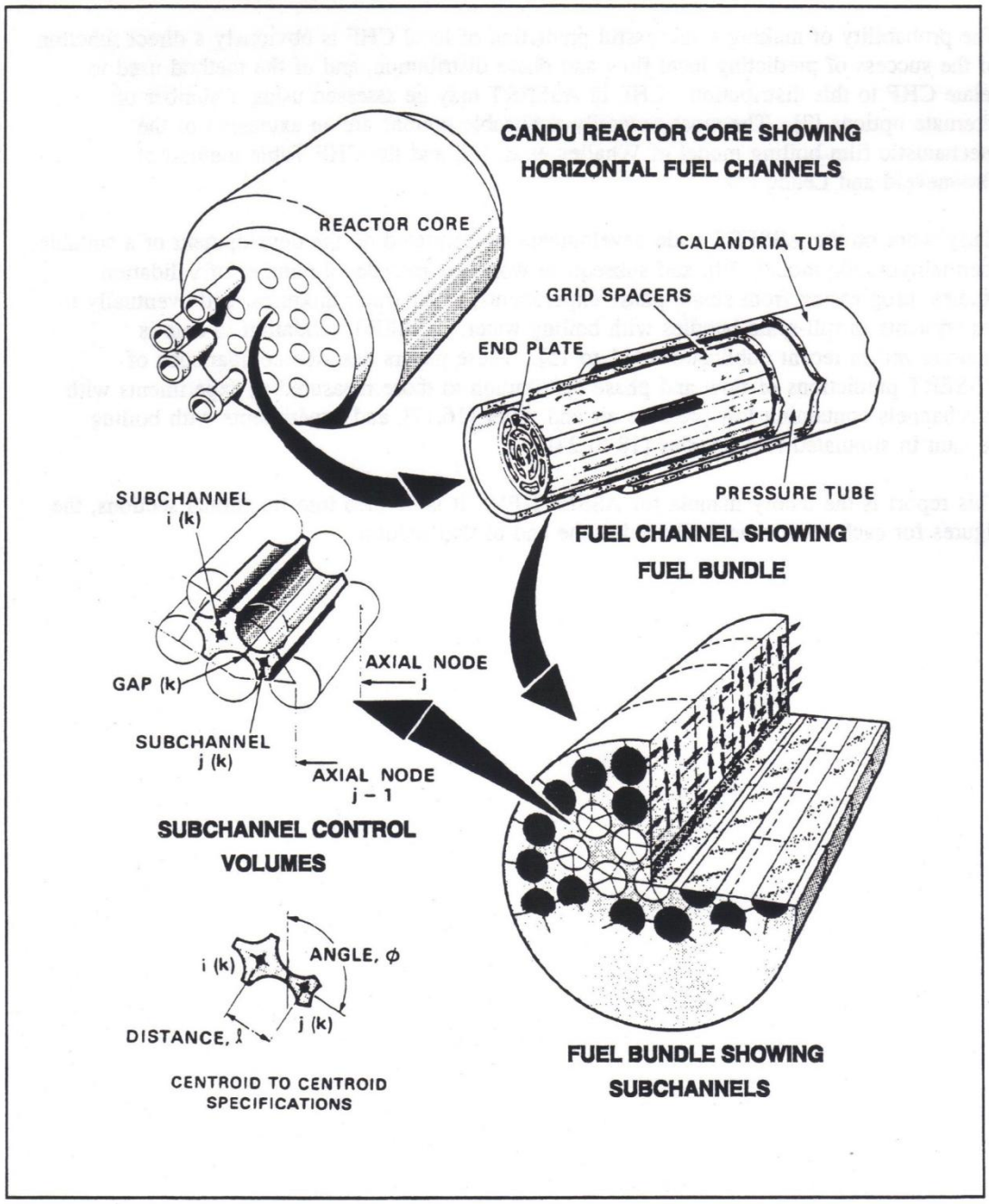

Figure 5 Definition of Subchannel Geometry in a CANDU Reactor

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Figure 6. shows subchannel and porous medium representation in a 7 rod bundle.

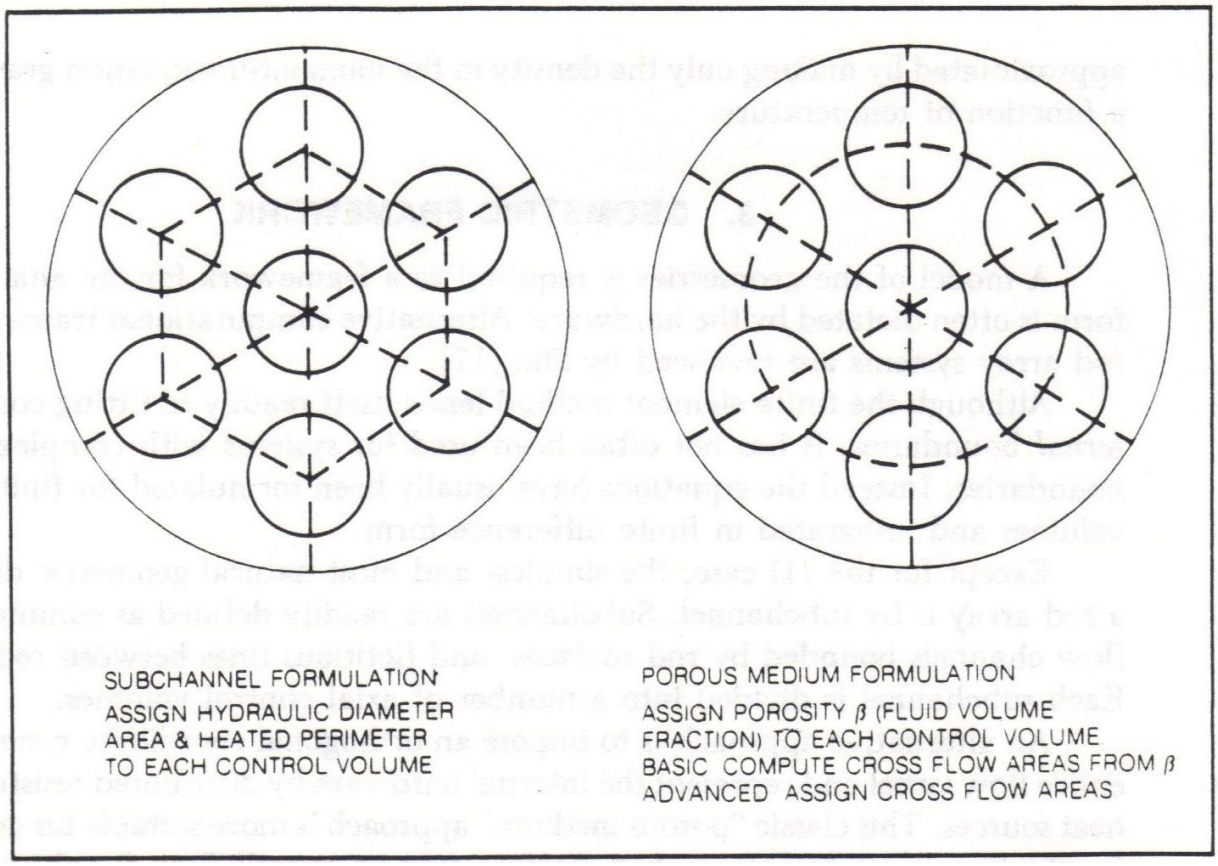


Figure 6 Protocol for Subchannel or Porous Medium Representation

Arbitrary Coordinate Systems - the equations may be written in general orthogonal or non-orthogonal coordinates that are then deformed to fit the geometry. This body-fitted method is now used in most commercial CFD codes. However, the mathematical implications are beyond the scope of the current discussion; see [21] for an introduction.

7. TWO-PHASE FLOW EQUATIONS

7.1 Homogeneous Equilibrium Model

The homogeneous or equilibrium model of two-phase flow requires considerably more constitutive relationships than the single-phase case, but can be handled by any of the numerical schemes already discussed. In this model, the two phases are assumed to be fully mixed such that they have the same temperature and velocity. The conservation equations for a homogeneous mixture are the same as for a single fluid, but require the extension of the equation of state to define saturation lines and two-phase quantities, and additional constitutive relationships to describe two-phase friction and heat transfer, and to define the relationship between weight and volume fractions, x and α. An overview of the model can be found in [23].

7.2 Extended Homogeneous Model

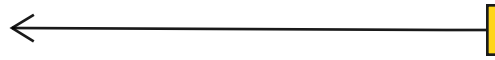
Some non-equilibrium features, such as the effect of subcooled boiling on heat transfer, density and pressure drop, and the effect of unequal velocity (slip) on density and pressure drop, can be added to the homogeneous model by means of additional algebraic equations, while still retaining the homogeneous conservation equations [23].

7.3 Non-Equilibrium Models

Non-equilibrium models of increasing complexity are obtained by introducing non-equilibrium effects individually. A non-equilibrium model utilises individual conservation equations for each phase. This permits the model to better approximate the general mechanics of a two-phase flow, hence it can better capture observed behavioral trends; however, many more constitutional relationships are now required to describe the frictional and heat transfer exchanges between the phases, and from each phase to the container. The state of development of such constitutive models is still behind that for equilibrium models, so considerable uncertainties still exist. To minimise these uncertainties, various intermediate forms of the non-equilibrium models have been utilised.

The equal velocity unequal temperature (EVUT) model permits the phases to have unequal temperatures, and hence requires two energy equations, one for each phase; see [13] for details.

The drift-velocity unequal temperature model (DVUT) adds another degree of freedom, by introducing individual phase velocities through a full-range drift-flux model. This now requires a further conservation equation; usually, the mixture mass continuity equation is replaced by one equation for each phase.

Finally, the full unequal velocity unequal temperature (UVUT) (two-fluid) model requires an individual mass, momentum and energy equation for each phase, and more constitutive relationships than one might at first realize. 

The general statement of the equations must now involve some additional concepts. First, the assumption of interpenetrating continua [24] permits conservation equations to be written for each phase as if each phase itself operates as a continuum interacting with another continuous phase, even under conditions such as bubbly flow and separated flow. Second, interactions between the fluid are described in terms of an interface, which must have some interfacial area, the definition of which is not inherent in the conservation equations, but requires further constitutive equations that vary with flow regime.

Various forms of the two-fluid equations are discussed in [24], and the general statement below can be seen to be an extension of Equations (29-31) written for two fluids (or two phases), k&l, as follows:

$$\frac{\partial(\alpha\rho)_k}{\partial t}+\frac{\partial(\alpha\rho v_i)_k}{\partial x_i}=\Gamma_{kl} \tag{82}$$

$$\frac{\partial(\alpha\rho v_i)_k}{\partial t}+\frac{\partial(\alpha\rho v_i v_j)_k}{\partial x_j}=-\alpha_k\frac{\partial P_k}{\partial x_i}-(P_k-P_l)\frac{\partial \alpha_k}{\partial x_k}-(\alpha\rho)_k g_i + [\tau'_{kw}+\tau'_{kl}+\Gamma_{kl}v_{kl}+\bar{\omega}_{kl}]_i \tag{83}$$

$$\frac{\partial(\alpha\rho e)_k}{\partial t}+\frac{\partial(\alpha\rho e v_i)_k}{\partial x_j}-\frac{\partial(\alpha P)_k}{\partial t}-(P_k-P_l)\frac{\partial \alpha_k}{\partial t}= q_{kw}+q_{kl}+[\tau'_{kl}v_{kl}+\Gamma_{kl}e_{kl}+v_k\bar{\omega}_{kl}]_i \tag{84}$$

The additional term in the mass equation is due to phase change. The additional terms in the momentum equation involve the pressure difference and shear stress between the fluids k&l, momentum transferred by phase change, and finally, a virtual mass term. The extra terms

Insert G

Figure 7 is a table showing which constitutive relations are required for each level of model from EVET through to UVUT.

Model	Homogenous	Extended Homogenous		EVUT	Drift Flux	Two Fluid
	EVET	uVET		EVUT	DFUT	UVUT
Mass Eqns	1	1		1	2	2
Mom Eqns	1	1 + Slip		1	1+ Drift	2
Enrg Eqns	1	1+Subc Boiling		2	2	2
mixt fric	x	x		x	x	
mixt heat	x	x				
slip/drift		x			x	
void		x				
liq heat				x	x	x
vap heat				x	x	x
int phs heat				x	x	x
int phs area				x	x	x
liq fric						x
vap fric						x
int phs fric						x

Figure 7 Constitutive Relations Required for EVET,UVET.....UVUT Models of the Conservation

appearing in the energy equation are analogous.

Additional constraints exist, in that the phase volume fractions must sum to unity, and the interphase relationships must be complementary, such that the individual phase equations, when added, return the standard mixture equations.

The above equations are stated as one set of conservation equations for each fluid, and many numerical solution schemes solve them in this form; however, other options can be exploited.

For example, the equations can be added and subtracted, such that the working equations to be solved are three mixture conservation equations and three equations expressed either in terms of differences, or describing one fluid only. Another approach is to resolve the two mass and two energy equations into a mixture mass equation and three energy equations (the mixture and each phase) [25]. This device adds the capability of considering options that have only liquid disequilibrium or both liquid and vapour disequilibrium. The use of mixture equations as one component part of the working equations can reduce the uncertainties in defining momentum and energy exchange between the phases from each phase to the surroundings, by using traditional mixture correlations for both momentum and energy, and then partitioning the energy and momentum transfer in the companion set of equations that captures the departure from equilibrium. This approach is used to provide options for choosing various levels of disequilibrium model in the ASSERT subchannel code [26], and the TUF system code [27].

Finally, it is often important to include the presence of any non-condensable gases in the solution, as they share the available flow area with the coolant. These are usually accounted for by a transport model that assumes they travel at the same speed as the vapour phase; hence it usually suffices to solve an additional differential equation expressing mass conservation of incondensables. However, an additional energy equation may be needed.

7.4 Numerical Solution and Hyperbolicity

As noted above, the inviscid equations are hyperbolic, and viscous terms in the one-dimensional thermalhydraulic equations are usually replaced by a correlation for frictional pressure drop; this renders the equations hyperbolic according to the above classification schemes. The equation system must have real eigenvalues to be hyperbolic. Certain forms of the two-fluid equations, particularly those with a single pressure, generate complex eigenvalues, which give the equations a partially elliptic character that results in an ill-posed initial-value problem. Some models choose the form of the virtual mass term and/or artificial viscosity terms, in a manner that ensure the equations remain well-posed (hyperbolic) during the evolution of the solution. The implications of hyperbolicity are still under debate [28].

While most 1-D two-fluid codes formulate the model in terms of Equations (82-84), and solve them in a semi-implicit manner, using a staggered grid, many differences have evolved in the

precise formulation, the choice of prime variables, the appropriate differencing of the equations and the choice of implicit terms. Particular codes are discussed in the next section.

7.5 Two-Step Methods

As mentioned above, even schemes that are designed to maximize implicitness are often subject to some time-step limit, due to numerical instability arising from the coupling of auxiliary systems in a manner that cannot be easily captured in the linearised Jacobian derivatives used to represent the local variation of constitutive relationships and of the equation of state. Some causes of such instability have been found to relate to a number of phenomena, such as: phase transitions that cause discontinuities in constitutive relationships, the progression of phase transition fronts though a finite grid system (water packing), or flow reversals that affect donor logic in the linearised terms and hence may deteriorate mass and energy conservation.

A number of two-step approaches have been proposed, that basically work as two-step predictor-correctors. Mahaffy [29] first used the two-step label for a predictor-corrector method involving a predictor step and a stabiliser step. The scheme was devised for the two-fluid equations, but also applied to homogeneous flow. This method is too involved to detail here. A simpler stabiliser step was proposed by Ransom [30], in the form of a subsequent mass correction equation that compensates for the difference in mass conservation caused by linearisation in the linearised implicit solution.

7.6 Three-Dimensional Methods

Again, three-dimensional methods generally follow one of the two principal PV variants [16,17]. The principle is much the same, except that the presence of two fluids increases the degrees of freedom that can be explored. The momentum equations may be formulated as (74), to provide an estimate of each velocity component, i, for each fluid, k, and differentiated as in (77):

Insert H

$$\delta((\alpha\rho v)_i)_k=[1/a_i[\Sigma_n\ b_n(\alpha\rho v)_n+\alpha c_i(\delta p_D-\delta p_U)]]_k \qquad (85)$$

The mass equations can be formulated to arrive at two residuals, D_k and D_l, for fluids k and l.

$$\left[V_i\ \frac{[(\alpha\rho)-(\alpha\rho)^0]_i}{\Delta t}+\Sigma_j[(A\alpha\rho v)_D-(A\alpha\rho v)_U]_j=D_i\right]_k \qquad (86)$$

The change in pressure is sought to drive the residual of the mixture mass equation $D=D_k+D_l$ to zero:

$$\delta D=\Sigma_k\left[V_i\frac{\delta(\alpha\rho)_i}{\delta t}+\Sigma_j[(A\alpha\rho v)_D-(A\alpha\rho v)_U)]_j\right]_k=-(D_k+D_l)_i \qquad (87)$$

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Figure 8 shows the scalar and vector control volumes required for a cartesian coordinate system.

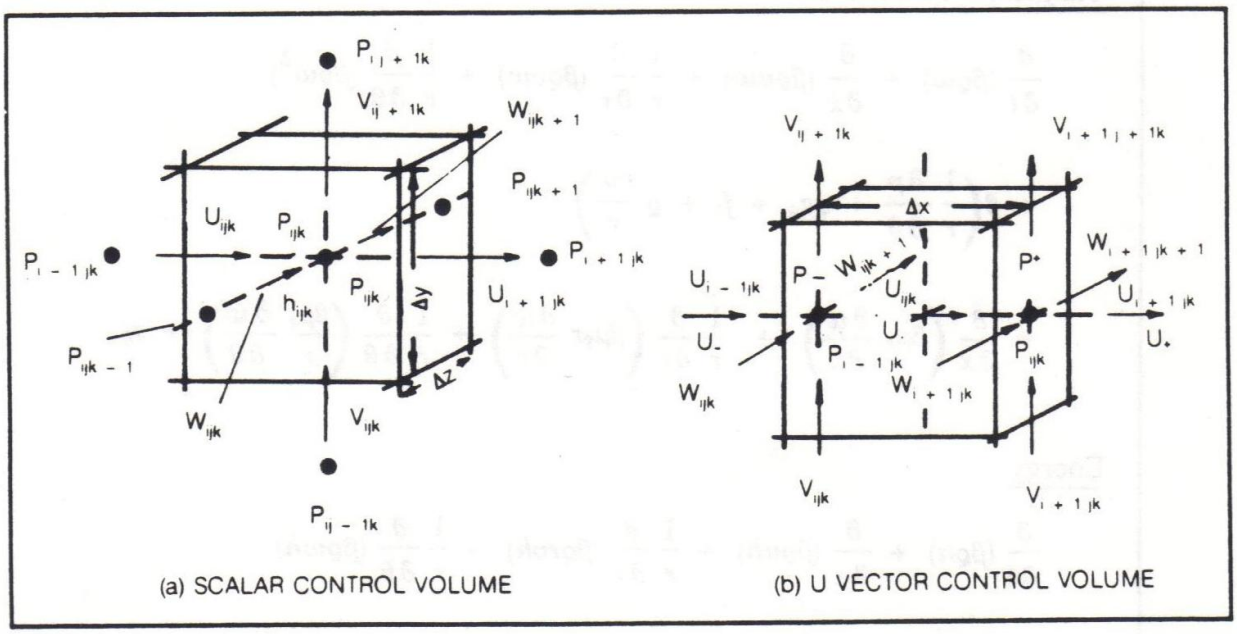

Figure 8 Staggered Grid Showing Scalar and Vector Control Volumes for 3D Cartesian

Hence a pressure equation similar in form to (78) is solved:

$$\overline{A}\ \overline{\delta P}=-\overline{D}=-[\overline{D_k}+\overline{D_l}] \tag{88}$$

and velocities are updated via (85). For fluids with widely disparate density, it can be advantageous to base the pressure equation on a volumetric continuity, as below:

$$\delta D'=\Sigma_k\left[V\frac{\delta(\alpha)_i}{\delta t}+\Sigma_j[(A\alpha u)_D-(A\alpha u)_U)]_j\right]_k=-(D'_k+D'_l)_i \tag{89}$$

The question of an equation defining the volumetric fraction has been addressed in many ways. One continuity equation can be used; however, it is better to use an equation that is implicit in both fluids. The IPSA method [31] is one option, and a simpler method with the same degree of implicitness can be formulated by subtracting the two volumetric continuity equations, to give a second linear combination [19]. This gives:

$$2V_i\frac{\delta(\alpha)_i}{\delta t}+\Sigma_j[[\alpha_v\ (v_v+v_l)]_D-[\alpha_v\ (v_v+v_l)]_U]_j=0 \tag{90}$$

Having new values for the flow field variables, the energy equation can now be solved, and the sequence is iterated. For boiling flows, improved coupling between energy and density must be established.

8. COMPUTER CODES FOR TWO-PHASE FLOW ANALYSIS

The following summarises the features of the principal computer codes used in analysis of CANDU[1] thermalhydraulics.

8.1 One-Dimensional System Codes

System codes have the capability of modelling flow and heat exchange in all components of the reactor coolant circuit, and its interaction with the rest of the system, including the neutronic feedback, fuel, pressure-tube, calandria tube, and the control system.

While it is possible to model each reactor channel, channels are usually analyzed in representative groups. Most of the coolant circuit is in single-phase flow; however, normal

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[1] CANDU: CANada Deuterium Uranium; registered trademark.

operating conditions permit some void generation in the fuel channels, and postulated accidents considered in safety analysis invariably lead to transients causing significant void generation, so all system codes need two-phase capabilities.

8.1.1 Two-Phase Codes

NUCIRC [32] is a steady-state system code used primarily in the analysis of critical channel power. NUCIRC has an equilibrium flow model, modified to account for subcooled boiling and slip, and their effects on void and pressure drop. NUCIRC has the capability to model the whole coolant circuit and can simultaneously model all the individual reactor channels.

SOPHT [33] is a transient system code and uses an equilibrium flow model, modified to account for subcooled boiling and slip, and their effects on void and pressure drop. SOPHT models all components in the circuit. The numerical solution algorithm follows the Porsching Flow-Based approach.

FIREBIRD [34] is a transient system code and uses an equilibrium flow model, modified to account for subcooled boiling and slip and their effects on void and pressure drop. It has similar capabilities to SOPHT.

SPORTS [35] was written specifically for transient analysis of two-phase flow in low-pressure pool reactors. It solves the extended homogeneous equations using an iterative implicit method. Although the neutron kinetics equations are solved in a semi-implicit manner in most system codes, work with SPORTS revealed that at low pressures these equations must also be treated fully implicitly, to avoid numeric oscillations [36].

8.1.2 Two-fluid Codes

RELAP5 is often referred to as a standard of comparison, and has been occasionally used in CANDU analysis [37]. RELAP5-Mod2 [30] uses the full six-equation model, with a single pressure and primary variables $[v_l, v_g, e_{ig}, e_{il}, P, \alpha_g]$. Individual phase pressures are extracted for stratified flows. Two options are available to avoid the material Courant limit: a semi-implicit two-step method, and a "nearly implicit" method that provides the maximum possible coupling available for the linearised equations. For the two-step method, the mass and momentum equations are first resolved in an implicit PV formulation, and then the energy equations are arranged in the semi-implicit form of (55), where $[\Phi]$ is $[P, \alpha_g, e_{ig}, e_{il}]$, and solved for the time step, using property derivatives based on the state equations, to provide the linearised (Jacobian) terms wherever possible.

CATHENA [38] uses the full six-equation model with two pressures, giving seven principal variables, which are reduced to six, $[v_l, v_g, h_g, h_l, P, \alpha_g]$, by using a constitutive relationship for interphase pressure difference. These are arranged in the semi-implicit form of (55), again with property derivatives used in supplying the Jacobian terms, and the resulting linear set is

solved in the time step by a sparse matrix package (the same package as in [6]). A stabilising corrector step based on mass conservation is applied. Time-step control is based on considerations of the rate of change of variables.

TUF [27] uses a full six-equation model with principal variables [M_m,M_g,E_m,E_g,W_m,v_r]. The solution method is a two-step method with an explicit predictor step and an implicit step that is a two-fluid extension of the Porsching flow-based method. TUF includes options for various levels of departure from equilibrium (see section 7.3).

All three of the above codes include equations for non-condensables. ← Insert I

8.2 Multidimensional Component Codes

Multidimensional analysis is not widely used in system codes, because of the increased complexity and expense of multidimensional solutions, but some multidimensional auxiliary features are often used (for example, conduction in the fuel model).

In general, multidimensional codes concentrate on particular components, such as the channel, steam generator, calandria, etc.

The **ASSERT** subchannel code [26] was written to model two-phase flow in the horizontal fuel channels of CANDU reactors. It uses the DFUT model, which allows the phases to have unequal temperatures and velocities. The definition of subchannel is the same as that used in COBRA-IV [39]; however, COBRA-IV uses the equilibrium model of two-phase flow. ASSERT has an equilibrium option that permits it to solve the same equations as COBRA-IV, but the nonequilibrium options permit ASSERT to mechanistically model the onset of subcooled boiling in particular subchannels, and the resulting redistribution of flow amongst the subchannels, and the progression towards stratification that occurs in horizontal channels at higher void fractions. ASSERT is used primarily in steady-state for analysis of critical heat flux (CHF) for various flow conditions, particularly in the case of variations of flux profile or pressure-tube geometry that are beyond the experimental data on CHF. The code also has the capability to do transients involving post-dryout and flow reversal; however, three-dimensional transients are expensive. ← Insert J

The **THIRST** code [40] is for analysis of the thermalhydraulics of steam generators. THIRST solves the extended homogeneous equations on a three-dimensional grid to obtain the distribution of flow and phases in the secondary (shell) side of a recirculating steam generator. Temperatures of the primary (tube) side is also computed, together with a calculation of recirculation ratio and steam production. Apart from analysis of steam-generator performance, THIRST is also used to compute local flow velocities and void fraction that are required as input for calculation of the vibration and wear of the tube arrays. An auxiliary code, **SLUDGE** [41], provides a calculation of the distribution and deposition of fouling matter within the steam generator, given the velocity fields from THIRST. ← Insert K

Insert I

The codes above all use a one dimensional model - z - of the coolant flow, but the complication of the data description is immense; Figure 9 shows a nodalisation for Darlington 4 [50]. The codes compute rod surface temperatures at location 'z'. Because the power profile in a bundle is non- uniform, it is possible to estimate surface temperatures of selected rods, particularly the hottest rod (the one with the highest power generation). Users should be aware that the actual hot rod temperature will be higher because flow distribution must de facto be neglected. Figure 10 shows some results from SOPHT [33,50].

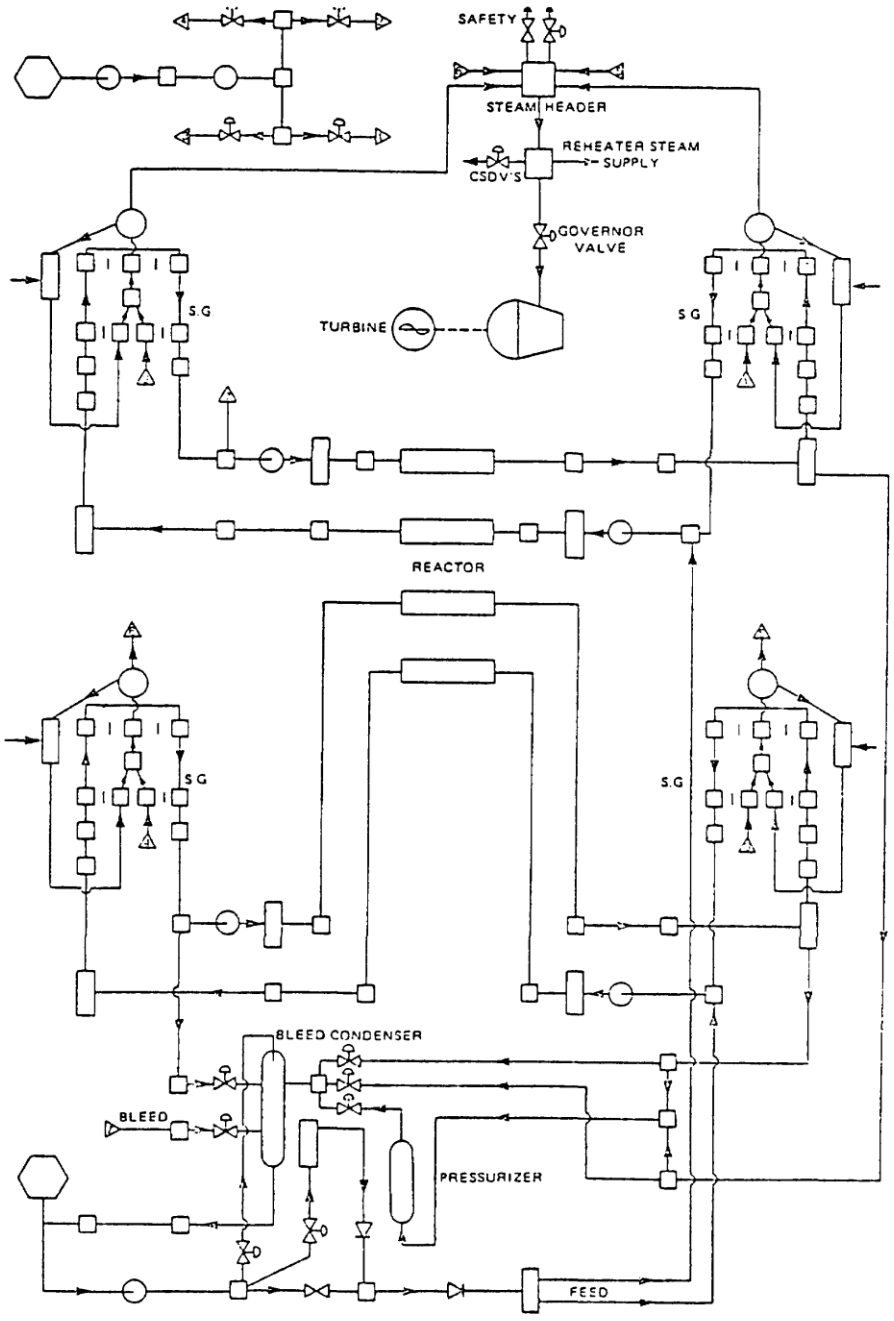

Figure 9 SOPHT nodalisation for Darlington 4

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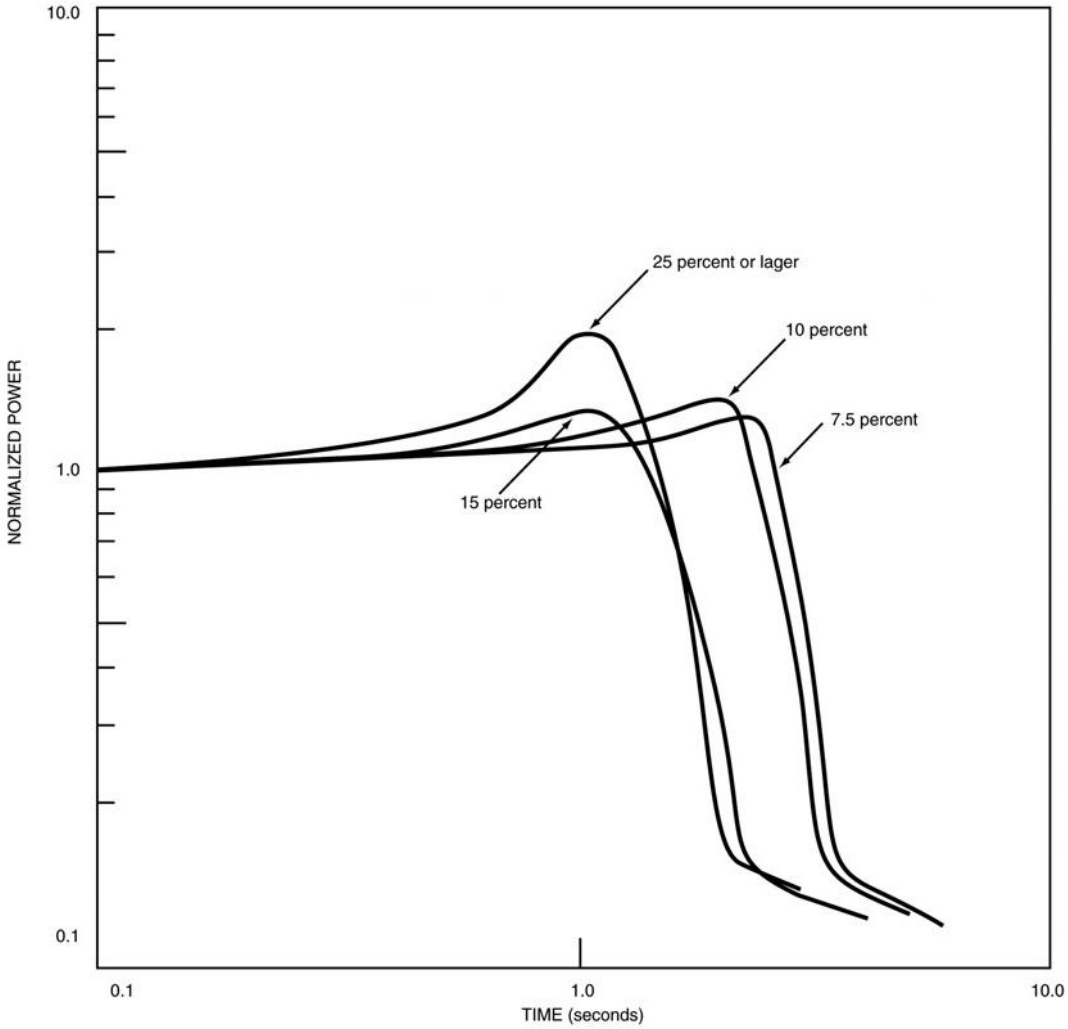

Figure 10 LOCA, SOPHT: Hot Element Power Transients for Inlet Header Breaks, Menely[50]

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Figure 11 shows an ASSERT study of the effect on CHF of pressure tube creep. The measured and modelled locations of dryout are shown for an electrically simulated CANDU bundle.

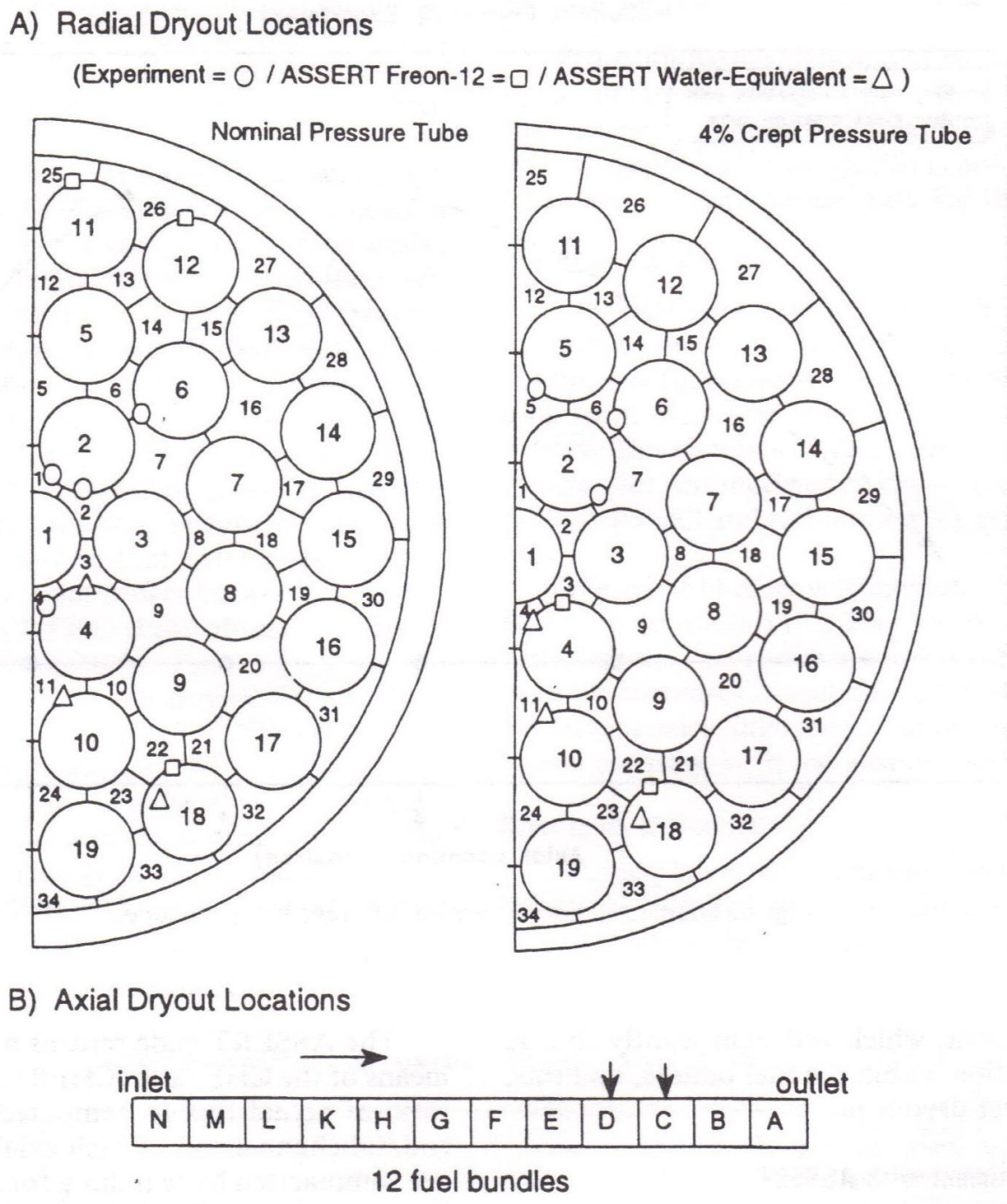

Figure 11 ASSERT Study of Effect of Crept PT on CHF

Insert J continued

Figure 12 shows a MAPLE X10 fuel channel with numbering for rods and subchannels.

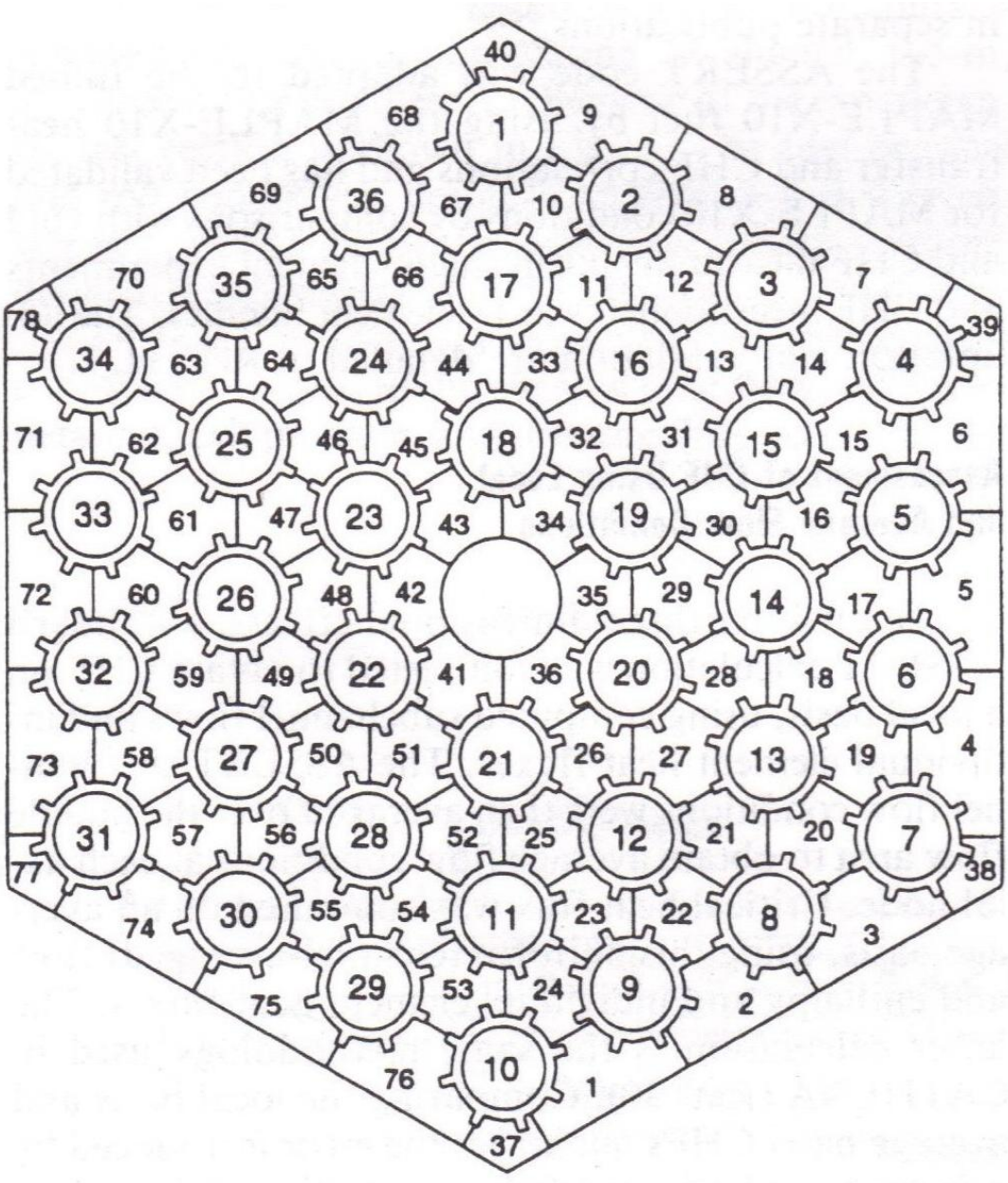

Figure 12 MAPLE X10 Fuel Channel with Numbering forSubchannels and Fuel Rods

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Figure 13. shows THIRST analysis of a steam generator secondary side flow using the porous medium approach to incorporate the hardware of the secondary side (a complex arrangement of inverted u-tubes with many stabiliser bars and a pre-heating heat exchanger).

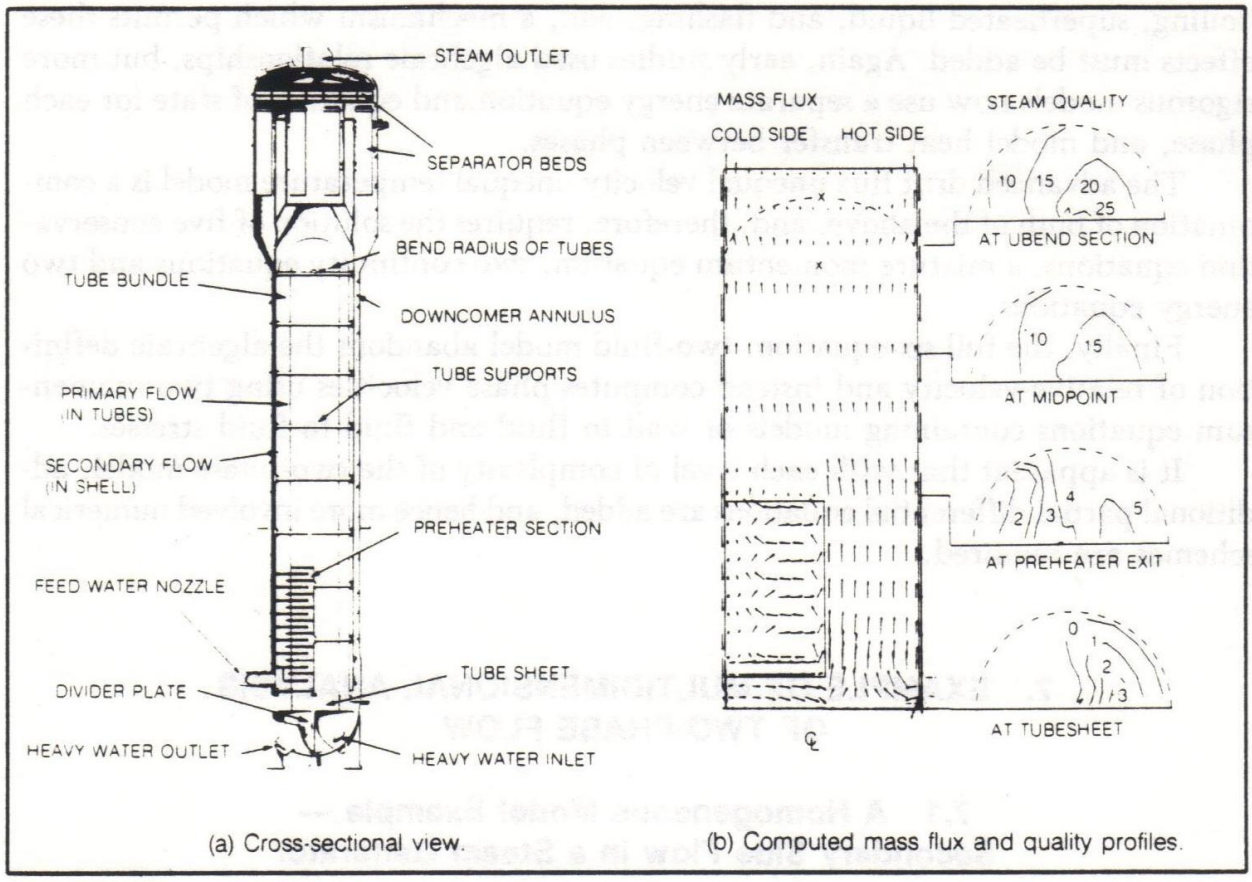
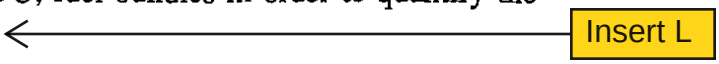


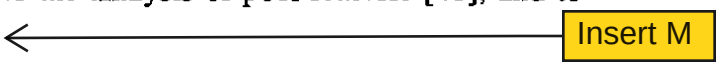
Figure 13 THIRST Study of Steam Generator Thermalhydraulics

8.3 Commercial Codes

Significant advances in CFD methodology in arbitrary coordinate systems, combined with the increased complexity required to incorporate these advances, has gradually removed the field from the realm of the general practitioner to that of the focussed specialist. This trend has spawned a significant increase in the number of advanced CFD codes offered on a commercial basis. Most of these codes are not sold on a black-box basis, but rather together with a certain amount of consulting support from the parent company. The performance of the codes for single-phase flow is well established, and their accuracy is primarily a function of the applicability of the turbulence model used. Usually, the codes contain a choice of turbulence model, thus shifting that responsibility to the user. We mention three here that have been used in analyses related to CANDU.

TASCFLOW [42] is a single-phase, three-dimensional CFD code for arbitrary geometries, offered by ASC. It has been applied successfully to very complex geometries. An early version of TASCFLOW forms the basis of the MODTURC program, that models moderator flow in CANDU calandrias [43]. TASCFLOW has also been used in modelling flow in conduit junctions [43], and past spacers in CANDU, fuel bundles in order to quantify the associated heat-transfer enhancement [44]. 

PHEONICS [45] is another three-dimensional CFD code for arbitrary geometries, written by CHAM; and has also been used for analysis of calandria flow [46]. PHEONICS advertises a fairly extensive two-fluid option.

FLOW-3D [47], a three-dimensional CFD code for arbitrary geometries, from CFDS, also has a two-fluid option. FLOW-3D has been applied to the analysis of pool reactors [48], and to model void distribution in channels [49]. 

9. CONCLUDING REMARKS

The preceding has reviewed the current state of numerical methods for solution of the thermalhydraulic equations. Most of the methods currently in use have their roots in numerical methodology that was developed in the 1970's and was hence focussed on the computing capabilities of that era, when limitations on available memory led to an emphasis of segmented methods over direct methods. As today's computers are not subject to such stringent storage limits, the trend in CFD software is towards more direct methods that maximize coupling, leading to significant reduction in the convergence problems that often hamper the segmented methods.

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Figure 14 shows results of TMODTURC 2D modelling of flows inside a CANDU calandria [43].

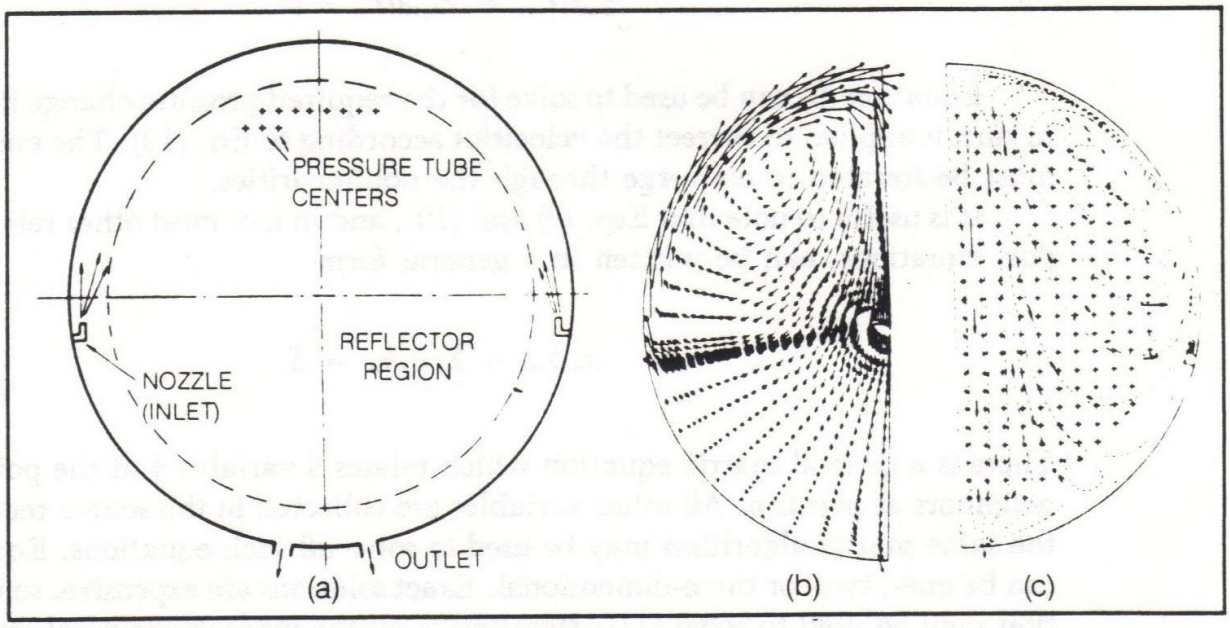

Figure 14 Pickering Calandria Experiments a>Simplified Front View b> Computed

Insert M

In such computation it is necessary to use some form of turbulence model for a two fluid system; this is easiest to address in bubbly flows such as [49] as one can legitimately state that the near wall turbulence is dictated by the continuous fluid and there is evidence that this does work fairly well for bubbly flows[19,51]; the technique is described in detail in [52].

FAITH [19] is a 3D @ Fluid CFD code developed by the author; it is not commercially available. Figure 15 shows computed redistribution of air and water in the Ecole Polytechnique subchannel experiments[53]. Finally Figure 16 [19]shows the fascinating redistribution of air and water in a vertical pipe, through a 90 degree bend to a horizontal pipe.The phases go through a complete swap as centrifugal acceleration moves the water radially until it is driven back by gravity in the horizontal section.

Insert M continued

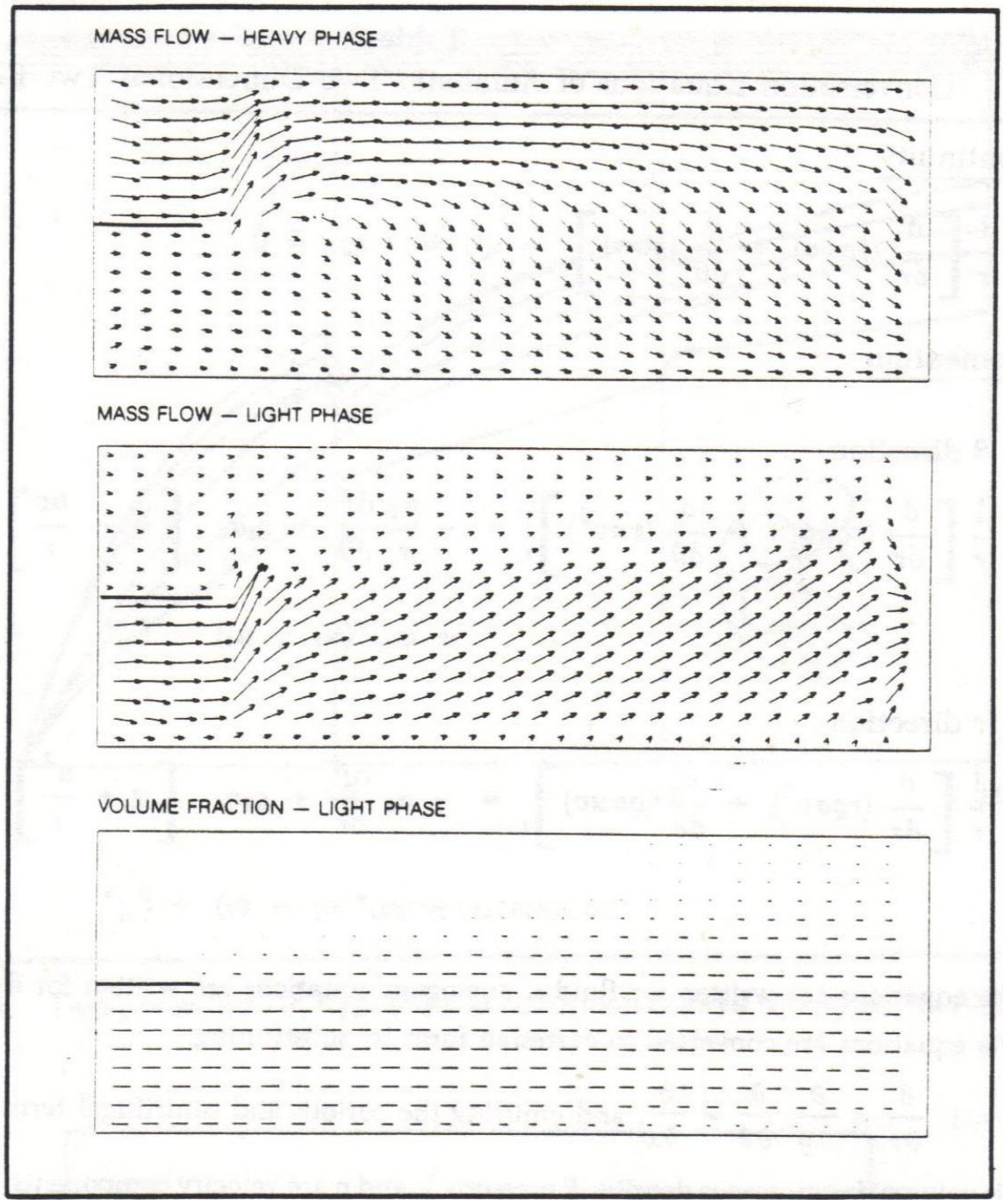

Figure 15 FAITH code Simulation of Air-Water Redistribution in

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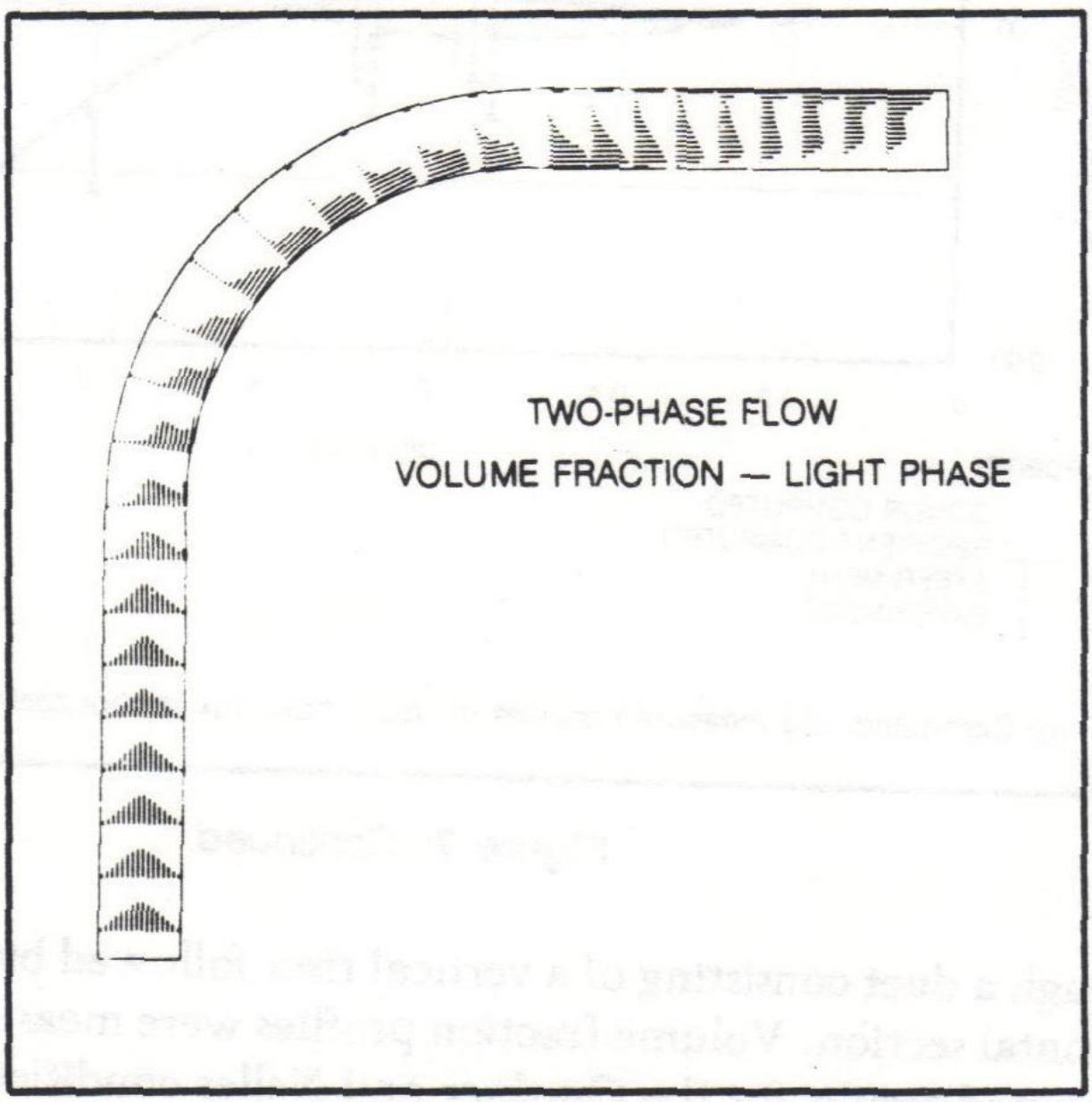

Figure 16 FAITH code Simulation of Air-Water Redistribution in

10. ACKNOWLEDGEMENTS

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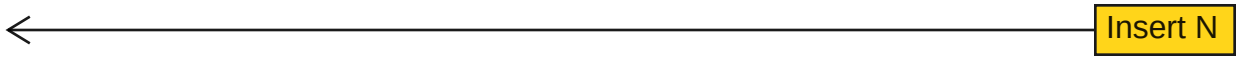

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