

BASIC EQUATIONS FOR THERMALHYDRAULIC SYSTEMS ANALYSIS

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ABSTRACT

This paper reviews the basic mass, momentum and energy equations used in typical computer codes for Heat Transport System simulation. The equations are derived from first principles and the necessary approximations lead to the requirements for empirical correlations. Closure is obtained by the equation of state.

1. INTRODUCTION

The known territory of the basic mass, energy and momentum conservation equations (Bird et al [1]) is explored, herein, from the perspective of thermalhydraulic systems analysis for nuclear reactors.

Invariably in the modelling of fluids, the conservation equations are cast in one of two main forms: integral or distributed approach, respectively (Currie [2]). The differential form sees infrequent use in the analysis of thermohydraulic systems since the cost and complexity of such a detailed analysis on even a single complex component of a system is enormous, which makes this route to the analysis of systems of such complex components unrealizable. Recourse is generally made to the integral or lumped form so that inter-relationships of various components comprising a system can be simulated. Necessarily, the models used for the individual components are much simpler than that of the detailed models based on the distributed approach. Great care must be taken to ensure that the simpler models of the integral approach are properly formulated and not misused.

It behooves us, then, to develop the models used in thermohydraulic systems analysis from first principles. This will provide a traceable and verifiable methodology to aid development and validation of system codes, to lucidate the necessary assumptions made, to show pitfalls, to show the common roots and geneology of specific tools like FLASH (3), SOPHT (4), RETRAN (5), FIREBIRD (6), etc., and to help guide future development.

The exploration proceeds by first establishing and discussing the general principle of conservation. Next, this general principle is applied in turn to mass, momentum and energy to arrive at the specific forms commonly seen in the systems approach. Closure is then given via the equation of state and by supporting empirical correlation. Finally, the ideas

developed are codified in a diagrammatical representation to aid in the physical interpretation of these systems of equations and to provide a summary of the main characteristics of fluid systems.

2. CONSERVATION.

We start, both historically and pedagogically, with a basic experimental observation:
"CONSERVATION".

This was, and is, most easily understood in terms of mass:

"WHAT GOES IN MUST COME OUT UNLESS IT STAYS THERE
OR IS GENERATED OR LOST SOMEHOW".

Although this should be self-evident, it is important to realize that this is an experimental observation.

If we further assume that we have a continuum, we can mathematically recast our basic experimental observation for any field variable, ψ :

$$\frac{D}{Dt} \iiint_V \psi dV = \iiint_V \Gamma dV + \iint_s S \cdot n ds, \quad (1)$$

where

- D/Dt = substantial derivative⁺ = change due to time variations plus change due to movement in space at the velocity of the field variable, ψ ,
- V = arbitrary fluid volume,
- Γ = net sum of local sources and local sinks of the field variable, ψ , within the volume V .
- ψ = field variable such as mass, momentum, energy, etc.
- t = time
- s = surface bounding the volume, V
- n = unit vector normal to the surface, and
- S = net sum of local sources and local sinks of the fluid variable, ψ , on the surface s .

We can now use Reynold's Transport Theorem (a mathematical identity) (Currie, [2]):

$$\frac{D}{Dt} \iiint_V \psi dV = \iiint_V \frac{\partial \psi}{\partial t} dV + \iint_s \psi V \cdot n ds \quad (2)$$

⁺For a lucid discussion of the three time derivatives, $\frac{\partial}{\partial t}$, $\frac{D}{Dt}$, $\frac{d}{dt}$, see Bird et al [1], page 73.

where

$\partial/\partial t$ = local time derivative, and
 \mathbf{V} = velocity of the field variable,

to give

$$\iiint_V \frac{\partial \psi}{\partial t} dV = - \iint_S \psi \mathbf{V} \cdot \mathbf{n} ds + \iiint_V \Gamma dV + \iint_S \mathbf{S} \cdot \mathbf{n} ds. \quad (3)$$

In words, this states that the change in the conserved field variable ψ in the volume V is due to surface flux plus sources minus sinks. We can use another mathematical identity (Gauss' Divergence Theorem):

$$\iint_S \mathbf{A} \cdot \mathbf{n} ds = \iiint_V \nabla \cdot \mathbf{A} dV, \quad (4)$$

where

\mathbf{A} = any vector, such as velocity, and
 ∇ = Del operator (eg. $\nabla = \partial/\partial x i + \partial/\partial y j + \dots$).

Thus equation (3) can be rewritten:

$$\iiint_V \frac{\partial \psi}{\partial t} dV = - \iiint_V \nabla \cdot \psi \mathbf{V} dV + \iiint_V \Gamma dV + \iiint_V \nabla \cdot \mathbf{S} dV. \quad (5)$$

If we assume that this statement is universally true, i.e. for any volume within the system under consideration, then the following identity must hold at each point in space:

$$\frac{\partial \psi}{\partial t} = -\nabla \cdot \psi \mathbf{V} + \Gamma + \nabla \cdot \mathbf{S}. \quad (6)$$

This is the distributed or microscopic form. Equation (3) is the lumped or macroscopic form. They are equivalent and one can move freely back and forth between the two forms as long as the field variables are continuous.

The above derivation path is not unique. One could start with an incremental volume and derive (1) via (6). It is largely a question of personal choice and the end use. One school of thought, attended by most scientists, applied mathematicians and academics, since they usually deal with the local or microscopic approach, focuses on the conversion of the surface integrals to volume integrals using Gauss' Theorem. The volume integrals are then dropped giving the partial differential or microscopic form. This path works well when a detailed analysis is desired, such as subchannel flow in fuel bundles, moderator circulation in the calandria, etc.

The second school, which sees more favour among engineers, particularly in the chemical industry, evaluates the surface integrals as they stand without converting to volume integrals. This leads to a lumped or macroscopic approach useful for network analysis, distillation towers, etc.

There exists a very large number of possible derivations, each with its own advantages and disadvantages. As more and more detail is picked up in each class of models, numerical means have to be used. In the limit of large numbers of nodes or mesh points, etc., both methods converge to the same solution.

Since the above equations are basic to all subsequent modelling of thermalhydraulic systems, one should keep in mind the basis for these equations:

1) Conservation as an experimental observation.

This is usually taken for granted. However, when the conservation equations for separate phases in a mixture are under consideration, the various sinks and sources of mass, momentum and energy are not entirely known and the interpretation of experimental data can be difficult because of the complexity. It helps to keep in mind the distinctly different roles that we have historically assigned to the players in the conservation process:

- a) the local time derivative, $\partial\psi/\partial t$,
- b) the advection term (flux), $\nabla \cdot \psi V$,
- c) the local sinks and sources, Γ , within a volume and
- d) the local sinks and sources, S , on the surface of a volume.

If a clarity of form is adopted by establishing and maintaining a one-to-one correspondence between the form and the physical processes, then a substantial pedagogical tool will have been achieved. This proves invaluable in experimental design (to zero in on a particular process or parameter), model formulation and interpretation, data analysis and presentation, correlation development, etc. A model could lose its generality because, for instance, fluxes across interfaces are written as a term in Γ , thus making the interfacial flux a local phenomena rather than a boundary phenomena. This may be acceptable for a single geometry but causes the model to break down when applied to diverse geometries.

2) The field variables are continuous within the volume V .

This is also usually taken for granted. But care must be exercised in multiphase flow where discontinuities abound. A common approach, taken to simplify the complexity of multiphase flow, is to average the terms in the conservation equations across the cross-sectional area of the flow path. One could speculate that the error introduced in this manner could separate the model from reality enough to make the solutions be "unreal", i.e. complex numbers, singularities, etc. Further, fluctuating parameters are often smoothed by averaging over an appropriate Δt . These averaged parameters and products of parameters are used in models and compared to experiments. But there is no guarantee that, for instance,

$$\frac{1}{\Delta t} \int_{\Delta t} \psi \mathbf{V} dt = \left(\frac{1}{\Delta t} \int_{\Delta t} \psi dt \right) \left(\frac{1}{\Delta t} \int_{\Delta t} \mathbf{V} dt \right).$$

Thus the use of time averaged parameters can lead to additional errors. Indeed, because of the possibility of error due to space and time discontinuities, several investigators have offered rigorous treatments for the distributed approach (see, for example, Delhaye [7]). There is no reason why these treatments could not be applied to the lumped approach, as well. But, at this time, there is little incentive to do so since grid coarseness and experimental data are larger sources of error. As always, the operative rule is - BUYER BEWARE.

We now proceed to treat the mass, momentum and energy equations in turn.

3. THE CONSERVATION OF MASS

Historically, mass was the first variable observed to be conserved:

$$\iiint_V \frac{\partial}{\partial t} (Y_k \rho_k) dV = - \iint_S Y_k \rho_k \mathbf{V}_k \cdot \mathbf{n} ds + \iiint_V \Gamma_k dV + \iint_S S_k \mathbf{n} \cdot ds \quad (7)$$

where

- ρ_k = density of phase k (1 = liquid, 2 = vapour),
- Y_k = volume fraction of phase, k, in volume V, and
- Γ_k, S_k = phase sinks and sources, including chemical and nuclear effects.

The individual densities are related as follows:

$$\bar{\rho} = Y_1 \rho_1 + Y_2 \rho_2 = (1 - \alpha) \rho_1 + \alpha \rho_2, \quad (8)$$

where

- $\bar{\rho}$ = average density, and
- α = void fraction.

The 'overbar', $\bar{\quad}$ serves, to remind us that the volume fraction weighted sum must be performed.

But adding both phases together, equation (7) becomes:

$$\begin{aligned} \iiint_V \frac{\partial}{\partial t} [(1 - \alpha) \rho_1 + \alpha \rho_2] dV = \\ - \iint_S [(1 - \alpha) \rho_1 \mathbf{V}_1 + \alpha \rho_2 \mathbf{V}_2] \cdot \mathbf{n} ds + \iiint_V (\Gamma_1 + \Gamma_2) dV. \end{aligned} \quad (9)$$

In our case, $\Gamma_1 = -\Gamma_2$ (liquid boils or vapour condenses) and $S_k = 0$ (no mass sources or sinks at surfaces). Therefore:

$$\iiint_V \frac{\partial \bar{\rho}}{\partial t} dV = - \iint_S \bar{\rho} \mathbf{V} \cdot \mathbf{n} ds, \quad (10)$$

where

$$\overline{\rho V} = (1 - \alpha) \rho_1 V_1 + \alpha \rho_2 V_2 . \quad (11)$$

If we apply Gauss' Theorem and drop the integrals we have:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \overline{\rho V} = 0 \quad (12)$$

or

$$\frac{\partial}{\partial t} [(1 - \alpha) \rho_1 + \alpha \rho_2] + \nabla \cdot [(1 - \alpha) \rho_1 V_1 + \alpha \rho_2 V_2] = 0 . \quad (13)$$

This is the distributed form useful for modelling detailed flow patterns such as in the calandria, vessels, steam generators and headers. Component codes such as THIRST [8] and COBRA [9] use this approach.

In contrast, system codes such as SOPHT [4] and FIREBIRD [6], both based on Porsching's work [3], use the lumped equations. These codes represent a hydraulic network of pipes by nodes joined by links. Mass, pressure and energy changes occur at the nodes. Momentum changes occur in the links. Thus the network is treated on a macroscopic scale requiring an integral approach to the fundamental equations. Flow details in pipes are not considered. That is, diffusion, dispersion, advection, flow regimes, flow profiles, etc. are not fundamentally accounted for but are covered by empirical correlations. Averaging techniques, commonly used in the distributed approach are not used in the lumped approach mainly because there is little incentive to do so. The main sources of error lie elsewhere, mainly in the coarseness of the discretization in the direction of flow (i.e. node size) and in friction factors and heat transfer coefficients.

Now, $\iiint_V \rho dV$ is the mass, M_i , in the volume, V_i , of the i th node. Also, for our case, the surface integral can be written as surface integrals over the individual flow paths into and out of the volume or node. That is,

$$- \int_S \overline{\rho V} \cdot \mathbf{n} ds = \sum_j \overline{\rho_j V_j} A_j , \quad (14)$$

where j represents inflow and outflow links with $V_j > 0$ for inflow and < 0 for outflow. Inherent in equation (11) is the assumption that the integral, $\iint_S \rho V \cdot \mathbf{n} ds$ can be replaced by the simple product $\rho_j V_j A_j$. This implies known or assumed (usually uniform) velocity and density profile across the face of the link (or pipe).

Thus we now have:

$$\frac{\partial M_i}{\partial t} = \sum_j \overline{\rho_j V_j} A_j \equiv \sum_j W_j , \quad (15)$$

where W_j is the mass flow. This is the typical representation in system codes. Thus for the node-link type equations, we must add two more assumptions:

- i) nodalization, and

ii) assumed velocity and density profile across the cross-section of a pipe.

These assumptions have far reaching ramifications that are not immediately obvious. No flow detail is considered as the fluid moves along a pipe. Therefore, no diffusion, dispersion, advection, flow profiles or flow regimes are explicitly permitted. This is not too crude an approximation for the calculation of pressure drops and flows but for modelling the propagation of disturbances, this approach is inadequate as it stands unless a large number of nodes and links are used.

To show this, consider a homogeneous or bubbly flow through a pipe, as in the two-phase regions of typical heat transport systems in nuclear reactors, modelled in system codes as nodes connected by links. Perfect mixing at the nodes is assumed. Flow in a pipe, however, has aspects of plug flow. That is, flow is transmitted along the pipe relatively undisturbed. If no diffusion or turbulent dispersion existed, a sharp discontinuity in a property would propagate undisturbed. If a single mixing tank (node) represented a section of pipe of volume, V , and volumetric flow, \dot{V} , then a step change to zero in a field property, C , (which could be concentration or density) entering the node would be an exponential by the time it left the node, that is:

$$C_{OUT} = C_{IN} e^{-t/\tau}$$

where $\tau = V/\dot{V}$; τ is also the transmission time for the plug flow model. If the pipe were modelled by two nodes in series,

$$C_{OUT\ NODE\ 2} = C_{IN\ NODE\ 1} \times (1 + 2t/\tau) e^{-2t/\tau},$$

and in general, for n nodes.

$$C_{OUT\ NODE} = C_{IN\ NODE\ 1} \times e^{-nt/\tau} \sum_{k=1}^n (nt/\tau)^{k-1} / (n-1);$$

Figure 1 compares the transmission of a step change for various numbers of nodes and the plug flow model. It is easy to see why the codes model void propagation poorly. A very large number of nodes are needed to transmit a disturbance without appreciable distortion. The phase relationships or timing, of the propagation is very important in determining the stability of a thermal hydraulic system. A pocket of void reaching a given destination at an earlier or later time may enhance or cancel the phenomenon in question. The smearing of a wave front alters the timing and gain and hence affects stability. The slow convergence of the mixing model to the plug flow model explains the typically slow convergence of such system codes.

Thus, nodalization creates a form of diffusion in much the same manner as finite difference schemes create numerical diffusion (see, for instance, Roache [10]).

Attaining convergence in nodalization is, in essence, converging the model to plug flow behaviour. But is the flow in typical heat transport systems plug flow?

Flow in the CANDU feeders (38 to 76 mm) at 15 M/sec may indeed be plug flow. But some turbulent mixing does take place. More importantly, the feeders are of varying length and the flow has a spectrum of qualities. This gives quite a spectrum in transit time. This will skew the propagation of a disturbance. Thus, depending on the transit time spectrum, a 5 node approximation (say) may be quite a good representation.

The risers and headers may also give more diffusion than plug flow. These pipes are large diameter and the flow is turbulent. Very little is known of flow regimes and propagation properties in these situations.

In short, careful attention should be given to nodalization for meaningful simulation, quite apart from the normal numerical concerns such as the Courant limit, etc.

To conclude our progressive simplification, we note the steady state form of equation (15):

$$\sum_j \overline{\rho_j V_j} A_j = \sum_j W_j = 0 \quad (16)$$

For a simple circular flow loop, the mass flow rate at steady state is a constant at any point in the loop. Local area and density variations thus give rise to velocity variations around the loop.

Local velocity then is:

$$V = \frac{W}{\rho A} \quad (17)$$

4. THE CONSERVATION OF MOMENTUM

Newton observed that momentum is conserved, i.e. a body moves in a straight line unless forced to do otherwise. This is equivalent to a force balance if the inertial force (a momentum sink of sorts) is recognized. In the integral sense, the rate of change of momentum is equal to the forces acting on the fluid. Thus:

$$\frac{D}{Dt} \iiint_V \rho_k V_k dV = \iint_S \sigma_k \cdot n ds + \iiint_V \rho_k f_k dV + \iiint_V M_k dV, \quad (18)$$

where

σ is the stress tensor (i.e., short range or surface effects including pressure, viscosity, etc.),

f is the long range or body force (i.e., gravity),

and

M is the momentum interchange function accounting for phase change effects.

Using Reynold's Transport Theorem, we get:

$$\begin{aligned} & \int \int \int_V \frac{\partial}{\partial t} (\gamma_k \rho_k V_k) dV + \int \int_S (\gamma_k \rho_k V_k) (V_k \cdot n) ds \\ &= \int \int_S \sigma_k \cdot n ds + \int \int \int_V \gamma_k \rho_k f_k dV + \int \int \int_V M_k dV . \end{aligned} \quad (19)$$

Adding both phases together as per the mass equation, we find:

$$\int \int \int_V \frac{\partial}{\partial t} \overline{\rho V} dV + \int \int_S \overline{\rho V} (\overline{V \cdot n}) ds = \int \int_S \overline{\sigma} \cdot n ds + \int \int \int_V \overline{\rho f} dV . \quad (20)$$

To get the microscopic form we use Gauss's theorem and drop the volume integral as before to leave:

$$\frac{\partial}{\partial t} (\overline{\rho V}) + \nabla \cdot \overline{\rho V V} = \nabla \cdot \overline{\sigma} + \overline{\rho f} . \quad (21)$$

The stress tensor, σ , can be split into the normal and shear components:

$$\sigma = -PI + \tau, \quad (22)$$

where P is the pressure, I is the unity tensor and τ is the shear stress tensor. This enables the explicit use of pressure and helps maintain our tenuous link with reality. Of course, it can equally be introduced in the integral form, Equation (20), or as a separate pressure for each phase in equation (19). At any rate, Equation (21) becomes:

$$\frac{\partial}{\partial t} (\overline{\rho V}) + \nabla \cdot \overline{\rho V V} = \nabla P + \nabla \cdot \tau + \overline{\rho f} . \quad (23)$$

This is the form commonly seen in the literature, useful for distributed modelling as per the mass conservation equation. The term, $\nabla \cdot \tau$, is usually replaced by an empirical relation. For the system codes using the node-link structure, we switch back to the macroscopic form, Equation (20).

If the surface integral for the advective term is performed over the inlet and outlet areas of the pipe (link) in question, then:

$$\int \int_S \overline{\rho V} (\overline{V \cdot n}) ds = \int \int_{A_{IN}} \overline{\rho V} (\overline{V \cdot n}) ds + \int \int_{A_{OUT}} \overline{\rho V} (\overline{V \cdot n}) ds , \quad (24)$$

where A_{IN} is the flow inlet area and A_{OUT} is the flow outlet area. If we assume the properties are constant over the areas, then:

$$\overline{V} \frac{\partial \overline{\rho V}}{\partial t} - A_{IN} \overline{\rho V V} + A_{OUT} \overline{\rho V V} = \int \int_S \overline{\sigma_k} \cdot n ds + \int \int \int_V \overline{\rho f} dV .$$

Alternatively we could perform a cross-sectional average of each term, usually denoted by $\langle \rangle$, where $\langle \rangle = 1/A \int \int_S (\cdot) ds$. If we assume the properties, V , ρ and A are constant along the length of the pipe, then the second and third terms cancel.

Equation (25) can be rewritten as:

$$\begin{aligned} \bar{v} \frac{\partial \bar{\rho} \bar{V}}{\partial t} &= - \iint_S \mathbf{P} \mathbf{I} \cdot \mathbf{n} \, ds + \iiint_V (\nabla \cdot \boldsymbol{\tau} + \bar{\rho} \mathbf{f}) \, dV \\ &= -A_{\text{OUT}} P_{\text{OUT}} + A_{\text{IN}} P_{\text{IN}} - \frac{\bar{v} \bar{\rho}}{L} \left(\frac{fL}{D} + k \right) \frac{V|V|}{2g_c} - LA \bar{\rho} \sin(\theta) g/g_c, \end{aligned} \quad (26)$$

where g_c is the gravitational constant, g is the acceleration due to gravity and where $\nabla \cdot \boldsymbol{\tau}$ and $\rho \mathbf{f}$ evaluated by empirical correlations (the standard friction factor) plus an elevation change term (θ is the angle w.r.t. the horizontal).

Assuming one dimensional flow and defining the mass flow as $W = \bar{\rho} \bar{V} A$, and L as the pipe length, Equation (26) becomes:

$$\frac{\partial W}{\partial t} = \frac{A}{L} \left[(P_{\text{IN}} - P_{\text{OUT}}) - \left(\frac{fL}{D} + k \right) \frac{W^2}{2g_c \rho A^2} \right] - A \rho g/g_c \sin(\theta), \quad (27)$$

which is the form typically used in system codes.

If circumstances require, extra terms can be added. For instance, if a pump is present this can be considered to be an external force acting through head, ΔP_{pump} . Equation (27) would then become:

$$L \frac{\partial W}{\partial t} = A_{\text{OUT}} P_{\text{OUT}} + A_{\text{IN}} P_{\text{IN}} + A \Delta P_{\text{pump}} + \dots \quad (28)$$

The momentum flux terms ($A \rho V^2$) in Equation (25) could also be added if large area or property changes were present.

In the steady state, for a constant area pipe with no pump and no elevation change:

$$P_{\text{IN}} - P_{\text{OUT}} = \rho \left(\frac{fL}{D} + k \right) \frac{V^2}{2g_c} = \left(\frac{fL}{D} + k \right) \frac{W^2}{2A^2 \rho g_c} \quad (29)$$

As a final note, the assumptions made for the mixture momentum equation are thus similar to those made for the mixture mass equation and the same comments apply. One cannot hope to accurately model such phenomena as void propagation and other two phase transient flow effects using lumped single phase equations unless a large number of nodes and links are used.

5. THE CONSERVATION OF ENERGY

By the early 1800's, philosophical jumps were made in recognizing that heat was not a substance and in the emergence of electromagnetic theory. The concept of energy as we now think of it was formulated and it was found that energy, too, was conserved, as long as we carefully identify all the different forms of energy (kinetic, chemical, potential, nuclear, internal, electromagnetic, ...).

The mathematical statement of the conservation of energy is:

$$\begin{aligned} \frac{D}{Dt} \iiint_V Y_k \rho_k (e_k + \frac{1}{2} V_k^2) dV = & - \iint_S q_k \cdot n ds + \iiint_V E_k dV, \\ & + \iiint_V Y_k \rho_k f_k \cdot V_k dV + \iint_S (\sigma_k \cdot n) \cdot V_k ds \end{aligned} \quad (30)$$

where

- e_k = internal energy of phase k,
- q_k = surface heat flux for phase k, and
- E_k = internal heat sources and sinks of phase k.

The left hand side is the substantial derivative of the internal plus kinetic energy.

The right hand side terms are, respectively:

- 1) surface heat flux,
- 2) internal sources and sinks,
- 3) work due to long range body forces (gravity, etc.),
- 4) work due to short range forces (surface tension, pressure, etc.).

Using Reynold's Transport Theorem again:

$$\begin{aligned} & \iiint_V \frac{\partial}{\partial t} [Y_k \rho_k (e_k + \frac{1}{2} V_k^2)] dV + \iint_S Y_k \rho_k (e_k + \frac{1}{2} V_k^2) V_k \cdot n ds \\ = & - \iint_S q_k \cdot n ds + \iiint_V E_k dV + \iiint_V Y_k \rho_k f_k \cdot V_k dV + \iint_S (\sigma_k \cdot n) \cdot V_k ds \end{aligned} \quad (31)$$

Summing over k, the mixture equation becomes:

$$\begin{aligned} & \iiint_V \frac{\partial}{\partial t} [\overline{\rho e} + \frac{1}{2} \overline{\rho V^2}] dV + \iint_S [\overline{\rho e} + \frac{1}{2} \overline{\rho V^2}] V \cdot n ds \\ = & - \iint_S q \cdot n ds + \iiint_V E dV + \iiint_V \overline{\rho f \cdot V} dV + \iint_S \overline{(\sigma \cdot n) \cdot V} ds, \end{aligned} \quad (32)$$

where

$$\overline{\rho e} = Y_1 \rho_1 e_1 + Y_2 \rho_2 e_2 \text{ and } E = E_1 + E_2, \text{ etc.}$$

Using Gauss' Theorem to change some of the surface integrals to volume integrals:

$$\begin{aligned} & \iiint_V \frac{\partial}{\partial t} [\overline{\rho e} + \frac{1}{2} \overline{\rho V^2}] dV + \iint_S \overline{\rho e V} \cdot n ds + \iiint_V \nabla \cdot \left[\frac{1}{2} \overline{\rho V^2 V} \right] dV \\ = & - \iint_S q \cdot n ds + \iiint_V E dV + \iiint_V \overline{\rho f \cdot V} dV + \iiint_V \nabla \cdot (\overline{\sigma \cdot V}) dV. \end{aligned} \quad (33)$$

Since

$$\sigma = -PI + \tau,$$

$$\iiint_V \nabla \cdot (\overline{\sigma \cdot V}) dV = \iiint_V [\nabla \cdot (\overline{\tau \cdot V}) - \nabla \cdot (\overline{PV})] dV.$$

This is the total energy equation, composed of thermal terms and mechanical terms. We can separate the two by first generating the mechanical terms from the momentum equation (Equation 20). Forming the dot product with velocity we get:

$$\begin{aligned} \iiint_V \frac{\partial}{\partial t} (\rho \mathbf{V}) \cdot \mathbf{V} dV + \iiint_V \mathbf{V} \cdot (\nabla \cdot \rho \mathbf{V} \mathbf{V}) dV = \iiint_V \mathbf{V} \cdot (\nabla \cdot \boldsymbol{\tau}) dV \\ - \iiint_V \mathbf{V} \cdot \nabla P dV + \iiint_V \rho \mathbf{f} \cdot \mathbf{V} dV. \end{aligned} \quad (34)$$

Now

$$\mathbf{V} \cdot (\nabla \cdot \boldsymbol{\tau}) = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{V}) - \boldsymbol{\tau} : \nabla \mathbf{V}, \quad (35)$$

$$\mathbf{V} \cdot \nabla P = \nabla \cdot (P \mathbf{V}) - P \nabla \cdot \mathbf{V}, \quad (36)$$

$$\mathbf{V} \cdot \frac{\partial}{\partial t} (\rho \mathbf{V}) = \frac{\partial}{\partial t} \left(\frac{1}{2} \rho \mathbf{V} \cdot \mathbf{V} \right) = \frac{\partial}{\partial t} \left(\frac{1}{2} \rho V^2 \right) \quad (37)$$

and

$$\mathbf{V} \cdot (\nabla \cdot \rho \mathbf{V} \mathbf{V}) = \nabla \cdot \left(\frac{1}{2} \rho V^2 \mathbf{V} \right) \quad (38)$$

Using these identities and subtracting Equation (34) from Equation (33), we get:

$$\begin{aligned} \iiint_V \frac{\partial}{\partial t} (\overline{\rho e}) dV + \iint_S \overline{\rho e \mathbf{V}} \cdot \mathbf{n} ds = - \iint_S \mathbf{q} \cdot \mathbf{n} ds \\ + \iiint_V E dV + \iiint_V \boldsymbol{\tau} : \nabla \mathbf{V} dV - \iiint_V \overline{P \nabla \cdot \mathbf{V}} dV. \end{aligned} \quad (34)$$

This is the thermal form of the energy equation. This form of the energy equation can be used to generate the thermal conductance equation for solids. By setting fluid velocity to zero and converting surface integrals to volume integrals we get the distributed form:

$$\frac{\partial}{\partial t} (\rho e) = -\nabla \cdot \mathbf{q} + E, \quad (40)$$

where E is the internal energy generation rate term.

From thermodynamics, for solids, we have:

$$\frac{\partial}{\partial t} (\rho e) = \rho \frac{\partial e}{\partial t} = \rho C_v \frac{\partial T}{\partial t} \quad (41)$$

and using Fourier's law for heat conduction:

$$\mathbf{q} = -k \nabla T, \quad (42)$$

we have the classical form of the heat conduction equation:

$$\begin{aligned} \rho C_v \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + E \\ = k \nabla^2 T + E \quad \text{for space independent } k. \end{aligned} \quad (43)$$

This is useful for determining the temperature distributions in boiler tube walls, piping walls and reactor fuel pencils. To generate the node-link forms we now turn back to the integral

form of Equation (39). If we assume that the density and enthalpy are uniform over the node (the volume in question), then

$$\iiint_V \frac{\partial}{\partial t} (\overline{\rho e}) dV = \frac{\partial U}{\partial t} \quad (44)$$

where

$$U \equiv \overline{V \rho e} = LA \overline{\rho e} \quad (45)$$

The integral of the transport term can be written over the flow surfaces:

$$\iint_S \overline{\rho e \mathbf{V} \cdot \mathbf{n}} ds = \iint_{A_1} \overline{\rho e \mathbf{V} \cdot \mathbf{n}} ds + \iint_{A_2} \overline{\rho e \mathbf{V} \cdot \mathbf{n}} ds + \dots, \quad (46)$$

where A_1, A_2 , etc. are the pipe flow cross-sectional areas. For inflow, $\mathbf{V} \cdot \mathbf{n}$ is negative. For outflow, $\mathbf{V} \cdot \mathbf{n}$ is positive. Assuming uniform velocity, enthalpy and density across the link (pipe) cross-section gives:

$$\begin{aligned} \iint_S \overline{\rho e \mathbf{V} \cdot \mathbf{n}} ds &= - \sum_{\text{IN FLOW}} \overline{\rho e \mathbf{V}} A_i + \sum_{\text{OUT FLOW}} \overline{\rho e \mathbf{V}} A_i \\ &= - \sum \overline{W_{\text{IN}} e_{\text{IN}}} + \sum \overline{W_{\text{OUT}} e_{\text{OUT}}} \end{aligned} \quad (47)$$

The heat flux and generation terms of the thermal energy equation can be lumped into a loosely defined heat source for the volume:

$$- \iint_S \mathbf{q} \cdot \mathbf{n} ds + \iiint_V E dV \equiv Q \quad (48)$$

Therefore, the thermal energy equation becomes:

$$\frac{\partial U}{\partial t} = \sum \overline{W_{\text{IN}} e_{\text{IN}}} - \sum \overline{W_{\text{OUT}} e_{\text{OUT}}} + Q + \iiint_V \overline{\tau : \nabla \mathbf{V}} dV - \iint_V \overline{P \nabla \cdot \mathbf{V}} dV \quad (49)$$

The last two terms are the irreversible and reversible internal energy conversion, respectively.

Some system codes track enthalpy rather than internal energy. Defining:

$$h = \text{enthalpy} \equiv e + P/\rho$$

and

$$H \equiv \overline{V \rho h} \quad (50)$$

we can rewrite Equation (39) as follows:

$$\begin{aligned} \iiint_V \frac{\partial (\overline{\rho h - P})}{\partial t} dV + \iint_S (\overline{\rho h - P}) \mathbf{V} \cdot \mathbf{n} ds \\ = - \iint_S \mathbf{q} \cdot \mathbf{n} ds + \iiint_V E dV + \iiint_V \overline{\tau : \nabla \mathbf{V}} dV - \iint_V \overline{P \nabla \cdot \mathbf{V}} dV \end{aligned} \quad (51)$$

Collecting the pressure terms and simplifying yields:

$$\begin{aligned}
& \iiint_V \frac{\partial}{\partial t} (\overline{\rho h}) dV + \iint_S \overline{\rho h \mathbf{V}} \cdot \mathbf{n} ds \\
&= - \iint_S \overline{\mathbf{q}} \cdot \mathbf{n} ds + \iiint_V \overline{E} dV + \iiint_V \overline{\boldsymbol{\tau} : \nabla \mathbf{V}} \\
&+ \iiint_V \frac{\partial P}{\partial t} dV + \iint_S \overline{P \mathbf{V}} \cdot \mathbf{n} ds - \iiint_V \overline{P \nabla \cdot \mathbf{V}} dV. \tag{52}
\end{aligned}$$

The surface integral over P can be transformed into a volume integral using Gauss' theorem and combined with the last term to give:

$$\begin{aligned}
\iint_S \overline{P \mathbf{V}} \cdot \mathbf{n} ds - \iiint_V \overline{P \nabla \cdot \mathbf{V}} dV &= \iiint_V \overline{\nabla \cdot (P \mathbf{V})} dV - \iiint_V \overline{P \nabla \cdot \mathbf{V}} dV \\
&= \iiint_V \overline{\mathbf{V} \cdot \nabla P} dV.
\end{aligned}$$

The enthalpy flux terms can be evaluated in the same manner that the energy flux terms were in Equations (46-47). Thus,

$$\iint_S \overline{\rho h \mathbf{V}} \cdot \mathbf{n} ds = - \sum \overline{W_{IN} h_{IN}} + \sum \overline{W_{OUT} h_{OUT}}. \tag{54}$$

Finally, using Equations (48, 50, 53-54), Equation (52) becomes:

$$\begin{aligned}
\frac{\partial H}{\partial t} &= - \sum \overline{W_{IN} h_{IN}} + \sum \overline{W_{OUT} h_{OUT}} + Q \\
&+ \iiint_V \overline{\boldsymbol{\tau} : \nabla \mathbf{V}} dV + \iiint_V \left(\frac{\partial P}{\partial t} + \overline{\mathbf{V} \cdot \nabla P} \right) dV \tag{55}
\end{aligned}$$

The integral term involving pressure is often neglected since it is usually negligible compared to the other terms. For instance, the typical CANDU Heat Transport System operates at a pressure of 10 MPa, a fluid velocity of ~10 m/s, and a pressure gradient of less than 70 kPa/m. This translates into roughly 10 kJ/kg while e is approximately 1000 kJ/kg.

The turbulent heating term is usually approximated by adding pump heat as a specific form of Q.

Equation (55) in the steady state, neglecting turbulent heating and the pressure terms, is the familiar:

$$Q = \sum \overline{W_{OUT} h_{OUT}} - \sum \overline{W_{IN} h_{IN}}. \tag{56}$$

For a reactor or a boiler (one flow in, one flow out):

$$Q = \overline{W(h_{OUT} - h_{IN})} = \overline{W C_p (T_{OUT} - T_{IN})}. \tag{57}$$

Another special case of equation (55) is obtained by expanding the term Q as per equation (48):

$$-\iint_S \mathbf{q} \cdot \mathbf{n} \, ds + \iiint_V E \, dV \equiv Q \quad (48)$$

Using Newton's Law of cooling for convection:

$$\mathbf{q} \cdot \mathbf{n} = h_N (T - T_s), \quad (58)$$

where

- $\mathbf{q} \cdot \mathbf{n}$ = heat flux normal to surface, s,
- T = Temperature of fluid,
- T_s = Temperature of surface (wall), and
- h_N = heat transfer coefficient,

Equation (55), neglecting the pressure terms, becomes:

$$\begin{aligned} \iiint_V \frac{\partial \rho h}{\partial t} - \iiint_V \frac{\partial P}{\partial t} \left(\equiv \iiint_V \frac{\partial \rho e}{\partial t} = \iiint_V \rho C_v \frac{\partial T}{\partial t} \right) \\ = \sum \overline{W_{IN} h_{IN}} - \sum \overline{W_{OUT} h_{OUT}} - Ah_N (T - T_s) \\ + \iiint_V \tau : \nabla \mathbf{V} \, dV \end{aligned} \quad (59)$$

which is useful for accounting for heat transfer between the fluid and the pipe or tube walls (eg: boiler heat transfer).

The heat transfer coefficient, h_N , is supplied through empirical relations. The turbulent heating term $\iiint_V \tau : \nabla \mathbf{V} \, dV$ generally can be neglected.

6. THE EQUATION OF STATE

From the conservation equations, we have three equations for each phase (mass, momentum and energy conservation) and four unknowns:

- 1) density, ρ or mass, $\forall \rho$,
- 2) velocity, V , or mass flow, W , or momentum, ρV ,
- 3) energy, e , or enthalpy, $h = e + P/\rho$, or temperature, $T = \text{fn}(e)$ or $\text{fn}(h)$, and
- 4) pressure, P .

The fourth equation required for closure is the equation of state:

$$P = \text{fn}(h, \rho) \text{ or } \text{fn}(T, \rho)$$

or

$$\rho = \text{fn}(P, T), \text{ etc.} \quad (60)$$

Thermodynamic equilibrium is usually assumed, as in the following. For water, H_2O or D_2O , tables of properties give the required functional relationship. Often, a curve fit of the tables is used. This data is input to the computer codes and utilized in table lookup schemes or directly via the parametric curve fits.

To illustrate the process, consider a fixed volume, V , having a mass of H_2O , M , and a specific enthalpy, h . The volume is usually a specified geometric input. The mass flows and enthalpy have, let's assume, been calculated from the simultaneous solution of the conservation equations. The state equation gives the pressure given the mass and enthalpy for that volume, as follows.

The density, ρ , is an average for that volume, and is calculated from:

$$\rho = M/V. \quad (61)$$

The pressure is guessed (as per the last time iteration, for instance) and the table lookup gives the associated density and specific enthalpies for liquid and vapour forms of H_2O . Since the average density is related to the specific densities by the relation:

$$\rho = \rho_f(1 - \alpha) + \rho_g \alpha, \quad (62)$$

that is, the average density is a volume weighted sum of the specific densities. The void fraction, α , is readily calculated. Given a relationship between void fraction, α , and weight fraction (quality), x , we have the quality, x . An example of such a relationship is the no-slip case:

$$\left(\frac{x}{1-x} \right) \left(\frac{1-\alpha}{\alpha} \right) \frac{\rho_f}{\rho_g} = 1. \quad (63)$$

The mixture enthalpy, h , is given by

$$h = h_f(1-x) + h_g x, \quad (64)$$

that is, the average or mixture enthalpy is a mass weighted sum of the specific enthalpies. This mixture enthalpy is compared to the given enthalpy and the guess at the pressure is updated accordingly until convergence is reached.

To help guide the search for the compatible combination of P , h and ρ , partial derivatives, such as $\partial P / \partial h|_p$, are often used to calculate the next guess.

If the fluid is calculated to be subcooled, then no positive quality or void exists. The slope of the property functions become very steep so that small variations in ρ or h can generate large variations in P . One solution to this problem is to start with the density, use it in a table lookup to give the saturation pressure and the saturation enthalpy. Then a correction to the pressure is made to correct for the fact that the actual enthalpy is less than the saturation enthalpy. Thus:

$$P = P_{SAT_f}(\rho) + \left. \frac{\partial P}{\partial h} \right|_p [h - h_{SAT_f}(\rho)]. \quad (65)$$

A similar process is used for single phase steam, giving:

$$P = P_{SAT_g}(\rho) + \left. \frac{\partial P}{\partial h} \right|_p [h - h_{SAT_g}(\rho)]. \quad (66)$$

Internal energy, e (or sometimes, u), is related to enthalpy, h as follows:

$$h = e + P/\rho \quad (67)$$

The above calculation of pressure is sometimes performed using the variable, e or u , rather than h . The choice is one of convenience or personal preference only.

7. EMPIRICAL CORRELATIONS

As previously discussed, supporting relations are required to provide the necessary information for the conservation and state equations. The primary areas where support is needed are:

- 1) relationship between quality and void fractions, i.e., slip velocities in two phase flow (to link the mass and energy conservation equations via the state equation);
- 2) the stress tensor, τ (effects of wall shear, turbulence, flow regime and fluid properties on momentum or, in a word: friction);
- 3) heat transfer coefficients (to give the heat energy transfer for a given temperature distribution in heat exchangers, including steam generators and reactors);
- 4) thermodynamic properties for the equation of state;
- 5) flow regime maps to guide the selection of empirical correlations appropriate to the flow regime in question;
- 6) special component data for pumps, valves, steam drums, pressurizers, bleed or degasser condensers, etc; and
- 7) critical heat flux information (this is not needed for the solution of the process equations but a measure of engineering limits is needed to guide the use of the solutions of the process equations as applied to process design.

The above list of correlations, large enough in its own right, is but a subset of the full list that would be required were it not for a number of key simplifying assumptions made in the derivation of the basic equations. The three major assumptions made for the primary heat transport system are:

- 1) one dimensional flow;
- 2) thermal equilibrium (except for the pressurizer under surge); and
- 3) one fluid model (i.e. mixture equations).

These are required because of state of the art limitations. References [11-21] are recommended for further reading.

8. SOLUTION OVERVIEW

Because of the complexity of solving the mass, momentum and energy equations plus supporting equations of state and empirical correlations all subject to initial and boundary conditions, it is quite easy to "not see the forest for the trees". A skeleton overview may help

in this regard. Figure 2 illustrates the equations and the information links between them. In words, the momentum equation gives the flows or velocities from one node to another, or from one grid point to another, based on a given pressure, flow, mass and energy distribution. The updated flows are used by the mass and energy equations to update the mass and energy contents at each location. This information is given to the equation of state to update the pressure distribution. This information, along with the new densities and energies are used by the momentum equation, and so on. In this manner, a time history of the fluid evolution is obtained. Of course, only the main variables are noted. The numerous and diverse empirical correlations require updates on the main variables and many secondary variables. This information also "flows" around the calculation.

A further point to note on the solution overview is that each phase in a multiphase flow has a main information flow path as shown in Figure 3. In the full UVUEUP (unequal velocity, energy and pressure) model, there are two distinct phases: one for the vapour phase and one for the liquid phase. If a simplified model was imposed, this essentially means that the planes would touch at some point. For instance, if equal pressure in both phases was assumed, then Figure 4 would result. Here, the equation of state is common to both planes.

The HEM (homogeneous equilibrium model) is the fully collapsed case where both planes collapse into one (Figure 2). You may find these images to be useful in conceptualizing the basic equations and how they fit together.

The precise solution procedure that you might employ is case dependent. At present, no general solution scheme exists because the nuances of specific problems are subtle and because one cannot usually afford to ignore the efficiency and cost savings gained by tuning a method to a particular case. The economics of using a case specific code are changing, however, with developments in the microcomputer field and with the realization that total design and analysis time can often be reduced by using a less efficient but more robust code. Codes such as SOPHT and FIREBIRD are a direct result of this realization. The near term evolution will likely be affected mostly by microcomputer developments.

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NOMENCLATURE

| | |
|---------------|--|
| A | area |
| \mathbf{A} | arbitrary vector |
| C | concentration |
| C_p | heat capacity at constant pressure |
| C_v | heat capacity at constant volume |
| e | specific internal energy |
| E | internal heat source or sink |
| f | friction factor |
| \mathbf{f} | long range or body force |
| g_c | gravitational constant |
| g | acceleration due to gravity |
| h | specific enthalpy |
| h_N | heat transfer coefficient |
| H | total enthalpy in volume, \mathcal{V} |
| I | unity tensor |
| k | head loss coefficient |
| L | length |
| M | mass in volume, \mathcal{V} |
| \mathbf{M} | momentum interchange vector |
| \mathbf{n} | unit vector normal to the surface |
| P | pressure |
| q | heat flux |
| Q | lumped heat source or sink |
| s | surface bounding volume, \mathcal{V} |
| S | surface sink or source |
| t | time |
| T | temperature |
| U | total internal energy in volume, \mathcal{V} |
| \mathcal{V} | arbitrary fluid volume |
| \mathbf{V} | velocity vector |
| W | mass flow |
| x | quality (weight fraction) |

$$Q = - \iint_S \mathbf{q} \cdot \mathbf{n} ds + \iiint_{\mathcal{V}} E d\mathcal{V}$$

Greek

| | |
|----------|----------------------------------|
| α | void fraction |
| γ | phase volume fraction |
| Γ | local sink or source |
| ψ | field variable |
| ρ | density |
| σ | stress tensor |
| θ | angle with respect to horizontal |
| τ | shear stress tensor |

Operators

$\frac{\partial}{\partial t}$ partial time derivative

$\frac{d}{dt}$ total time derivative

$\frac{D}{Dt}$ substantial time derivative

∇ Del operator

$\iiint_V () dV$ volume integral

$\iint_S () ds$ surface integral

$(\overline{ })$ sum over the phases

$\langle () \rangle = \frac{1}{A} \iint_S () ds =$ cross-sectional average

Subscripts

| | |
|-----|-------------------------------|
| f | liquid (fluid) phase |
| g | vapour (gaseous) phase |
| i | summation index for nodes |
| j | summation index for links |
| k | 1, 2 (1 = liquid, 2 = vapour) |
| S | surface |
| SAT | saturated |
| IN | ingoing |
| OUT | outgoing |

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