CHAPTER 10

BASIC EQUATIONS

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SUMMARY

This chapter 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 empirical correlations. Closure is obtained by the equation of state.

10.1 DEVELOPMENT OF THE BASIC EQUATIONS

Fluid flow and heat transfer, the phenomena of concern in the systems analysis of process systems, are governed by the conservation laws for mass, energy and momentum (Bird et al., 1960), the constitutive laws or state equations plus numerous supporting empirical relationships.

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 fact.

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

$$\frac{D}{Dt}\int\int\int_{\forall} \psi \, d\forall = \int\int\int_{\forall} \Gamma \, d\forall \tag{1}$$

where

D/Dt = total or substantial derivative (= change due to time variations plus change due to movement in space)

$\forall$ = volume

Γ = sum of (local sources - minus local sinks)

ψ = field variable such as mass, momentum, energy, etc.

t = time

We can now use Reynold's Transport Theorem (a mathematical identity) (Currie, 1974):

$$\frac{D}{Dt}\iiint_{\forall} \psi \, d\forall = \iiint_{\forall} \frac{\partial \psi}{\partial t} d\forall + \iint_{S} \psi \, \mathbf{V} \cdot \mathbf{n} \, ds \tag{2}$$

where

$\partial/\partial t$ = local time derivative

S = surface bounding the volume, $\forall$

V = velocity of the field variable

n = unit vector normal to the surface;

to give

$$\iiint_{\forall} \frac{\partial \psi}{\partial t} d\forall = -\iint_{S} \psi \, \mathbf{V} \cdot \mathbf{n} \, ds + \iiint_{\forall} \Gamma d\forall \, . \tag{3}$$

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

$$\iint_{S} \mathbf{A} \cdot \mathbf{n} \, ds = \iiint_{\forall} \nabla \cdot \mathbf{A} \, d\forall \tag{4}$$

where

A = any vector, such as velocity

∇ = Del operator (eg. $\nabla = \partial/\partial x \, \mathbf{i} + \partial/\partial y \, \mathbf{j} + \dots$) .

Thus equation (3) can be rewritten:

$$\iiint_{\forall} \frac{\partial \psi}{\partial t} d\forall = -\iiint_{\forall} \nabla \cdot \psi \, \mathbf{V} \, d\forall + \iiint_{\forall} \Gamma d\forall \tag{5}$$

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:

$$\frac{\partial \psi}{\partial t} = -\nabla \cdot \psi \, \mathbf{V} + \Gamma \tag{6}$$

This is the microscopic form. Equation (3) is the 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 most 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 (i.e. SOPHT), 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 fact.

   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), $\nabla\cdot\psi\mathbf{V}$, and
   c) the local sinks and sources, Γ.

   Models often lose their 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 $\forall$.

   This is also usually taken for granted. But care must be excercised 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,

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

Thus the use of time averaged parameters can lead to additional errors. As always, the operative rule is - BUYER BEWARE.

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

10.2 THE CONSERVATION OF MASS

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

$$\iiint_{\forall}\frac{\partial}{\partial t}(\gamma_k\,\rho_k)\,d\forall = -\iint_S \gamma_k\,\rho_k\,\mathbf{V}_k\cdot\mathbf{n}\,ds + \iiint_{\forall}\Gamma_k\,d\forall\,, \tag{7}$$

where

ρ_k = density of phase k (1 = liquid, 2 = vapour)

γ_k = volume fraction of phase, k, in volume $\forall$, and

Γ_k = phase sinks and sources, including chemical and nuclear effects.

The individual densities are related as follows:

$$\overline{\rho} = \gamma_1\rho_1 + \gamma_2\rho_2 = (1-\epsilon)\,\rho_1 + \epsilon\,\rho_2 \tag{8}$$

where

$\overline{\rho}$ = average density, and

ϵ = void fraction.

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

$$\iiint_{\forall}\frac{\partial}{\partial t}[(1-\epsilon)\,\rho_1 + \epsilon\,\rho_2]\,d\forall =$$

$$-\iint_S [(1-\epsilon)\,\rho_1\,\mathbf{V}_1 + \epsilon\,\rho_2\,\mathbf{V}_2]\cdot\mathbf{n}\,ds + \iiint_{\forall}(\Gamma_1+\Gamma_2)\,d\forall \tag{9}$$

In our case, $\Gamma_1 = -\Gamma_2$ (liquid boils or vapour condenses). Therefore:

$$\iiint_{\forall}\frac{\partial\overline{\rho}}{\partial t}\,d\forall = -\iint_S \overline{\rho\mathbf{V}}\cdot\mathbf{n}\,ds \tag{10}$$

where

$$\overline{\rho\mathbf{V}} = (1-\epsilon)\,\rho_1\mathbf{V}_1 + \epsilon\,\rho_2\mathbf{V}_2 \tag{11}$$

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

$$\frac{\partial\overline{\rho}}{\partial t} + \nabla\cdot\overline{\rho\mathbf{V}} = 0 \tag{12}$$

or

$$\frac{D\overline{\rho}}{Dt} = 0\,. \tag{13}$$

This is the microscopic form useful for modelling detailed flow patterns such as in the calandria, vessels, steam generators and headers. Component codes such as MODCIRC, THIRST and COBRA use the microscopic approach.

In contrast, system codes such as SOPHT and FIREBIRD use the macroscopic equations. These codes represent a hydraulic network of pipes by nodes joined by links. Mass 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 <u>not</u> considered. That is, diffusion, dispersion, advection, flow regimes, flow profiles, etc. are not fundamentally accounted for but are covered by empirical correlations and averaging techniques.

Now, $\iiint_{\forall} \overline{\rho} d\forall$ is the mass, M_i, in the volume, $\forall_i$, where i represents the node. Also, for our case, the surface integral can be written as surface integrals over the individual paths into and out of the volume or node. That is,

$$-\iint_S \overline{\rho \mathbf{V}} \cdot \mathbf{n}\, ds = \sum_j \overline{\rho_j V_j} A_j , \tag{14}$$

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, $\iint_S \overline{\rho \mathbf{V}} \cdot \mathbf{n} ds$ can be replaced by the simple product $\overline{\rho_j V_j} A_j$. This implies a uniform velocity and density profile across the face of the link (or pipe).

Thus we now have:

$$\frac{\partial M_i}{\partial t} = \sum_j \overline{\rho_j V_j} A_j \equiv \sum W_j , \tag{15}$$

where W_j is the mass flowrate. This is the precise representation in SOPHT. For the node-link type equations, we must add two more assumptions:

i) nodalization

ii) uniform velocity and density 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. No diffusion, dispersion, advection, flow profiles or flow regimes are permitted. This is not too crude an approximation for the calculation of pressure drops and flow rates but for modelling the propagation of disturbances, this approach is inadequate as it stands unless a large number of nodes and links are used.

A further simplification of equation (15) is the steady state:

$$\sum_j \overline{\rho_j V_j} A_j \equiv \sum W_j = 0 . \tag{16}$$

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:

$$V = \frac{W}{\rho A} \tag{17}$$

10.3 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 inertial forces (a momentum sink of sorts) are recognized. In the integral sense, the rate of change of momentum is equal to the forces acting on the fluid. Thus:

$$\frac{D}{Dt}\iiint_{\forall} \gamma_k \rho_k \mathbf{V}_k \, d\forall = \iint_S \boldsymbol{\sigma}_k \cdot \mathbf{n} \, ds + \iiint_{\forall} \gamma_k \rho_k \mathbf{f}_k \, d\forall + \iiint_{\forall} \mathbf{M}_k \, d\forall \ , \tag{18}$$

where

$\boldsymbol{\sigma}$ is the stress tensor (i.e., short range or surface effects including pressure, viscosity, etc.)

$\mathbf{f}$ is the long range or body force (i.e., gravity)

and

$\mathbf{M}$ is the momentum interchange function accounting for phase change effects.

Using Reynold's Transport Theorem, we get:

$$\iiint_{\forall} \frac{\partial}{\partial t}(\gamma_k \rho_k \mathbf{V}_k) \, d\forall + \iint_S (\gamma_k \rho_k \mathbf{V}_k)(\mathbf{V}_k \cdot \mathbf{n}) \, ds \tag{19}$$

$$= \iint_S \boldsymbol{\sigma}_k \cdot \mathbf{n} \, ds + \iiint_{\forall} \gamma_k \rho_k \mathbf{f}_k \, d\forall + \iiint_{\forall} \mathbf{M}_k \, d\forall \ .$$

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

$$\iiint_{\forall} \frac{\partial}{\partial t} \overline{\rho \mathbf{V}} \, d\forall + \iint_S \overline{\rho \mathbf{V} (\mathbf{V} \cdot \mathbf{n})} \, ds = \iint_S \boldsymbol{\sigma} \cdot \mathbf{n} \, ds + \iiint_{\forall} \overline{\rho \mathbf{f}} \, d\forall \ . \tag{20}$$

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

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

The stress tensor, $\boldsymbol{\sigma}$, can be split into the normal and shear components.

$$\boldsymbol{\sigma} = -PI + \tau, \tag{22}$$

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 macroscopic form, equation (20), or as a separate pressure for each phase in equation (19). At any rate, equation (21) becomes:

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

This is the form commonly seen in the literature, useful for microscopic 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:

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

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:

$$\forall\frac{\partial\overline{\rho\mathbf{V}}}{\partial t} - A_{IN}\overline{\rho_{IN}V_{IN}V_{IN}} + A_{OUT}\overline{\rho_{OUT}V_{OUT}V_{OUT}} = \int\!\!\int_S \sigma\cdot\mathbf{n}\,ds + \int\!\!\int\!\!\int_\forall \overline{\rho\mathbf{f}}\,d\forall\,. \tag{25}$$

Alternatively we could perform a cross-sectional average of each term, usually denoted by $< >$, where $<()> = 1/A \int\!\!\int_s ()\,ds$. 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:

$$\forall\frac{\partial\overline{\rho\mathbf{V}}}{\partial t} = -\int\!\!\int_S P I\cdot\mathbf{n}\,ds + \int\!\!\int\!\!\int_\forall (\nabla\cdot\tau + \overline{\rho\mathbf{f}})\,d\forall$$

$$= -A_{OUT}\mathbf{P}_{OUT} + A_{IN}\mathbf{P}_{IN} - \frac{\forall\overline{\rho}}{L}\left(\frac{fL}{D} + k\right)\frac{\mathbf{V}|\mathbf{V}|}{2g_c} - LA\overline{\rho}\sin(\theta)\,\mathbf{g}/g_c\,, \tag{26}$$

where g_c is the gravitational constant, $\mathbf{g}$ is the acceleration due to gravity and where $\nabla\cdot\tau + \overline{\rho\mathbf{f}}$ are lumped together and 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 rate as $W \equiv \overline{\rho V}A$, and L as the pipe length, Equation (26) becomes:

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

which is the form used in SOPHT.

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:

$$L\frac{\partial W}{\partial t} = A_{OUT}P_{OUT} + A_{IN}P_{IN} + A\Delta P_{pump} + \ldots\,. \tag{28}$$

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:

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

As a final note, the assumptions made for the mixture momentum equation are thus similar to those mode 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.

10.4 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 <u>all</u> the different forms of energy (kinetic, chemical, potential, nuclear, internal, electromagnetic, ...).

The mathematical statement of the conservation of energy is:

$$\frac{D}{Dt}\iiint_{\forall} \gamma_k \rho_k \left(e_k + \frac{1}{2}V_k^2\right) d\forall = -\iint_S \mathbf{q}_k \cdot \mathbf{n}\, ds + \iiint_{\forall} E_k\, d\forall \ ,$$

$$+ \iiint_{\forall} \gamma_k \rho_k \mathbf{f}_k \cdot \mathbf{V}_k \, d\forall + \iint_S (\sigma_k \cdot \mathbf{n}) \cdot \mathbf{V}_k \, ds \tag{30}$$

where

e_k = internal energy of 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:

$$\iiint_{\forall} \frac{\partial}{\partial t}[\gamma_k \rho_k (e_k + \frac{1}{2} V_k^2)]\, d\forall + \iint_S \gamma_k \rho_k (e_k + \frac{1}{2} V_k^2)\mathbf{V}_k \cdot \mathbf{n}\, ds$$

$$= - \iint_S \mathbf{q}_k \cdot \mathbf{n}\, ds + \iiint_{\forall} E_k\, d\forall + \iiint_{\forall} \gamma_k \rho_k \mathbf{f}_k \cdot \mathbf{V}_k\, d\forall + \iint_S (\boldsymbol{\sigma}_k \cdot \mathbf{n}) \cdot \mathbf{V}_k ds \qquad (31)$$

Summing over k, the mixture equation becomes:

$$\iiint_{\forall} \frac{\partial}{\partial t}[\overline{\rho e} + \frac{1}{2} \overline{\rho V^2}]\, d\forall + \iint_S \overline{[\rho e + \frac{1}{2} \rho V^2]\, \mathbf{V} \cdot \mathbf{n}}\, ds$$

$$= - \iint_S \mathbf{q} \cdot \mathbf{n}\, ds + \iiint_{\forall} E\, d\forall + \iiint_{\forall} \overline{\rho \mathbf{f} \cdot \mathbf{V}}\, d\forall + \iint_S \overline{(\boldsymbol{\sigma} \cdot \mathbf{n}) \cdot \mathbf{V}} ds\, , \qquad (32)$$

where

$$\overline{\rho e} = \gamma_1 \rho_1 e_1 + \gamma_2 \rho_2 e_2 \text{ and } E = E_1 + E_2, \text{ etc.}$$

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

$$\iiint_{\forall} \frac{\partial}{\partial t}[\overline{\rho e} + \frac{1}{2} \overline{\rho V^2}]\, d\forall + \iint_S \overline{\rho e \mathbf{V}} \cdot \mathbf{n}\, ds + \iiint_{\forall} \nabla \cdot \left[\overline{\frac{1}{2} \rho V^2 \mathbf{V}} \right] d\forall$$

$$= - \iint_S \mathbf{q} \cdot \mathbf{n}\, ds + \iiint_{\forall} E\, d\forall + \iiint_{\forall} \overline{\rho \mathbf{f} \cdot \mathbf{V}}\, d\forall + \iiint_{\forall} \nabla \cdot \overline{(\boldsymbol{\sigma} \cdot \mathbf{V})}\, d\forall\, . \qquad (33)$$

Since

$$\sigma = -P\mathbf{I} + \tau,$$

$$\iiint_{\forall} \nabla \cdot (\overline{\sigma \cdot \mathbf{V}})\, d\forall = \iiint_{\forall} [\nabla \cdot (\overline{\tau \cdot \mathbf{V}}) - \nabla \cdot \overline{(P\mathbf{V})}]\, d\forall\, .$$

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:

$$\iiint_{\forall} \frac{\partial}{\partial t} \overline{(\rho \mathbf{V}) \cdot \mathbf{V}}\, d\forall + \iiint_{\forall} \overline{\mathbf{V} \cdot (\nabla \cdot \rho \mathbf{V}\mathbf{V})} d\forall = \iiint_{\forall} \overline{\mathbf{V} \cdot (\nabla \cdot \tau)} d\forall$$

$$- \iiint_{\forall} \overline{\mathbf{V} \cdot \nabla \cdot P\mathbf{I}}\, d\forall + \iiint_{\forall} \overline{\rho \mathbf{f} \cdot \mathbf{V}}\, d\forall\, . \qquad (34)$$

Now

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

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

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

and

$$\mathbf{V} \cdot (\nabla \cdot \rho \mathbf{V}\mathbf{V}) = \nabla \cdot (1/2\, \rho V^2\, \mathbf{V}). \qquad (38)$$

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

$$\iiint_{\forall} \frac{\partial}{\partial t}\overline{(\rho e)}\, d\forall + \iint_{S} \overline{\rho e\, \mathbf{V}} \cdot \mathbf{n}\, ds = - \iint_{S} \mathbf{q} \cdot \mathbf{n}\, ds$$

$$+ \iiint_{\forall} E\, d\forall + \iiint_{\forall} \overline{\tau : \nabla \mathbf{V}}\, d\forall - \iiint_{\forall} \overline{P \nabla \cdot \mathbf{V}}\, d\forall \, . \tag{39}$$

This is the thermal form of the energy equation. This form of the energy equation 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 microscopic form:

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

where E is the internal energy generation rate term.

From thermodynamics, for solids, we have:

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

and using Fourier's law for heat conduction:

$$\mathbf{q} = - k \nabla T, \tag{42}$$

we have the classical form of the heat conduction equation:

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + E$$

$$= k \nabla^2 T + E \qquad \text{for space independent k.} \tag{43}$$

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

$$\iiint_{\forall} \frac{\partial}{\partial t} \overline{(\rho e)}\, d\forall = \frac{\partial U}{\partial t} \, , \tag{44}$$

where

$$U \equiv \forall \overline{\rho e} = L A \overline{\rho e}. \tag{45}$$

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

$$\iint_{S} \overline{\rho e\, \mathbf{V}} \cdot \mathbf{n}\, ds = \iint_{A_1} \overline{\rho e\, \mathbf{V}} \cdot \mathbf{n}\, ds + \iint_{A_2} \overline{\rho e\, \mathbf{V}} \cdot \mathbf{n}\, ds + \ldots , \tag{46}$$

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:

$$\iint_S \overline{\rho e \mathbf{V}} \cdot \mathbf{n}\, ds = - \sum_{\text{IN FLOW}} \overline{\rho e V} A_i + \sum_{\text{OUT FLOW}} \overline{\rho e V} A_i$$

$$= - \sum \overline{W_{IN} e_{IN}} + \sum \overline{W_{OUT} e_{OUT}} \,. \tag{47}$$

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

$$- \iint_S q \cdot n\, ds + \iiint_{\forall} E\, d\forall \equiv Q \,. \tag{48}$$

Therefore, the thermal energy equation becomes:

$$\frac{\partial U}{\partial t} = \sum \overline{W_{IN} e_{IN}} - \sum \overline{W_{OUT} e_{OUT}} + Q + \iiint_{\forall} \overline{\tau : \nabla \mathbf{V}}\, d\forall - \iiint_{\forall} \overline{P \nabla \cdot \mathbf{V}}\, d\forall \tag{49}$$

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

SOPHT uses:

$$\frac{\partial U'}{\partial t} = \sum \overline{W_{IN} h_{IN}} - \sum \overline{W_{OUT} h_{OUT}} + Q \,, \tag{50}$$

where

$$U' = \forall \overline{\rho h}$$

$$h = \text{enthalpy} \equiv e + P/\rho. \tag{51}$$

By rearranging the reversible energy term of Equation (49), U and U′ can be compared. Thus, using Gauss' Theorem:

$$\iiint_{\forall} \overline{P\ \nabla \cdot \mathbf{V}}\, d\forall = \iiint_{\forall} \overline{P/\rho\, (\rho \nabla \cdot \mathbf{V})}\, d\forall = \iint_S \overline{P/\rho\, (\rho \mathbf{V} \cdot \mathbf{n})}\, ds \tag{52}$$

(NOTE: assumes no spatial variation in P & ρ)

Performing the surface integrals over the inflows and outflows gives:

$$\iiint_{\forall} \overline{P\ \nabla \cdot \mathbf{V}}\, d\forall = \sum \overline{(P/\rho)(\rho V)} A \Big|_{IN} + \sum \overline{(P/\rho)(\rho V)} A \Big|_{OUT}$$

$$= - \sum \overline{P_{IN} W_{IN}/\rho_{IN}} + \sum \overline{P_{OUT} W_{OUT}/\rho_{OUT}} \,, \tag{53}$$

where

$$\overline{W/\rho} = \frac{\Upsilon_1 \rho_1 V_1 A}{\rho_1} + \frac{\Upsilon_2 \rho_2 V_2 A}{\rho_2} \,.$$

Therefore,

$$\sum \overline{W_{IN}\, e_{IN}} - \sum \overline{W_{OUT}\, e_{OUT}} - \iiint_{\forall} \overline{P\, \nabla \cdot \mathbf{V}}\, d\forall$$

$$= \sum \overline{W_{IN}\,(e_{IN} + P_{IN}/\rho_{IN})} + \sum \overline{W_{OUT}\,(e_{OUT} + P_{OUT}/\rho_{OUT})}$$

$$= \sum \overline{W_{IN}\, h_{IN}} - \sum \overline{W_{OUT}\, h_{OUT}}\,. \tag{54}$$

where

$$\overline{Wh} = \gamma_1\, \rho_1\, V_1\, Ah_1 + \gamma_2\, \rho_2\, V_2\, Ah_2.$$

Equation (31) can be written as:

$$\frac{\partial U}{\partial t} = \sum \overline{W_{IN}\, h_{IN}} - \overline{W_{OUT}\, h_{OUT}} + Q + \iiint_{\forall} \overline{\tau : \nabla \mathbf{V}}\, d\forall \tag{55}$$

$$= \frac{\partial U'}{\partial t} - \forall\, \frac{\partial P}{\partial t}\,.$$

Therefore, comparing Equations (50) and (55), SOPHT has neglected the irreversible conversion to internal energy or turbulent heating. A lumped approximation is made to this in SOPHT by adding the pump heat to the node downstream of the pump.

The term, $\partial P/\partial t$, in equation (55) is neglected in SOPHT.

At a pressure 10 MPa, which is typical for the CANDU Primary Heat Transport, this converts to 10 kJ/kg while e is approximately 1000 kJ/kg. Thus the discrepancy of the P/ρ term is negligible.

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

$$Q = \Sigma\, W_{OUT}\, h_{OUT} - \Sigma\, W_{IN}\, h_{IN}. \tag{56}$$

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

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

as we have seen in Chapter 1.

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

$$-\iint_{S} \mathbf{q} \cdot \mathbf{n}\, ds + \iiint_{\forall} E\, d\forall \equiv Q\,. \tag{48}$$

Using Newton's Law of cooling for convection:

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

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) becomes:

$$\forall \frac{\overline{\partial \rho h}}{\partial t} - \forall \frac{\partial P}{\partial t} \left(\equiv \forall \frac{\partial \rho e}{\partial t} \simeq \forall \rho C_v \frac{\partial T}{\partial t} \right)$$

$$= \sum \overline{W_{IN} h_{IN}} - \sum \overline{W_{OUT} h_{OUT}} - A h_N (T - T_S) + \forall E$$

$$+ \iiint_{\forall} \overline{\boldsymbol{\tau} : \nabla \mathbf{V}} \, d\forall \qquad (59)$$

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 $\iiint_{\forall} \boldsymbol{\tau} : \nabla \mathbf{V} \, d\forall$ generally can be neglected.

10.5 THE EQUATION OF STATE (see Vlachopoulos, 1980 for instance)

The equation of state determines the relationship between density and the thermodynamic pressure and temperature, i.e. $\rho = \rho(P,T)$.

This relationship is extremely complicated for liquids, solids and during phase changes.

The equation of state for a perfect gas is

$$P = \rho R T \qquad (60)$$

where

p = pressure

R = $\mathcal{R}$/Molecular weight

T = absolute temperature

$\mathcal{R}$ = 8,314 J/kg-mol·K (universal gas constant)

ρ = density

Obviously R depends on the particular gas.

It can be shown that for an adiabatic frictionless process (isentropic) in a perfect gas we have the relationship

$$P \rho^{-k} = \text{constant} \qquad (61)$$

where $k = C_p/C_v$.

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 rate, W, or momentum, ρV

3) energy, e, or enthalpy, $h = e + P/\rho$, or temperature, $T = fn(e)$ or $fn(h)$

4) pressure, P.

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

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

or

$$\rho = fn\,(P,T), \text{ etc.} \qquad (62)$$

Thermodynamic equilibrium is usually assumed, as in the following. For water, H_20 or D_20, 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, $\forall$, having a mass of H_20, 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:

$$\rho = M/\forall. \qquad (63)$$

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_20. Since the average density is related to the specific densities by the relation:

$$\rho = \rho_\ell (1 - \epsilon) + \rho_v \epsilon, \qquad (64)$$

that is, the average density is a volume weighted sum of the specific densities. The void fraction, ϵ, is readily calculated. Given a relationship between void fraction, ϵ, and weight fraction (quality), x, we have the quality, x.

The mixture enthalpy, h, is given by

$$h = h_\ell (1 - x) + h_v x \qquad (65)$$

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 $\partial P/\partial h|_\rho$, 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:

$$P = P_{SAT_f}(\rho) + \left.\frac{\partial P}{\partial h}\right|_{\rho} [h - h_{SAT_f}(\rho)] \ . \tag{66}$$

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

$$P = P_{SAT_g}(\rho) + \left.\frac{\partial P}{\partial h}\right|_{\rho} [h - h_{SAT_g}(\rho)] \ . \tag{67}$$

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

$$h = e + P/\rho \tag{68}$$

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.

10.6 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 condensors, etc.
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.

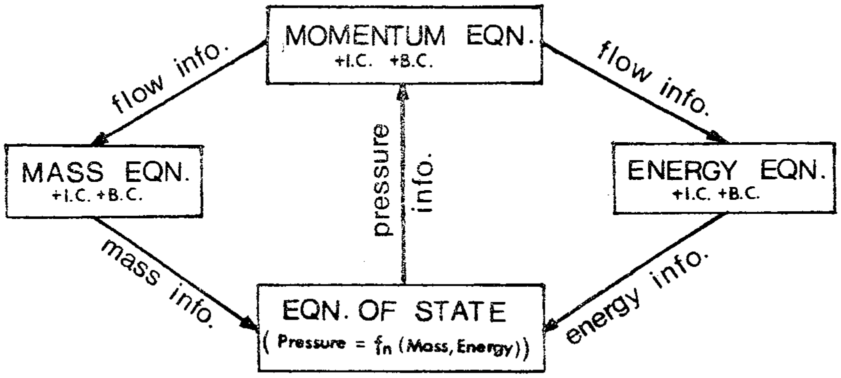
The above list of correlations, large enough in its own right, is but a subset of the full list that would be required were it not for a number of key simplifying assumptions made in the derivation of the basic equations. The three major assumptions made for the primary heat transport system are:

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

These are required because of state of the art limitations. The references listed are recommended for further reading.

10.7 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. Illustrated below are 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.

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.

Subsequent chapters will show how the basic equations developed herein, are brought to life.

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