Chapter 2 Basic Equations for Thermalhydraulic Systems Analysis

2.1 Introduction

2.1.1 Chapter Content

This chapter presents the basic mass, momentum and energy equations used in typical computer codes for thermalhydraulic 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.

The known territory of the basic mass, energy and momentum conservation equations (Bird et al [BIR60]) 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 (Currie [CUR74]): integral or distributed approach, as illustrated in figure 2.1. The differential form sees infrequent use in the analysis of thermalhydraulic 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 thermalhydraulic systems analysis from first principles. This will provide a traceable and verifiable methodology to aid development and validation of system codes, to elucidate the necessary assumptions made, to show pitfalls, to show the common roots and genealogy of specific tools like FLASH [POR69], SOPHT [CHA75a, CHA75b, CHA77a, CHA77b, SKE75, SKE80], RETRAN [AGE82], FIREBIRD [LIN79], CATHENA [HAN95], etc., and to help guide future development.

2.1.2 Learning Outcomes

The overall objectives for this chapter are as follows:

Objective 2.1	The student should be able to identify the terms and symbols used in thermalhydraulics.					
Condition	Closed book written examination.					
Standard	100% on key terms and symbols.					
Related concept(s)	Fundamental hydraulic and heat transfer phenomena.					
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a	a				

Objective 2.2	The student should be able to distinguish between the differential and integral form and be able to choose, with justification, the correct form to use in various situations.					
Condition	Closed book written or oral examination.					
Standard	100%.					
Related concept(s)	Mathematical forms of the conservation equation.					
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a	a	a			

Objective 2.3	The student should be able to recall typical values and units of parameters.					
Condition	Closed book written or oral examination.					
Standard	100% on key terms and symbols.					
Related concept(s)						
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a					

Objective 2.4	The student should be able to recognize key physical phenomena.					
Condition	Open book written or oral examination.					
Standard	100% on key items, supporting material used only as memory triggers.					
Related concept(s)						
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a					

Objective 2.5	The student should be able to recognize the coupling between mass, momentum, energy and pressure in thermalhydraulic systems.					
Condition	Closed book written or oral examination.					
Standard	100%.					
Related concept(s)						
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a					

Objective 2.6	The student should be able to choose approximations as appropriate (# of dimesions, transient or steady state, averaging, spatial resolution, etc.) with justification.					
Condition	Open book written or oral examination.					
Standard	75%.					
Related concept(s)						
Classification	Knowledge	Comprehension	Application	Analysis	Synthesis	Evaluation
Weight	a	a	a	a		a

2.1.3 The Chapter Layout

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 correlations. 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.

2.2 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 <u>experimental</u> observation.

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

$$\frac{D}{Dt}\iiint_V \psi\, dV = \iiint_V \Gamma\, dV + \iint_S \mathbf{S}\cdot\mathbf{n}\, ds \tag{1}$$

where

D/Dt = substantial derivative[1] = 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 discussed in detail in appendix 2):

$$\frac{D}{Dt}\iiint_V \psi\, dV = \iiint_V \frac{\partial\psi}{\partial t}\, dV + \iint_S \psi\mathbf{v}\cdot\mathbf{n}\, ds \tag{2}$$

where

$\partial/\partial t$ = local time derivative, and
v = velocity of the field variable.

to give

$$\iiint_V \frac{\partial\psi}{\partial t}\, dV = -\iint_S \psi\,\mathbf{v}\cdot\mathbf{n}\, ds + \iiint_V \Gamma\, dV + \iint_S \mathbf{S}\cdot\mathbf{n}\, ds\,. \tag{3}$$

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):

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[1] For a lucid discussion of the three time derivatives, $\frac{\partial}{\partial t}$, $\frac{D}{\partial t}$, $\frac{d}{dt}$, see [BIR60, pp 73-74], reproduced as appendix 1.

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

where

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

Thus equation 3 can be rewritten:

$$\iiint_V \frac{\partial \psi}{\partial t} dV = - \iiint_S \nabla \cdot \psi \, \mathbf{v} \, dV + \iiint_V \Gamma \, dV + \iiint_V \nabla \cdot \mathbf{S} \, dV . \qquad (5)$$

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:

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

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 <u>all</u> 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), $\nabla \cdot \psi \mathbf{v}$.

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,

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

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 [DEL81]). 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.

2.3 Conservation of Mass

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

$$\iiint_V \frac{\partial}{\partial t}(\gamma_k\, \rho_k)\, dV = -\iint_S \gamma_k\, \rho_k\, \mathbf{v}_k \cdot \mathbf{n}\, ds + \iiint_V \Gamma_k\, dV + \iint_s S_k\, \mathbf{n} \cdot ds \qquad (7)$$

where

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

γ_k = volume fraction of phase, k, in volume V, and

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

The average density is defined as:

$$\rho = \gamma_1\, \rho_1 + \gamma_2\, \rho_2 = (1 - \alpha)\, \rho_1 + \alpha\, \rho_2, \qquad (8)$$

where

ρ = average density, and
α = void fraction.

Adding both phases together, equation 7 becomes:

$$\iiint_V \frac{\partial}{\partial t}\left[(1-\alpha)\rho_1 + \alpha\rho_2\right] dV = -\iint_S \left[(1-\alpha)\rho_1 \mathbf{v}_1 + \alpha\rho_2 \mathbf{v}_2\right]\cdot \mathbf{n}\, ds$$
$$+ \iiint_V (\Gamma_1 + \Gamma_2)\, dV + \iint_S (S_1 + S_2)\cdot \mathbf{n}\, ds. \tag{9}$$

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

$$\iiint_V \frac{\partial \rho}{\partial t}\, dV = -\iint_S \rho\, \mathbf{v}\cdot \mathbf{n}\, ds \tag{10}$$

where

$$\rho\, \mathbf{v} = (1-\alpha)\rho_1 \mathbf{v}_1 + \alpha\rho_2 \mathbf{v}_2 . \tag{11}$$

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

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

or

$$\frac{\partial \rho}{\partial t}\left[(1-\alpha)\rho_1 + \alpha\rho_2\right] + \nabla\cdot\left[(1-\alpha)\rho_1 \mathbf{v}_1 + \alpha\rho_2 \mathbf{v}_2\right] = 0 . \tag{13}$$

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 [CAR81a] and COBRA [BNW76] use this approach.

In contrast, system codes such as SOPHT [CHA77a], based on Porsching's work [POR71], use the lumped equations. These codes represent a hydraulic network of pipes by nodes joined by links, discussed in detail in chapter 3. 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 <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. 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, $\iiint \rho dV$ is the mass, M_i, in the volume, V_i, of the ith 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,

$$-\iint_S \rho\, \mathbf{v}\cdot\mathbf{n}\, ds = \sum_j \rho_j v_j A_j . \tag{14}$$

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, $\iint_S \rho\, \mathbf{v}\cdot\mathbf{n}\, ds$ can be replaced by the simple product $\rho_j\, \mathbf{v}_j\, A_j$. This implies known or assumed (usually uniform) velocity and density profiles across the face of the link (or pipe).

Thus we now have:

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

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 may not be immediately obvious. This is discussed in more detail in chapter 3.

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

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

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:

$$v = \frac{W}{\rho A} . \tag{17}$$

2.4 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:

$$\frac{D}{Dt}\iiint_V \gamma_k\, \rho_k\, v_k\, dV = \iint_S \sigma_k \cdot \mathbf{n}\, ds + \iiint_V \gamma_k\, \rho_k\, \mathbf{f}_k\, dV + \iiint_V \mathbf{M}_k\, dV , \tag{18}$$

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:

$$\iiint_V \frac{\partial}{\partial t}(\gamma_k\, \rho_k\, \mathbf{v}_k)\, dV + \iint_S (\gamma_k\, \rho_k\, \mathbf{v}_k)(\mathbf{v}_k \cdot \mathbf{n})\, ds$$
$$= \iint_S \sigma_k \cdot \mathbf{n}\, ds + \iiint_V \gamma_k\, \rho_k\, \mathbf{f}_k\, dV + \iiint_V \mathbf{M}_k\, dV. \qquad (19)$$

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

$$\iiint_V \frac{\partial}{\partial t}\rho\, \mathbf{v}\, dV + \iint_S \rho\, \mathbf{v}\, (\mathbf{v}\cdot\mathbf{n})\, ds = \iint_S \sigma \cdot \mathbf{n}\, ds + \iiint_V \rho\, \mathbf{f}\, dV. \qquad (20)$$

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

$$\frac{\partial}{\partial t}(\rho\, \mathbf{v}) + \nabla\cdot\rho\, \mathbf{v}\, \mathbf{v} = \nabla\cdot\sigma + \rho\, \mathbf{f}. \qquad (21)$$

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

$$\sigma = -P\mathbf{I} + \tau, \qquad (22)$$

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:

$$\frac{\partial}{\partial t}(\rho\, \mathbf{v}) + \nabla\cdot\rho\, \mathbf{v}\, \mathbf{v} = -\nabla P + \nabla\cdot\tau + \rho\, \mathbf{f}. \qquad (23)$$

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:

$$\iint_S \rho\, \mathbf{v}\, (\mathbf{v}\cdot\mathbf{n})\, ds = \iint_{A_{IN}} \rho\, \mathbf{v}\, (\mathbf{v}\cdot\mathbf{n})\, ds + \iint_{A_{OUT}} \rho\, \mathbf{v}\, (\mathbf{v}\cdot\mathbf{n})\, ds, \qquad (24)$$

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:

$$V\frac{\partial \rho\, v}{\partial t} - A_{IN}\, \rho_{IN}\, v_{IN}\, v_{IN} + A_{OUT}\, \rho_{OUT}\, v_{OUT}\, v_{OUT} = \iint_S \sigma_k\cdot\mathbf{n}\, ds + \iiint_V \rho\, \mathbf{f}\, dV. \qquad (25)$$

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

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

where g_c is the gravitational constant, g is the acceleration due to gravity and where $\nabla \cdot \tau$ and ρf evaluated by empirical correlations (the standard friction factor) plus an elevation change term (θ is the angle w.r.t. the horizontal). Note that is $A_{OUT} \neq A_{IN}$ then, even for constant pressure, there is a net force on the volume causing it to accelerate if it were not restrained. In a restrained system such as HTS piping, the piping supports exert an equal and opposite force on the volume. Thus when the area differences are explicitly modelled, the appropriate body forces must be included. Generally, it is simpler to use an average or representative area for the IN and OUT surfaces and to add entrance and exit frictional losses explicitly in the (fl/D+k) term.

Assuming one dimensional flow and defining the mass flow as $W \equiv \rho V A$, 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 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:

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

The momentum flux terms ($A\rho v^2$) in equation 25 could also be added if large area or property changes were present or the effect could be included in the friction term.

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

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

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.

2.5 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:

$$\frac{D}{Dt}\iiint_V \gamma_k \rho_k \left(e_k + \frac{1}{2} v_k^2\right) dV = -\iint_S \mathbf{q}_k \cdot \mathbf{n}\, ds + \iiint_V E_k\, dV + \iiint_V \gamma_k \rho_k \mathbf{f}_k \cdot \mathbf{v}_k\, dV + \iint_S (\sigma_k \cdot \mathbf{n}) \cdot \mathbf{v}_k\, ds . \qquad (30)$$

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:

$$\iiint_V \frac{\partial}{\partial t}\left[\gamma_k \rho_k \left(e_k + \frac{1}{2} v_k^2\right)\right] dV + \iint_S \gamma_k \rho_k \left(e_k + \frac{1}{2} v_k^2\right) \mathbf{v}_k \cdot \mathbf{n}\, ds = -\iint_S \mathbf{q}_k \cdot \mathbf{n}\, ds + \iiint_V E_k\, dV + \iiint_V \gamma_k \rho_k \mathbf{f}_k \cdot \mathbf{v}_k\, dV + \iint_S (\sigma_k \cdot \mathbf{n}) \cdot \mathbf{v}_k\, ds . \qquad (31)$$

Summing over k, the mixture equation becomes:

$$\iiint_V \frac{\partial}{\partial t}\left[\rho e + \frac{1}{2} \rho v^2\right] dV + \iint_S \left[\rho e + \frac{1}{2} \rho v^2\right] \mathbf{v} \cdot \mathbf{n}\, ds = -\iint_S \mathbf{q} \cdot \mathbf{n}\, ds + \iiint_V E\, dV + \iiint_V \rho\, \mathbf{f} \cdot \mathbf{v}\, dV + \iint_S (\sigma \cdot \mathbf{v}) \cdot \mathbf{v}\, ds . \qquad (32)$$

where

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

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

$$\iiint_V \frac{\partial}{\partial t}\left[\rho e + \frac{1}{2}\rho v^2\right] dV + \iint_S \rho e\, \mathbf{v}\cdot\mathbf{n}\, ds + \iiint_V \nabla\cdot\left[\frac{1}{2}\rho v^2\, \mathbf{v}\right] dV$$

$$= -\iint_S \mathbf{q}\cdot\mathbf{n}\, ds + \iiint_V E\, dV + \iiint_V \rho\, \mathbf{f}\cdot\mathbf{v}\, dV + \iiint_V \nabla\cdot(\sigma\cdot\mathbf{v})\, dV. \tag{33}$$

Since

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

$$\iiint_V \nabla\cdot(\sigma\cdot\mathbf{v})\, dV = \iiint_V \left[\nabla\cdot(\tau\cdot\mathbf{v}) - \nabla\cdot(P\,\mathbf{v})\right] dV.$$

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:

$$\iiint_V \frac{\partial}{\partial t}(\rho\,\mathbf{v})\cdot\mathbf{v}\, dV + \iiint_V \mathbf{v}\cdot(\nabla\cdot\rho\,\mathbf{v}\,\mathbf{v})\, dV = \iiint_V \mathbf{v}\cdot(\nabla\cdot\tau)\, dV$$

$$- \iiint_V \mathbf{v}\cdot\nabla P\, dV + \iiint_V \rho\, \mathbf{f}\cdot\mathbf{v}\, dV. \tag{34}$$

Now

$$\mathbf{v}\cdot(\nabla\cdot\tau) = \nabla(\tau\cdot\mathbf{v}) - \tau : \nabla\mathbf{v}, \tag{35}$$

$$\mathbf{v}\cdot\nabla P = \nabla\cdot(P\,\mathbf{v}) - P\,\nabla\cdot\mathbf{v}, \tag{36}$$

$$\mathbf{v}\cdot\frac{\partial}{\partial t}(\rho\,\mathbf{v}) = \frac{\partial}{\partial t}\left(\frac{1}{2}\rho\,\mathbf{v}\cdot\mathbf{v}\right) = \frac{\partial}{\partial t}\left(\frac{1}{2}\rho\, v^2\right) \tag{37}$$

and

$$\mathbf{v}\cdot(\nabla\cdot\rho\,\mathbf{v}\,\mathbf{v}) = \nabla\cdot\left(\frac{1}{2}\rho\, v^2\,\mathbf{v}\right). \tag{38}$$

Using these identities and subtracting equation 34 from equation 33, we get:

$$\iiint_V \frac{\partial}{\partial t}(\rho\, e)\, dV + \iint_S \rho\, e\, \mathbf{v}\cdot\mathbf{n}\, ds = -\iint_S \mathbf{q}\cdot\mathbf{n}\, ds$$

$$+ \iiint_V E\, dV + \iiint_V \tau : \nabla\mathbf{v}\, dV - \iiint_V P\,\nabla\cdot\mathbf{v}\, dV. \tag{39}$$

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:

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

where E is the internal energy generation rate term.

From thermodynamics, for solids, we have:

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

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:

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

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

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

where

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

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

$$\iint_S \rho e \mathbf{v} \cdot \mathbf{n}\, ds = \iint_{A_1} \rho e \mathbf{v} \cdot \mathbf{n}\, ds + \iint_{A_2} \rho e \mathbf{v} \cdot \mathbf{n}\, ds + \ldots.. \tag{46}$$

where A_1, A_2, etc., are the pipe flow cross-sectional areas. For inflow, v·**n** is negative. For outflow, v·**n** is positive. Assuming uniform velocity, enthalpy and density across the link (pipe) cross-section gives:

$$\begin{aligned} \iint_S \rho e \mathbf{v} \cdot \mathbf{n}\, ds &= -\sum_{\text{IN FLOW}} \rho e v A_i - \sum_{\text{OUT FLOW}} \rho e v A_i \\ &= -\sum W_{IN} e_{IN} + \sum W_{OUT} e_{OUT}. \end{aligned} \tag{47}$$

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

$$-\iint_S \mathbf{q} \cdot \mathbf{n}\, ds - \iiint_V E\, dV \equiv Q. \tag{48}$$

Therefore, the thermal energy equation becomes:

$$\frac{\partial U}{\partial t} = \sum W_{IN}\, e_{IN} - \sum W_{OUT}\, e_{OUT} + Q + \iiint_V \tau : \nabla \mathbf{v}\, dV - \iiint_V P \nabla \cdot \mathbf{v}\, dV . \tag{49}$$

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

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

$$h = \text{enthalpy} \equiv e + P/\rho \quad \textit{and} \quad H = V \rho h . \tag{50}$$

we can rewrite equation 39 as follows:

$$\begin{aligned} \iiint_V \frac{\partial (\rho h - P)}{\partial t}\, dV + \iint_s (\rho h - P) \mathbf{v} \cdot \mathbf{n}\, ds &= - \iint_S \mathbf{q} \cdot \mathbf{n}\, ds \\ &- \iiint_V E\, dV + \iiint_V \tau : \nabla \mathbf{v}\, dV - \int_V P \nabla \cdot \mathbf{v}\, dV . \end{aligned} \tag{51}$$

Collecting the pressure terms and simplifying yields:

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

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

$$\begin{aligned} \iint_S P \mathbf{v} \cdot \mathbf{n}\, ds - \iiint_V P \nabla \cdot \mathbf{v}\, dV &= \iiint_V \nabla \cdot (P \mathbf{v})\, dV - \iiint_V P \nabla \cdot \mathbf{v}\, dV \\ &= \iiint_V \mathbf{v} \cdot \nabla P\, dV . \end{aligned} \tag{53}$$

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

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

Finally, using equations 48, 50, 53-54, equation 52 becomes:

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

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:

$$Q = \sum W_{OUT} h_{OUT} - \sum W_{IN} h_{IN} . \qquad (56)$$

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

$$Q = W(h_{OUT} - h_{IN}) \equiv W C_p (T_{OUT} - T_{IN}) \text{ in single phase.} \qquad (57)$$

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

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

Using Newton's Law of cooling for convection:

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

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:

$$V \frac{\partial \rho h}{\partial t} - V \frac{\partial P}{\partial t} \left(\equiv V \frac{\partial \rho e}{\partial t} \simeq V \rho C_v \frac{\partial T}{\partial t} \right) = \sum W_{IN} h_{IN} - \sum W_{OUT} h_{OUT}$$
$$- A h_N (T - T_S) + V E + \iiint_V \tau : \nabla \mathbf{v} \, dV . \qquad (59)$$

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 $\iiint_V \tau : \nabla \mathbf{v} \, dV$ generally can be neglected or added as a pump heat term.

2.6 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, $V\rho$,
2) velocity, v, or mass flow, W, or momentum, ρv,
3) energy, e, or enthalpy, $h = e + P/\rho$, or temperature, $T = fn(e)$ or $fn(h)$, and
4) pressure, P.

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

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

Thermodynamic equilibrium is usually assumed. 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.

The equation of state is discussed in detail in chapter 4.

2.7 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 enthalpy 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 insurge); and
3) one fluid model (i.e. mixture equations).

These are required because of state of the art limitations (however, two fluid models ae being used increasingly in recent years.). Empirical correlations are discussed in more detail in chapter 7.

2.8 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 2.2 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. The new mass and energy are given to the equation of state to update the pressure distribution. The new pressure, 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 2.3. 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 2.4 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 2.2). 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 CATHENA [HAN95] are a direct result of this realization. The near term evolution will likely be affected mostly by microcomputer developments.

2.9 Exercises

1. For a pool-type research reactor as shown in figure 2.5, which form of the mass, momentum and energy conservation equations are the appropriate ones to use for the following cases:
   a. Pipe connecting the pool to the Hold Up Tank (HUT)
   b. Mixing within the HUT
   c. Pipe connecting the HUT to the Heat Exchanger (HX)
   d. The HX
   e. Flow through the fuel assemblies.
   f. The Pool

   For each case, write out the appropriate equations.

2. For the same pool-type reactor:
   a. Derive the simple steady state overall reactor core heat balance equation relating the reactor power, core flow and core ΔT. Defend your assumptions.
   b. Would the reactor coolant outlet ΔT change very much when the reactor power changes? Explain.
   c. Derive the simple steady state equation to determine the Heat Transport System flow. Defend your assumptions.
   d. Would the reactor coolant flow change very much when the reactor power or temperature changes? Explain.
   e. Based on the above, in modelling which needs to be determined first, the heat transfer situation or the hydraulic situation?

3. Referring to figure 2.2:
   a. Explain the inter-relationship between the mass, momentum and energy equations and the equation of state.
   b. For the integral form, devise a simple solution scheme for the transient equations. Show what equations are being solved and how they are being solved. Flow chart your scheme.

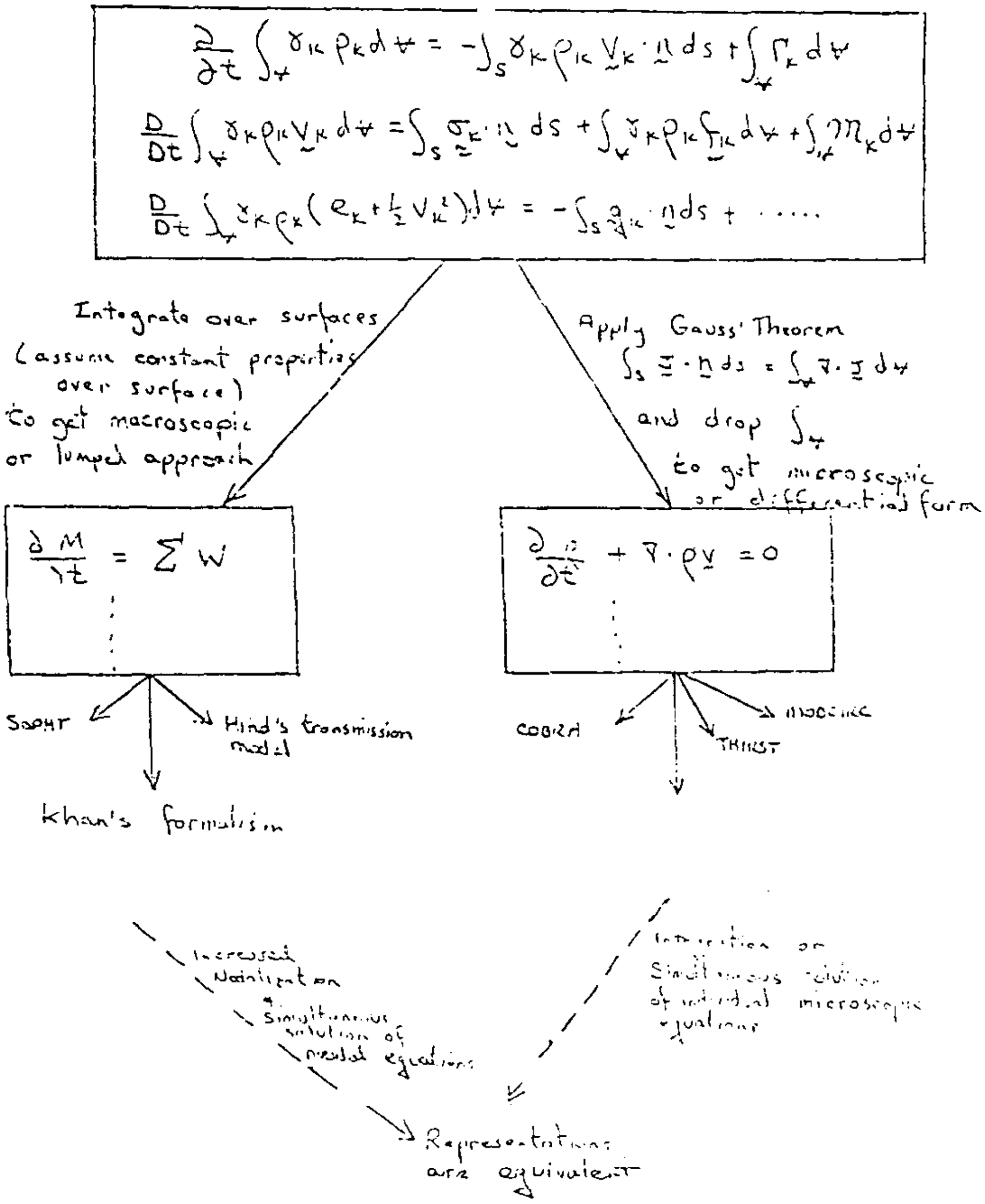

Figure 2.1 Derivation path.

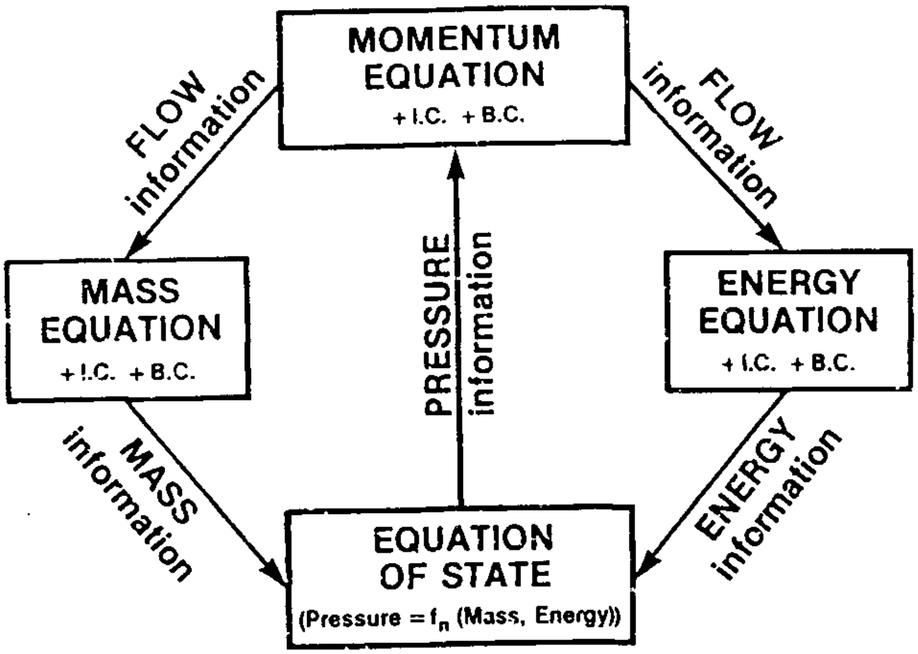

Figure 2.2 The four cornerstone single phase flow equations and the flow of information between them.

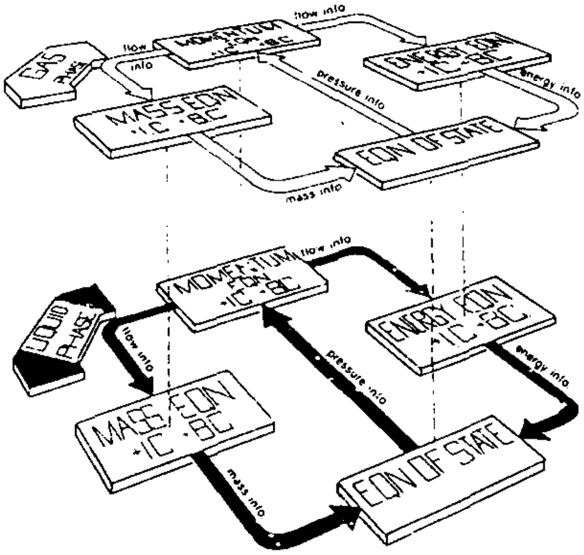

Figure 2.3 The four cornerstone equations for the full two-fluid model.

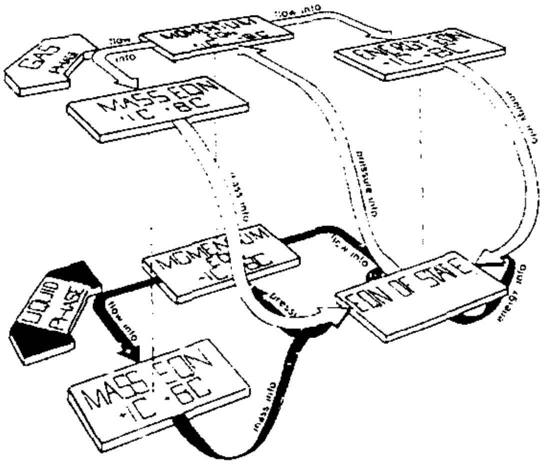

Figure 2.4 The four cornerstone equations for the two-fluid model with equal pressure of the two phases.

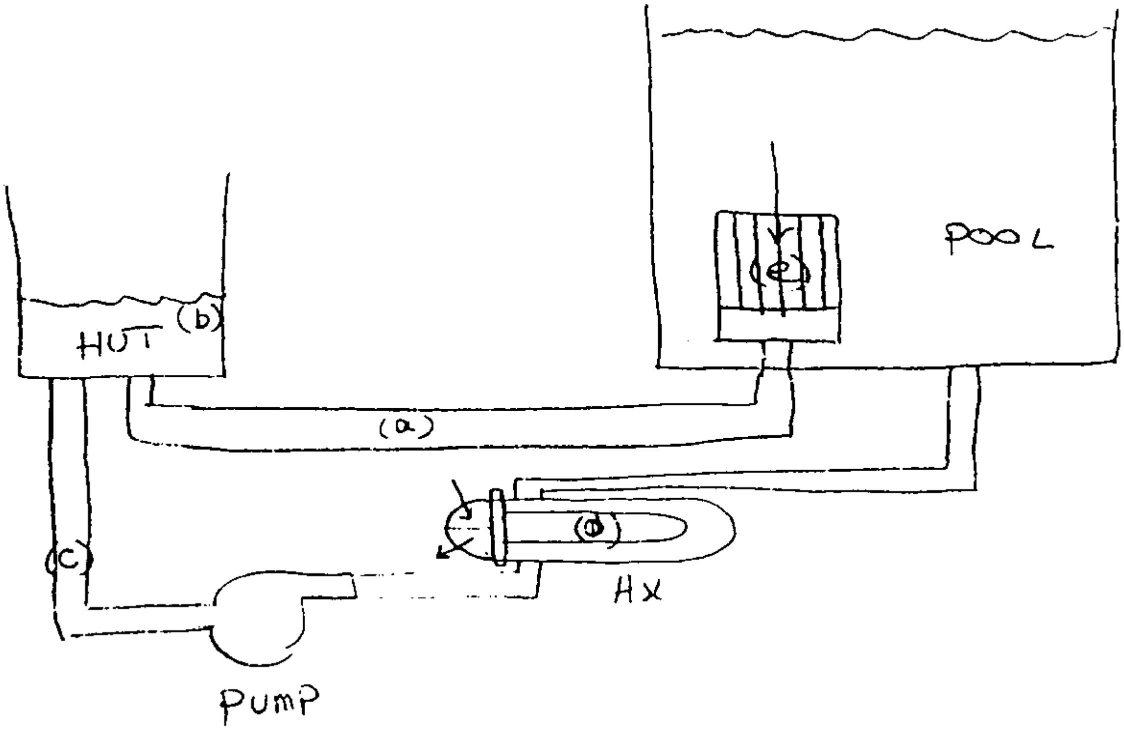

Figure 2.5 Simple pool-type research reactor.