

FIGURE 1: Transmission of a step change using the plug flow model and the mixing tank model (1 to 50 tanks).

FIGURE 2: The four cornerstone single-phase flow equations and the flow of information between them.

FIGURE 3: The eight cornerstone two-phase flow equations and the flow of information between them.

FIGURE 4: A special case of the general two-phase flow equations.

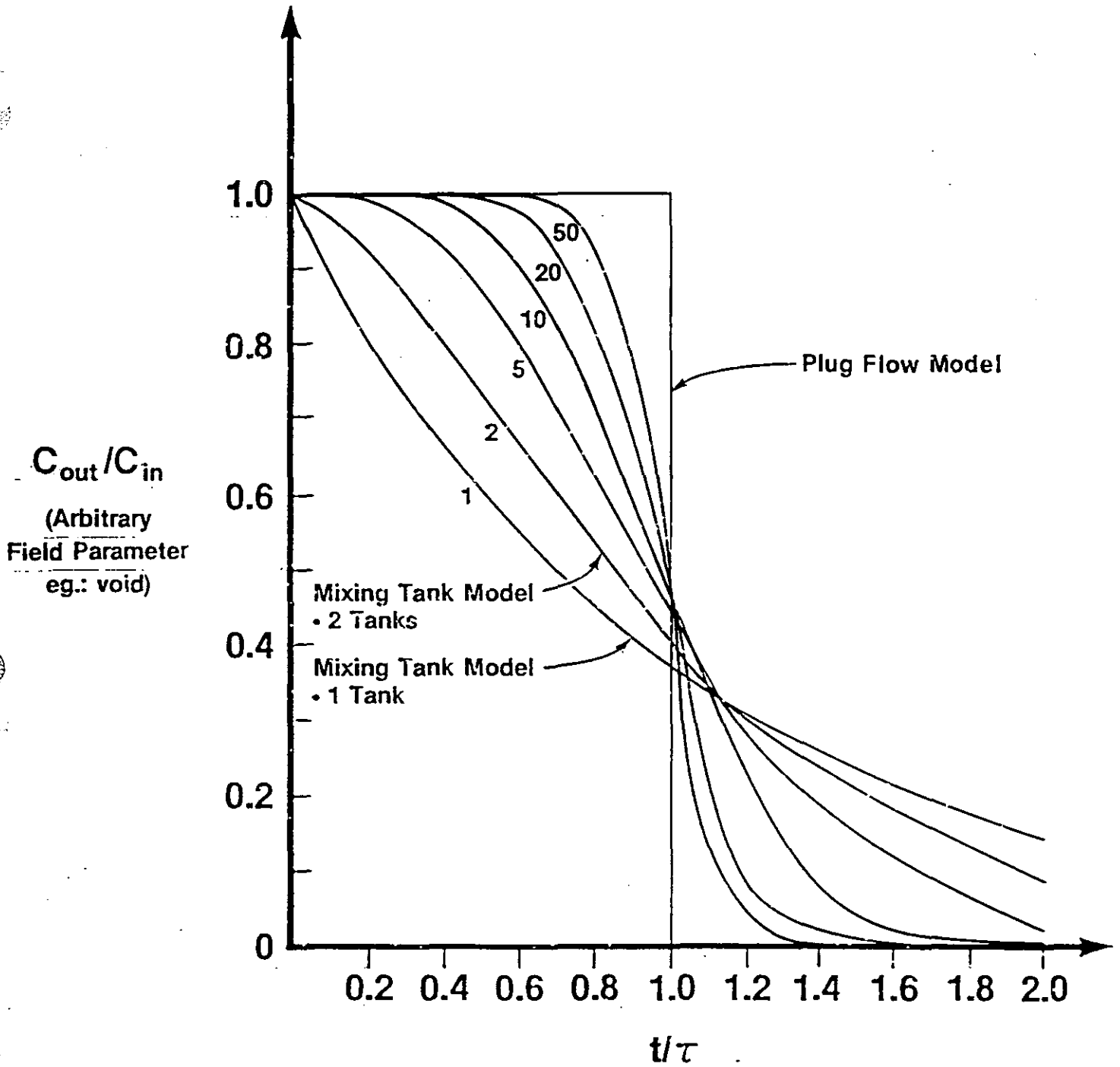


FIGURE 1 Transmission of a step change using the Plug Flow Model and the Mixing Tank Model (1 to 50 Tanks)

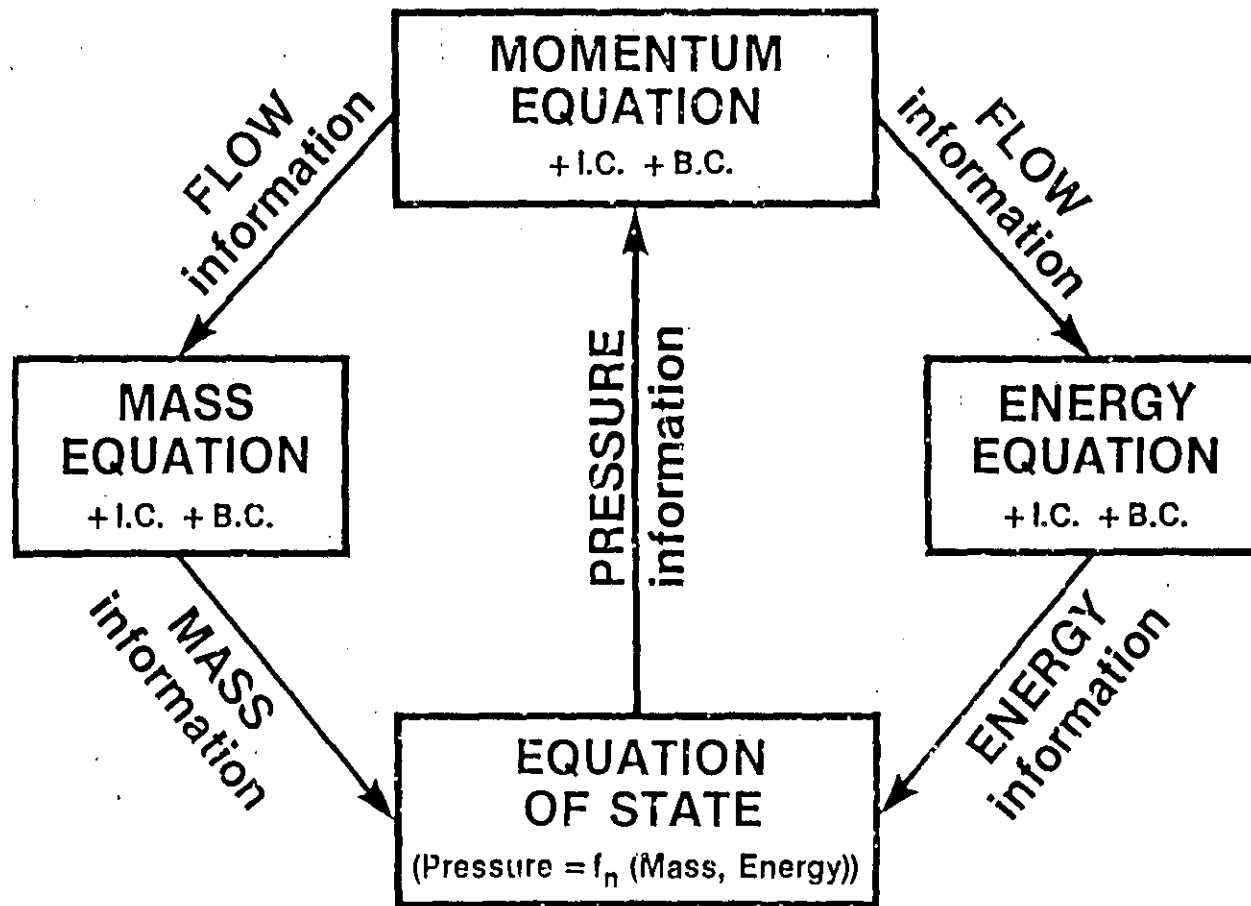
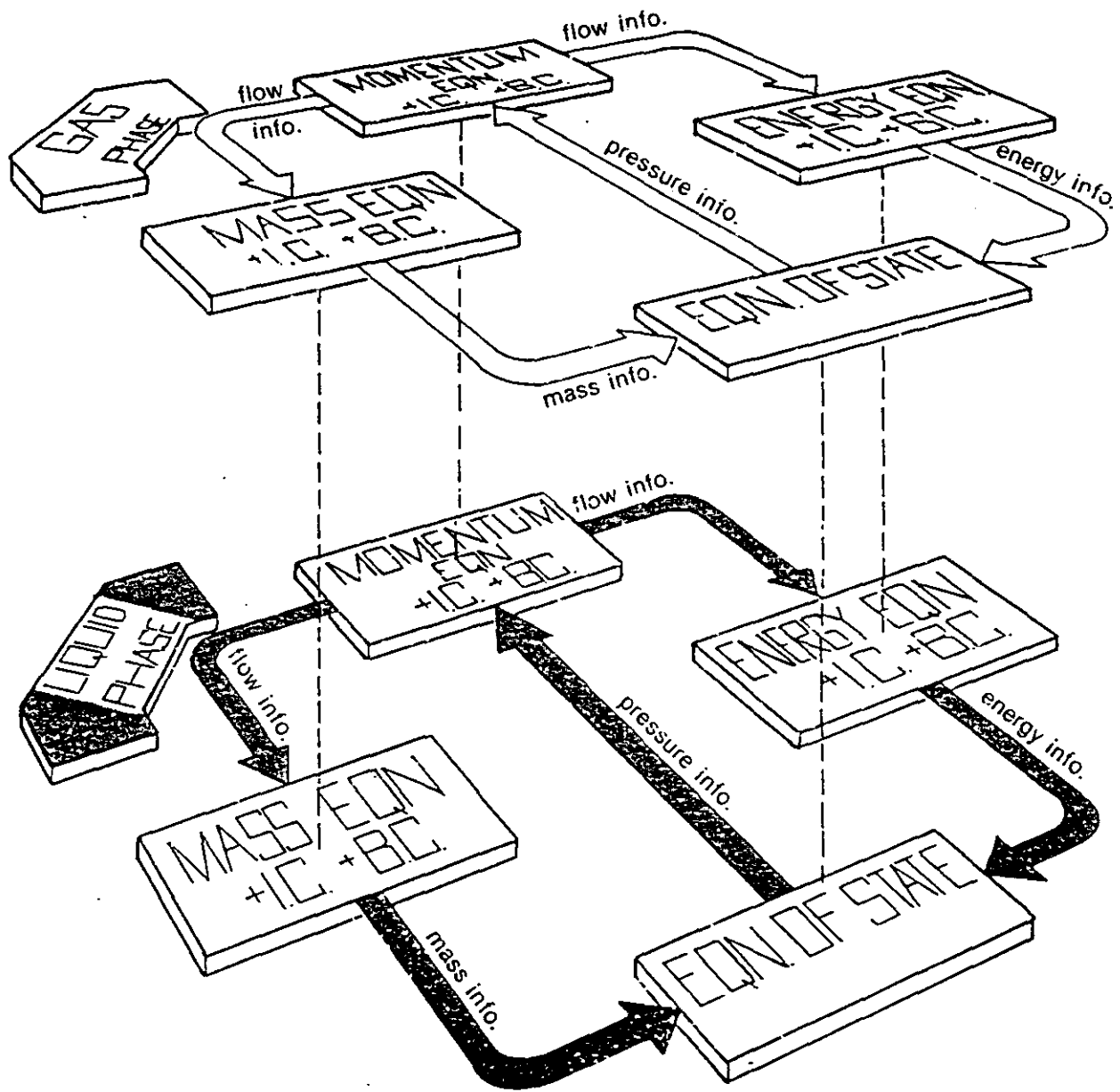
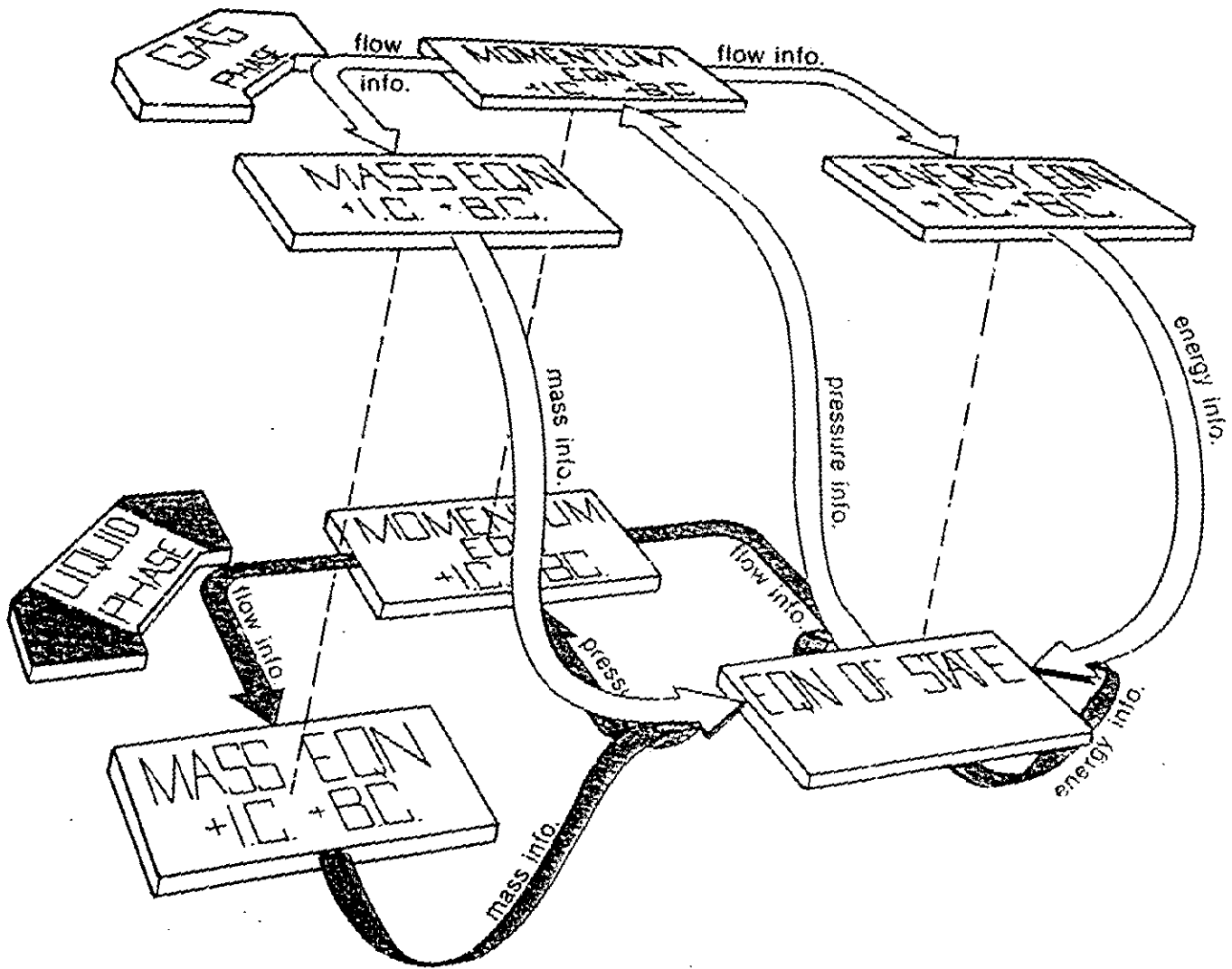


FIGURE 2 The four cornerstone single-phase flow equations and the flow of information between them.





$$\frac{x}{1-x} \frac{(1-\alpha) p_r}{\alpha} \frac{p_v}{p_w} = (1-x) \alpha p_w$$

$$x p_r - x \alpha p_r = \alpha p_w - x \alpha p_w$$

$$\textcircled{1} \quad i \equiv \frac{p_v x}{p_v \alpha + p_r (1-\alpha)}$$

$$\textcircled{2} \quad x p_v \alpha + x p_r (1-\alpha) = p_v x \quad \text{--- now gather } p_r \text{ \& } p_w \text{ terms}$$

$$\textcircled{3} \quad x p_r - x \alpha p_r = \alpha p_w - x \alpha p_w$$

$$\textcircled{4} \quad x p_r (1-\alpha) = \alpha p_w (1-x)$$

$$\textcircled{5} \quad \frac{x}{(1-x)} \frac{(1-\alpha) p_r}{\alpha} \frac{p_v}{p_w} = 1$$

To solve in terms of α :

$$\textcircled{4} \quad \rightarrow x p_r - \alpha x p_r = \alpha p_w (1-x)$$

$$x p_r = \alpha [x p_r + p_w - p_w x]$$

$$\alpha = \frac{x}{x + \frac{p_w}{p_r} - \frac{p_w}{p_r} x}$$

$$= \frac{x}{x \left[1 - \frac{p_w}{p_r} \right] + \frac{p_w}{p_r}} = \frac{x p_w}{x p_w + p_w - p_w x}$$

$$= \frac{x p_w}{(1-x) p_w + x p_w}$$

THE RATE METHOD — GENERALIZED

In the following, the case of two-phase equilibrium is considered first in order to illustrate the method. Subsequently, the equations are extended to cover single phase and two-phase non-equilibrium fluid.

Two-Phase Equilibrium

For a two-phase homogeneous mixture we have:

$$v = v_f + x v_{fg} \quad (26)$$

$$h = h_f + x h_{fg} \quad (27)$$

where $v_{fg} \equiv v_g - v_f$ and $h_{fg} \equiv h_g - h_f$.

We wish to relate rates of change of pressure to rates of change in v and h . Specifically, we desire:

$$\frac{dP}{dt} = G_1 \frac{dv}{dt} + G_2 \frac{dh}{dt} \quad (28)$$

since dv/dt and dh/dt (or equivalently, dM/dt and dH/dt) are available from the mass and enthalpy conservation equations. First concentrating on the case of constant v (or v), to obtain G_2 , we differentiate equation 27 to give:

$$\frac{dh}{dt} = \left[\frac{\partial h_f}{\partial P} + h_{fg} \frac{\partial x}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] \frac{dP}{dt} \quad (29)$$

Using equation 26, holding v constant: (i.e. $v = \text{constant}$)

$$\frac{dx}{dP} = \frac{\partial \left(\frac{v - v_f}{v_{fg}} \right)}{\partial P} = - \frac{1}{v_{fg}} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right]$$

$$\begin{aligned} v \frac{\partial \left(\frac{1}{v_{fg}} \right)}{\partial P} &= - \frac{(v - v_f) \partial v_{fg}}{v_{fg}^2 \partial P} \\ &= \frac{x}{v_{fg}} \frac{\partial v_{fg}}{\partial P} \end{aligned} \quad (30)$$

Substituting this into equation 29 gives:

$$\frac{dh}{dt} = \left\{ \frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} - \frac{h_{fg}}{v_{fg}} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\} \frac{dP}{dt} \quad (31)$$

or equally:

$$\frac{dP}{dt} = \frac{v_{fg}}{\left\{ v_{fg} \left[\frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] - h_{fg} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\}} \frac{dh}{dt}$$

$$= \frac{v_{fg}}{\{\text{DENOMINATOR}\}} \frac{dh}{dt} = G_2 \frac{dh}{dt} \quad (32)$$

This gives the pressure rate response due to an enthalpy rate change, holding p constant.

If we repeat the above but holding h constant we find:

$\frac{\partial e}{\partial t} = \frac{\partial v}{\partial t} = -\frac{1}{v^2} \frac{\partial v}{\partial t}$
 or $-\frac{1}{v^2} \frac{\partial v}{\partial t} = \frac{\partial v}{\partial t}$

$$\frac{dP}{dt} = \frac{-h_{fg}}{\{\text{DENOMINATOR}\}} \frac{dv}{dt} = \frac{h_{fg} v^2}{\{\text{DENOMINATOR}\}} \frac{d\rho}{dt} = G_1 \frac{d\rho}{dt} \quad (33)$$

Note that G_1 and G_2 are functions that depend only on the local saturation fluid properties and their slopes at the local pressure.

Combining equation 32 and 33 to get the total pressure rate response when both h and ρ are varying:

$$\frac{dP}{dt} = G_1(P, x) \frac{d\rho}{dt} + G_2(P, x) \frac{dh}{dt} \quad (34)$$

This is the rate form of the equation of state for two-phase equilibrium fluid in terms of the intensive rate properties, $d\rho/dt$ and dh/dt , which are obtained from the continuity equations.

Equation (34) can be cast in the extensive form by noting that, since $\rho = M/V$ and

$$h = H/M,$$

$\frac{\partial M}{\partial t} = v \frac{\partial \rho}{\partial t} + \rho \frac{\partial v}{\partial t}$

$$\frac{d\rho}{dt} = \frac{1}{V} \frac{dM}{dt} - \frac{M}{V^2} \frac{dV}{dt} \quad (35)$$

$\frac{\partial H}{\partial t} = M \frac{\partial h}{\partial t} + h \frac{\partial M}{\partial t}$

$$\frac{dh}{dt} = \frac{1}{M} \frac{dH}{dt} - \frac{H}{M^2} \frac{dM}{dt} \quad (36)$$

Substituting into equation 34 and collecting terms:

$$\frac{dP}{dt} = \left(\frac{G_1}{V} - \frac{G_2 H}{M^2} \right) \frac{dM}{dt} + \frac{G_2}{M} \frac{dH}{dt} - \frac{G_1 M}{V^2} \frac{dV}{dt} \quad (37)$$

After some simplification and rearrangement we find:

$(h_g - h_f) v_{fg}^2 - h (v_g - v_f)$
 $(h_g - h_f) (v_f + x(v_g - v_f)) - (h_f + x(h_g - h_f)) (v_g - v_f)$
 $h_g v_f + h_f v_f - h_f v_g + h_f v_f$

$$\frac{dP}{dt} = \frac{F_1 \frac{dM}{dt} + F_2 \frac{dH}{dt} + F_3 \frac{dV}{dt}}{M_g F_4 + M_f F_5} \quad (38)$$

$\frac{dP}{dt} = M_1 \left(h_{fg} \frac{v_f^2}{V} - \frac{H}{M^2} v_{fg} \right) \frac{dM}{dt}$
 $(M) v_{fg} \left\{ \frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right\} - h_{fg} \left\{ \frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right\}$

where:

$$\begin{aligned}
 F_1 &= h_g v_f - h_f v_g \\
 F_2 &= v_g - v_f \\
 F_3 &= h_f - h_g \\
 F_4 &= \frac{\partial h_g}{\partial P} (v_g - v_f) - \frac{\partial v_f}{\partial P} (h_g - h_f) \\
 F_5 &= \frac{\partial h_f}{\partial P} (v_g - v_f) - \frac{\partial v_f}{\partial P} (h_g - h_f)
 \end{aligned} \tag{39}$$

$$M_g = x M$$

and

$$M_f = (1-x) M.$$

The F functions are smooth, slowly varying functions of pressure (see Figures 6-10) provided good curve fits are used. The latest steam tables (Haar, 1984) were used to fit saturated properties to less than 1/4% accuracy using low order polynomials and exponentials (Garland and Hoskins, 1988). Considerable effort was spent on obtaining accuracy and continuous derivatives over the full pressure range. The fact that good fits are available means that the F functions are well behaved which in turn makes the rate form of the equation of state extremely well behaved, as shown later.

The G functions are also well behaved for the same reasons.

The F and G functions have direct physical interpretations which aid in generating intuition. The F functions relate changes in the extensive properties, M, H and V, to changes in pressure. The G functions related changes in the intensive properties, ρ and h, to changes in pressure. Often, a simple numerical evaluation of these functions during a simulation aids in developing an appreciation of the changing roles of the key actors in a dynamic simulation.

For instance, because F_1 is negative, we immediately see that adding mass to a fixed volume of liquid with fixed total enthalpy will cause a depressurization (because the specific

enthalpy, $h = H/M$, is decreased). But, since G_1 is positive, an increase in density in a fluid of fixed specific enthalpy causes a pressurization.

Single-Phase, Non-Equilibrium (Subcooled and Superheated)

For the single-phase subcooled or superheated case, we do not have to account for the sorting out between phases as we did for the two phase case. thus the derivation is more direct and less complex. We could simply use:

$$P = \pi(\rho, h) \quad (40)$$

to give:

$$\frac{dP}{dt} = \left. \frac{\partial P}{\partial \rho} \right|_h \frac{d\rho}{dt} + \left. \frac{\partial P}{\partial h} \right|_\rho \frac{dh}{dt} \quad (41)$$

but, since the steam tables are given as a function of P and T , the slopes in equation 41 are not easily obtained. To cast the pressure rate equation in terms of the independent variables, P and T , consider:

$$\rho = \rho(P, T) \quad (42)$$

and

$$h = h(P, T) \quad (43)$$

Note that the non-equilibrium case requires the explicit tracking of the temperature in addition to pressure. Taking derivatives of Equations 42 and 43:

$$\frac{d\rho}{dt} = \left. \frac{\partial \rho}{\partial P} \right|_T \frac{dP}{dt} + \left. \frac{\partial \rho}{\partial T} \right|_P \frac{dT}{dt} \quad (44)$$

and

$$\frac{dh}{dt} = \left. \frac{\partial h}{\partial P} \right|_T \frac{dP}{dt} + \left. \frac{\partial h}{\partial T} \right|_P \frac{dT}{dt} \quad (45)$$

But we desire:

$$\frac{dP}{dt} = G_{1P} \frac{d\rho}{dt} + G_{2P} \frac{dh}{dt} \quad (46)$$

and

$$\frac{dT}{dt} = G_{1T} \frac{d\rho}{dt} + G_{2T} \frac{dh}{dt} \quad (47)$$

This is easily obtained by solving equation 44 and 45 for dP/dt and dT/dt to yield:

$$\frac{dP}{dt} = \frac{\left(\frac{\partial h}{\partial T} \right)_P \frac{d\rho}{dt} - \left(\frac{\partial \rho}{\partial T} \right)_P \frac{dh}{dt}}{\left(\frac{\partial \rho}{\partial P} \right)_T \frac{dh}{dt} - \left(\frac{\partial h}{\partial P} \right)_T \frac{d\rho}{dt}} \quad (48)$$

and

$$\frac{dT}{dt} = \frac{\left(\frac{\partial h}{\partial P} \right)_T \frac{d\rho}{dt} - \left(\frac{\partial \rho}{\partial P} \right)_T \frac{dh}{dt}}{\left(\frac{\partial \rho}{\partial T} \right)_P \frac{dh}{dt} - \left(\frac{\partial h}{\partial T} \right)_P \frac{d\rho}{dt}} \quad (49)$$

which is the intensive form we desire.

The extensive form is obtained as for the two-phase equilibrium case. Equations 35 and 36 are substituted into equations 48 and 49 and after rearrangement we find:

$$\frac{dP}{dt} = \frac{F_{1P} \frac{dM}{dt} + F_{2P} \frac{dH}{dt} + F_{3P} \frac{dV}{dt}}{M_v F_{4P} + M_l F_{5P}} = \left(\frac{G_{1P}}{V} - \frac{G_{2P} H}{M^2} \right) \frac{dM}{dt} + \frac{G_{2P} H}{M^2} \frac{dH}{dt} - \frac{G_{3P} M}{V^2} \frac{dV}{dt} \quad (50)$$

and

$$\frac{dT}{dt} = \frac{F_{1T} \frac{dM}{dt} + F_{2T} \frac{dH}{dt} + F_{3T} \frac{dV}{dt}}{M_v F_{4T} + M_l F_{5T}} \quad (51)$$

where

$$F_{1P} = \rho \left(\frac{\partial h}{\partial T} \right)_P - h \left(\frac{\partial \rho}{\partial T} \right)_P$$

$$F_{2P} = - \left(\frac{\partial \rho}{\partial T} \right)_P$$

$$F_{3P} = - \rho^2 \left(\frac{\partial h}{\partial T} \right)_P$$

$$F_{4P} = 0$$

subcooled

$$= \left(\frac{d\rho}{dP} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{dh}{dP} \right)_T$$

superheated

(52)

$$F_{5P} = \left(\frac{d\rho}{dP} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{dh}{dP} \right)_T$$

subcooled

$$= 0$$

superheated

$$M_v = \text{mass of vapor phase} = 0 \text{ subcooled} \\ = M \text{ superheated}$$

$$M_l = \text{mass of liquid phase} = M \text{ subcooled} \\ = 0 \text{ superheated}$$

$$F_{1T} = \rho \left(\frac{\partial h}{\partial P} \right)_T - h \left(\frac{\partial \rho}{\partial P} \right)_T$$

$$F_{2T} = - \left(\frac{\partial \rho}{\partial P} \right)_T$$

$$F_{3T} = - \rho \left(\frac{\partial h}{\partial P} \right)_T$$

$$F_{4T} = - F_{4P}$$

$$F_{5T} = - F_{5P}$$

Two-Phase Non-Equilibrium

The rate form for the equation of state for the two-phase non-equilibrium case is a simple extension of the single-phase non-equilibrium case. The liquid and vapor phases are treated independently to give:

$$\frac{dP_k}{dt} = G_{1P}^k \frac{d\rho_k}{dt} + G_{2P}^k \frac{dh_k}{dt} \quad (53)$$

$$\frac{dT_k}{dt} = G_{1T}^k \frac{d\rho_k}{dt} + G_{2T}^k \frac{dh_k}{dt} \quad (54)$$

where k represents either l or v for the liquid or vapor phases respectively. In general, the 6 equation model (3 continuity equations for each phase) would be used for the general unequal temperature, unequal velocity, unequal pressure situation. Thus $d\rho_k/dt$ and dh_k/dt are available to the rate form of the equation of state.

Case	Functions	F_1	F_2	F_3	F_4	F_5
2 ϕ equilibrium (all derivatives along saturation line)		$h_g v_f - h_f v_g$	v_{fg}	h_{fg}	$\frac{\partial h_g}{\partial P} v_{fg} - \frac{\partial v_g}{\partial P} h_{fg}$	$\frac{\partial h_f}{\partial P} v_{fg} - \frac{\partial v_f}{\partial P} h_{fg}$
1 ϕ non-equilibrium pressure		$\rho \left(\frac{\partial h}{\partial T} \right)_P - h \left(\frac{\partial \rho}{\partial T} \right)_P$	$-\left(\frac{\partial \rho}{\partial T} \right)_P$	$-\rho^2 \left(\frac{\partial h}{\partial T} \right)_P$	$\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \frac{\partial \rho}{\partial T} \left(\frac{\partial h}{\partial P} \right)_T$ 0 subcooled superheated	$\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \frac{\partial \rho}{\partial T} \left(\frac{\partial h}{\partial P} \right)_T$ subcooled 0 superheated
1 ϕ non-equilibrium temperature		$\rho \left(\frac{\partial h}{\partial P} \right)_T - h \left(\frac{\partial \rho}{\partial P} \right)_T$	$-\left(\frac{\partial \rho}{\partial P} \right)_T$	$-\rho^2 \left(\frac{\partial h}{\partial P} \right)_T$	$-F_{4P}$	$-F_{5P}$

Case	Functions	G_1	G_2
2 ϕ equilibrium (all derivatives along saturation line)		$\frac{h_{fg} v^2}{\left\{ v_{fg} \left[\frac{\partial h_{fg}}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] - h_{fg} \left[\frac{\partial v_P}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\}}$	$\frac{v_{fg}}{\left\{ v_{fg} \left[\frac{\partial h_f}{\partial P} + x \frac{\partial h_{fg}}{\partial P} \right] - h_{fg} \left[\frac{\partial v_f}{\partial P} + x \frac{\partial v_{fg}}{\partial P} \right] \right\}}$
1 ϕ non-equilibrium pressure		$\frac{\left(\frac{\partial h}{\partial T} \right)_P}{\left[\left(\frac{\partial \rho}{\partial T} \right)_T \left(\frac{\partial h}{\partial P} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T \right]}$	$\frac{-\left(\frac{\partial \rho}{\partial T} \right)_P}{\left[\left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P - \left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T \right]}$
1 ϕ non-equilibrium temperature		$\frac{\left(\frac{\partial h}{\partial P} \right)_T}{\left[\left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T - \left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P \right]}$	$\frac{-\left(\frac{\partial \rho}{\partial P} \right)_T}{\left[\left(\frac{\partial \rho}{\partial T} \right)_P \left(\frac{\partial h}{\partial P} \right)_T - \left(\frac{\partial \rho}{\partial P} \right)_T \left(\frac{\partial h}{\partial T} \right)_P \right]}$