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THE DEVELOPMENT OF A NON-ITERATIVE EQUATION OF STATE FOR TWO-PHASE FLOW SYSTEMS

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ABSTRACT

A form of the equation of state is analytically derived in this paper. From this form, the value of the time rate of change of pressure can be solved directly, without any iteration numerical scheme. Applications of this non-iterative equation of state to two-phase modelling are generally discussed. Finally, the possibility of solving the non-iterative equation of state simultaneously with the governing equations and the possibility of utilizing the equation as a mechanism of time-step control are indicated.

1.0 INTRODUCTION

The equation of state is an important aspect of two-phase flow modelling. A considerable portion of simulation computer time is devoted to the solving of the equation of state. Unfortunately, it has not received sufficient attention in the recent rapid development of the two-phase flow modelling. This paper is intended to initiate a discussion on how to improve the method of solving the equation of state, such that the efficiency of the overall two-phase flow modelling can further be improved.

A general review on the nature of the equation of state and existing methods of solving the equation of state is briefly reviewed in Section 2.0. A new form of the equation of state, from which the value of the time rate of change of pressure can be solved directly, is analytically derived in Section 3.0. Some comments on how the new form of the equation of state can be applied to two-phase flow modelling is presented in Section 4.0. A method of solving the two-phase flow model governing equations as well as the equation of state simultaneously is discussed in Section 5.0. Finally, in the same section, the possibility of utilizing the new form of equation of state for variable time-step control is indicated.

2.0 EQUATION OF STATE

From a thermodynamics view point, the equation of state of a substance is a relationship between any four thermodynamic properties of the substance, three of which are independent. An example of the equation of state involves pressure P, volume V, temperature T and mass of a system:

$$f(P,V,T,M) = 0$$

If any three of the four properties are fixed, the fourth is determined.

The equation of state can also be written in a form which depends only on the nature of the system and not on how much of the substance is present, hence all extensive properties are replaced by their corresponding specific values. Thus

$$f(P,v,T) = 0$$

is the specific value form of the above equation of state, where v is the specific volume. If any two of the thermodynamic properties are fixed, the third is determined.

In two-phase flow modelling, the equation of state is used as a constitutive equation to supplement the calculation of the governing equations, which are the equations for the conservation of mass, momentum and energy. Figure 1 is a schematic representation of information flow among the governing equations as well as the equation of state. Basically, the equation of state receives information about mass M (or its change ΔM) and energy E (or its change ΔE) as independent variables. Given the

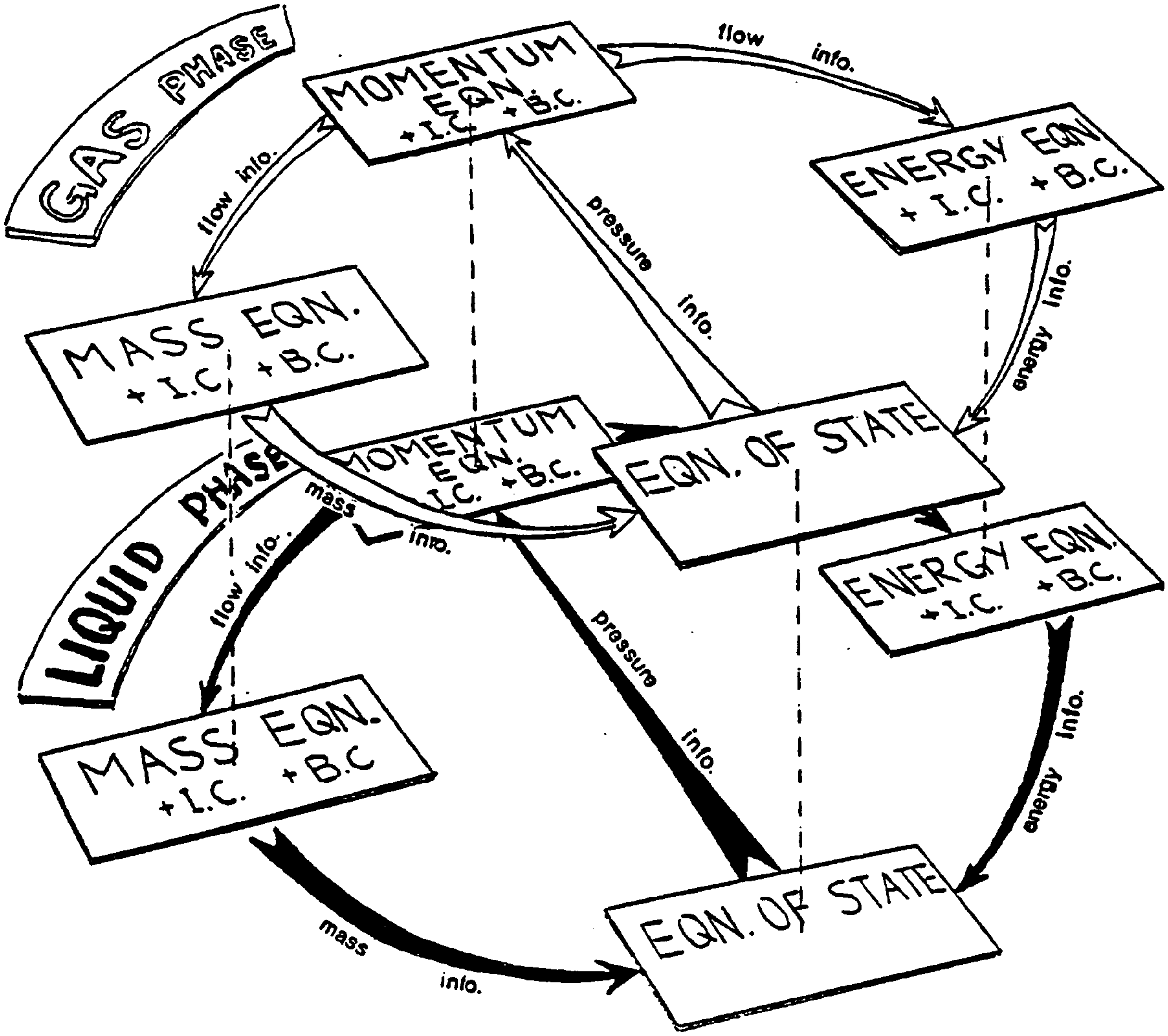

FIGURE 1 : Schematic Of Information Flow In Two-phase Flow Models

value of the volume of the system under consideration, V, the equation of state then calculates a new value of pressure P (or ΔP, its increment from its previous value). For example, the equation of state could take the form:

$$P = P_1(M,E,V)$$

or in specific values form:

$$P = P_2\ (\phi,e)$$

where ϕ represents mass (density ρ or specific volume v) and e is the specific value of E.

The new value of P is then fed into the momentum equation, and the numerical process is repeated for another time step.

In addition to the determination of P, the equation of state also calculate the new value of temperature T. Values of P and T are in turn used to calculate values of other thermodynamic properties which do not explicitly appear in the governing equations, but whose values are needed in further calculation. For example, if the enthalpy equation is used as the governing equation representing the energy, then the equation of state may take the form:

$$P = P(\rho,h)$$

where h is the specific enthalpy. If, furthermore, the value of the specific internal energy u is needed, then it can be calculated as

$$u = u(P,T)$$

It is noted, however, that for a saturated fluid, the value of the temperature fully depends on the saturation pressure.

Hence another independent parameter is needed in the above equation. The gas phase quality x is commonly used. Thus

$$u = u(P,x)$$

Given values of pressure, temperature or quality, the calculations of other thermodynamic properties are usually straightforward. On the other hand, the determination of pressure from known values of other thermodynamic properties is not, at least in the currently adopted methods. The rest of this paper therefore concentrates on how to predict new values of pressure of a two-phase system as a result of changes in mass and energy content of the system.

There are basically two forms of the equation of state: the instantaneous form and the differential form. The former generally takes the expression:

$$P = P_1(\Phi_1,\Phi_2,V) \qquad (1a)$$

where Φ_1 is the mass M and Φ_2 represents energy (enthalpy H or internal energy U). In terms of specific values, this is generally expressed as:

$$P = P_2(\phi_1,\phi_2) \qquad (1b)$$

where ϕ_1 represent density ρ or specific volume v, and ϕ_2 represent specific enthalpy h or specific internal energy u).

The differential form of equation of state is usually written in terms of time derivatives:

$$\frac{\partial P}{\partial t} = f_1\left(\frac{\partial \Phi_1}{\partial t}, \frac{\partial \Phi_2}{\partial t}, \frac{\partial V}{\partial t}\right) \qquad (2a)$$

or in specific values form:

$$\frac{\partial P}{\partial t} = f_2 \left(\frac{\partial \phi_1}{\partial t} , \frac{\partial \phi_2}{\partial t}\right) \qquad (2b)$$

The form chosen for a particular calculation is, of course, situation dependent. Eqn. (1) is usually used for a single control volume, where the exchange of mass and energy with external environment are treated as boundary conditions. In addition to being simpler, it does not have the usual error of numerical integration. However, the prediction of pressure is usually less continuous in time than that determined by using eqn. (2). On the other hand, eqn. (2) is usually used in nodal structure or differential type of calculation. It has an advantage that it can be used as the basis for time-step control in numerical calculation. This point will be elaborated in Section 5.0.

Another reason for adopting the form of eqn. (2) is as follows. When the conservation of mass, energy and momentum are written in differential or nodal forms, for example in the solution method of Porsching et al. [1], a pressure gradient term in the momentum balance is required to be written at the new time level by use of a Taylor series expansion about the old time level. This expansion requires partial derivatives of pressure, with respect of fluid mass, $\left(\frac{\partial P}{\partial \phi_1}\right)_{\phi_2}$ and with respect to energy, $\left(\frac{\partial P}{\partial \phi_2}\right)_{\phi_1}$. It is therefore natural to formulate the equation of state in such a way that these partial derivatives of pressure can be utilized:

$$\frac{\partial P}{\partial t} = \left(\frac{\partial P}{\partial \phi_1}\right)_{\phi_2} \frac{\partial \phi_1}{\partial t} + \left(\frac{\partial P}{\partial \phi_2}\right)_{\phi_1} \frac{\partial \phi_2}{\partial t}$$

At present, the equation of state such as eqn. (1) and eqn. (2) are usually solved by iterative numerical techniques. For example, an equation of eqn. (1a) type could be written in the form of:

$$V = v_f M_f + v_g M_g \tag{3a}$$

$$M = M_f + M_g \tag{3b}$$

$$U = u_f M_f + u_g M_g \tag{3c}$$

where M_f and M_g are, respectively, the mass of the liquid phase fluid and mass of the gas phase fluid in the system. v_f and v_g are, respectively, the saturated liquid and vapor specific volume. u_f and u_g are, restively, the saturated liquid and vapor specific internal energy. These fluid thermodynamic properties are functions of pressure, P, only. Since values of V, M and U are inputted into the equation of state, there are basically three unknowns in the above set of three equations.

To initiate the iteration, a tentative value of P is used to estimate M_f and M_g from eqn. (3a) and eqn. (3b). These approximate values of P, M_f and M_g are then used to estimate the value of the internal energy from eqn. (3c). The estimated value of the internal energy is compared to the actual value of U. Any discrepancies are fed back to the guessing mechanism to produce the next approximated value of P.

A similar "search and match" approach is also used in solving the equation of state of the eqn. (2) type. Sometimes, more sophisticated techniques, such as the method of small perturbation, are used. Several thermodynamic properties are "perturbed" from their initial values by small deviations. Partial derivatives involving these properties are then estimated by table look-up. They are in turn used to find the approximate value of P[2].

However, the authors believe that the use of these iterative methods can be eliminated if the equation of state is recast, such that the value of pressure P or the time derivative of P can be solved directly. The time derivative form of such an equation of state is developed in the next section.

3.0 The Derivations of the Non-iterative Equations of State In Time Derivative Forms

Two equations of the forms like eqn. (2a) and (2b) are analytically derived in this section. They are

$$\frac{\partial P}{\partial t} = \frac{F_1(P)\frac{\partial M}{\partial t} + F_2(P)\frac{\partial H}{\partial t} + F_3(P)\frac{\partial V}{\partial t}}{M_gF_4(P) + M_fF_5(P)} \qquad (5)$$

and
$$\frac{\partial P}{\partial t} = G_1(P,X)\frac{\partial \rho}{\partial t} + G_2(P,X)\frac{\partial h}{\partial t} \qquad (6)$$

The F_i (P)'s where i=1 to 5, are functions of several thermodynamic properties. They depend only on pressure. Similarly, G_1 (P,x) and G_2 (P,x) are thermodynamic functions which depend only on pressure and quality. When eqn. (5) or eqn. (6) are used these functions can be determined directly, hence eliminating iterations when solving for $\frac{\partial P}{\partial t}$

The choice of ρ to represent mass in eqn. (6) and the choice of enthalpy to represent energy in eqn. (5) and eqn. (6) is not unique. Similar expressions written in terms of other parameters (such as v and u) can be derived following the same procedure described below.

Consider an arbitrary volume of two-phase fluid as a thermodynamic system. It is assumed that both phase are at saturation under a uniform saturation pressure P. The total mass of the fluid, M, the total enthalpy in the system, H, the volume of the system, V and the quality of the gas phase x can be expressed as follow:

$$M = M_g + M_f \tag{7}$$

$$H = M_g h_g + M_f h_f \tag{8}$$

where h_g and h_f are the specific enthalpy of the saturated gas and saturated liquid respectively, at pressure P.

$$V = M_g v_g + M_f v_f \tag{9}$$

where v_g and v_f are the specific volume of the saturated gas and saturated liquid respectively, at pressure p.

and $$x = \frac{M_g}{M} \tag{10}$$

Taking the derivatives of eqn. (7), (8) and (9) with respect to time, give

$$\frac{\partial M}{\partial t} = \dot{M}_g + \dot{M}_f \tag{11}$$

$$\frac{\partial H}{\partial t} = M_g \frac{\partial h_g}{\partial t} + \dot{M}_g\, h_g + M_f \frac{\partial h_f}{\partial t} + \dot{M}_f\, h_f \tag{12}$$

$$\frac{\partial V}{\partial t} = M_g \frac{\partial v_g}{\partial t} + \dot{M}_g\, v_g + M_f \frac{\partial v_f}{\partial t} + \dot{M}_f\, v_f \tag{13}$$

where $$\dot{M}_g = \frac{\partial M_g}{\partial t} \quad ; \quad \dot{M}_f = \frac{\partial M_f}{\partial t}$$

Using the definition h = u + Pv, eqn. (12) can further be written as:

$$\frac{\partial H}{\partial t} = M_g \frac{\partial u_g}{\partial t} + M_g P \frac{\partial v_g}{\partial t} + M_g v_g \frac{\partial P}{\partial t} + \dot{M}_g u_g$$

$$+ \dot{M}_g P v_g + M_f \frac{\partial u_f}{\partial t} + M_f P \frac{\partial v_f}{\partial t} + M_f v_f \frac{\partial P}{\partial t}$$

$$+ \dot{M}_f u_f + \dot{M}_f P v f$$

Expressing $\frac{\partial u_g}{\partial t} = \frac{du_g}{dP}\,\frac{\partial P}{\partial t}$

and $\frac{\partial u_f}{\partial t} = \frac{du_f}{dP}\,\frac{\partial P}{\partial t}$

the above equation can be re-arranged to give

$$M_g(\frac{du_g}{dP} + v_g)\,\frac{\partial P}{\partial t} + M_f(\frac{du_f}{dP} + v_f)\,\frac{\partial P}{\partial t} + \dot{M}_g\,u_g$$

$$+ \dot{M}_f u_f + P\{M_g\,\frac{\partial v_g}{\partial t} + \dot{M}_g v_g + M_f\frac{\partial v_f}{\partial t} + \dot{M}_f v_f\}$$

$$= \frac{\partial H}{\partial t}$$

The last term in the left hand side of this equation can be identified as the product of P and $\frac{\partial V}{\partial t}$ (eqn. (13). Thus:

$$\{M_g\,(\frac{du_g}{dP} + v_g) + M_f(\frac{du_f}{dP} + v_f)\}\,\frac{\partial P}{\partial t}$$

$$+ \dot{M}_g u_g + \dot{M}_f u_f = \frac{\partial H}{\partial t} - P\,\frac{\partial V}{\partial t} \qquad (14)$$

Multiplying eqn. (11) by u_f

$$\dot{M}_g u_f + \dot{M}_f u_f = \frac{\partial M}{\partial t}\,u_f$$

Substituting this in eqn. (14) yields:

$$\{M_g\,(\frac{du_g}{dP} + v_g) + M_f(\frac{du_f}{dP} + v_f)\}\,\frac{\partial P}{\partial t} + \dot{M}_g(u_g - u_f)$$

$$= \frac{\partial H}{\partial t} - P\,\frac{\partial V}{\partial t} - \frac{\partial M}{\partial t}\,u_f \qquad (15)$$

The derivatives of the specific volume with respect to t in eqn. (13) can also be expressed differently:

$$\frac{\partial v_g}{\partial t} = \frac{dv_g}{dP}\frac{\partial P}{\partial t}$$

$$\frac{\partial v_f}{\partial t} = \frac{dv_f}{dP}\frac{\partial P}{\partial t}$$

Eqn. (11) is now multiplied by v_f:

$$\dot{M}_g\ v_f + \dot{M}_f v_f = \frac{\partial M}{\partial t}\ v_f$$

The preceding equation is substituted from eqn. (13) to yield

$$\left(M_g \frac{dv_g}{dP} + M_f \frac{dv_f}{dP}\right)\frac{\partial P}{\partial t} + \dot{M}_g\ (v_g - v_f)$$

$$= \frac{\partial V}{\partial t} - \frac{\partial M}{\partial t}\ v_f \qquad (16)$$

Multiplying eqn. (15) by $(v_g - v_f)$ and eqn. (16) by $(u_g - u_f)$, and combining them to eliminate $\dot{M}_g$, the eqn. (5) sought at the beginning of this section is now obtained:

$$\frac{\partial P}{\partial t} = \frac{F_1(P)\dfrac{\partial M}{\partial t} + F_2(P)\dfrac{\partial H}{\partial t} + F_3(P)\dfrac{\partial V}{\partial t}}{M_g F_4(P) + M_f F_5(P)} \qquad (5)$$

where $F_1(P) = v_f(u_g - u_f) - u_f(v_g - v_f)$

$= h_g v_f - h_f v_g$

$F_2(P) = v_g - v_f$

$F_3(P) = -\ (h_g - h_f)$

$$F_4(P) = \left(\frac{du_g}{dP} + v_g\right)(v_g - v_f) - \frac{dv_g}{dP}\ (u_g - u_f)$$

$$= \frac{dh_g}{dP}\ (v_g - v_f) - \frac{dv_g}{dP}\ (h_g - h_f)$$

$$F_5(P) = (\frac{du_f}{dP} + v_f)(v_g - v_f) - \frac{dv_f}{dP}(u_g - u_f)$$

$$\frac{dh_f}{dP}(v_g - v_f) - \frac{dv_f}{dP}(h_g - h_f)$$

It is noted that F_i (P), i=1,5, are just some combinations of saturated values of thermodynamic properties and hence are dependent only on pressure. Values of F_i (P)'s for heavy water have been calculated using correlations suggested by Firla (3). They are shown in Fig. 2 to Fig. 6 as smooth continuous functions of P.

Eqn. (6) can be derived from eqn. (5) by averaging the thermodynamic properties in the system. The averaged specific volume of the fluid, v and the average specific enthalpy, h are defined as follows:

$$v = x\,v_g + (1-x)\,v_f$$
$$h = x\,h_g + (1-x)\,h_f$$

By substituting H with Mh, V with Mv, M_g with xM and M_f with (1-x)M, eqn. (5) can be written as:

$$\frac{\partial P}{\partial t} = \frac{[F_1(P) + F_2(P)h + F_3(P)v]\frac{\partial M}{\partial t} + F_2(P)\frac{\partial h}{\partial t}M + F_3(P)\frac{\partial v}{\partial t}M}{xMF_4(P) + (1-x)MF_5(P)} \qquad (17)$$

However, $F_1(P) + F_2(P)\,h + F_3(P)\,v$

$$= h_g v_f - h_f v_g + (v_g - v_f)[xh_g + (1-x)h_f] - (h_g - h_f)[xv_g + (1-x)v_f]$$

which can be shown to be zero.

Equation (17) is therefore written as:

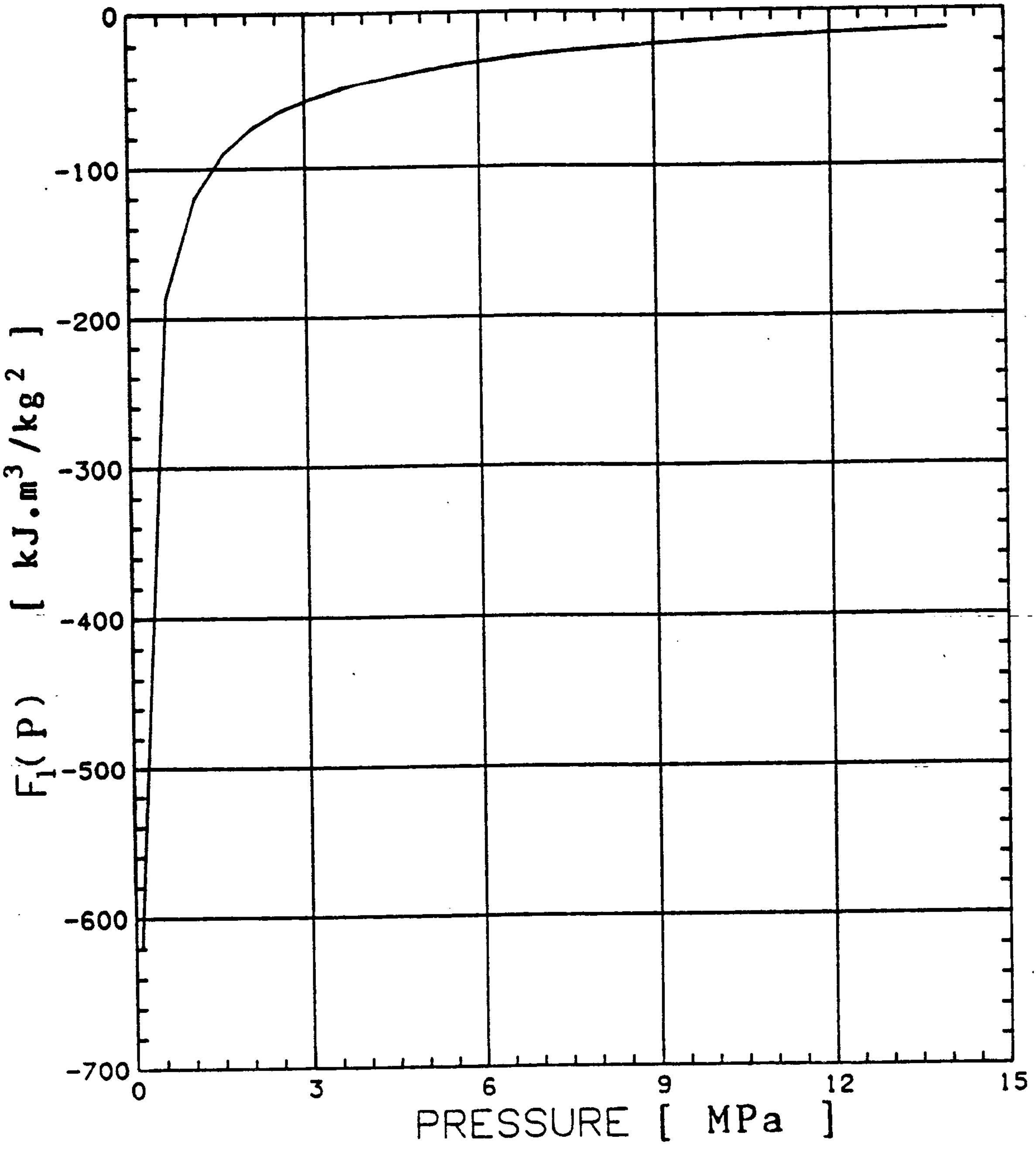

FIGURE 2 : Characteristic Of Thermodynamic Function $F_1(P)$

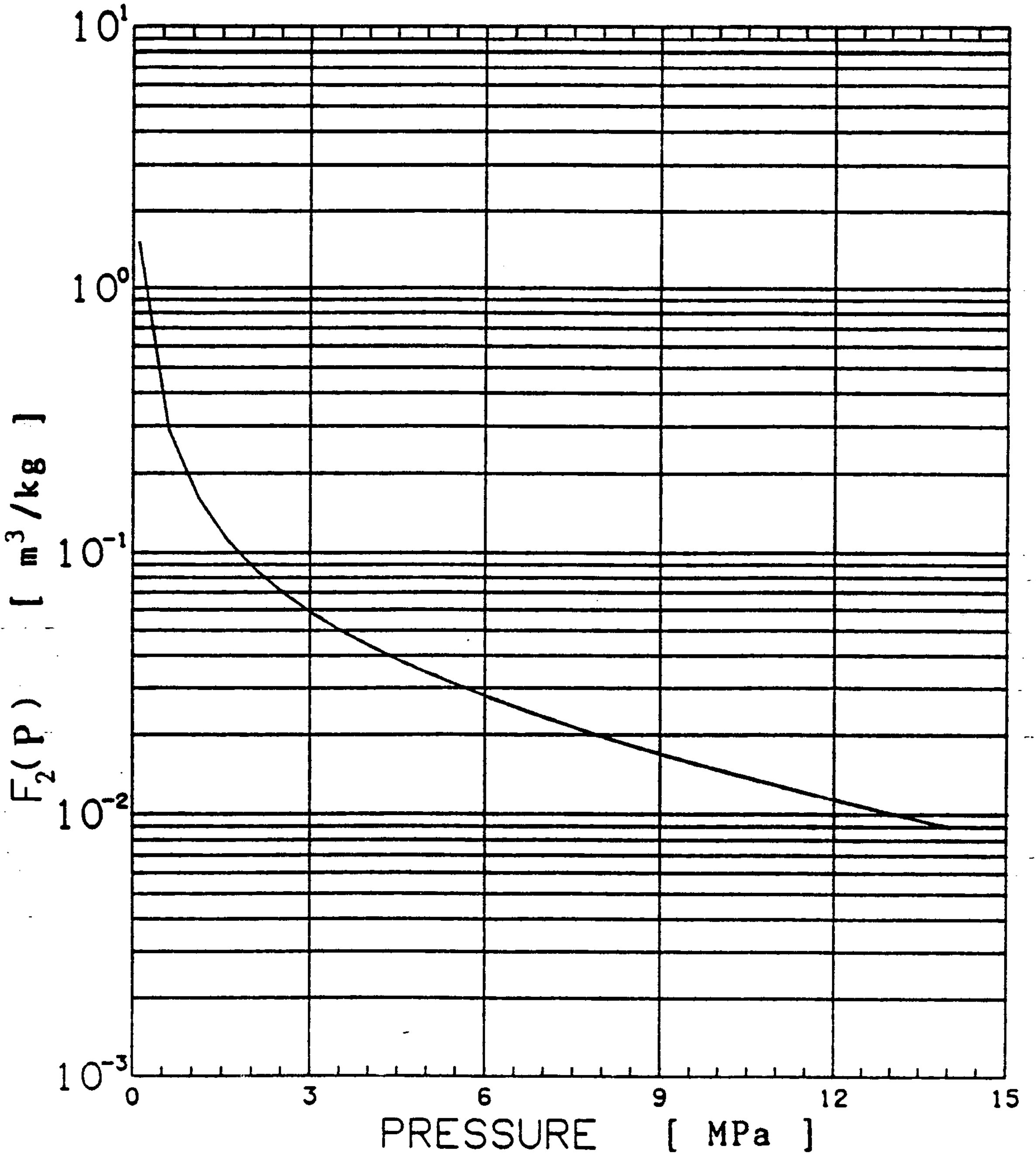

FIGURE 3 : Characteristic Of Thermodynamic Function $F_2(P)$

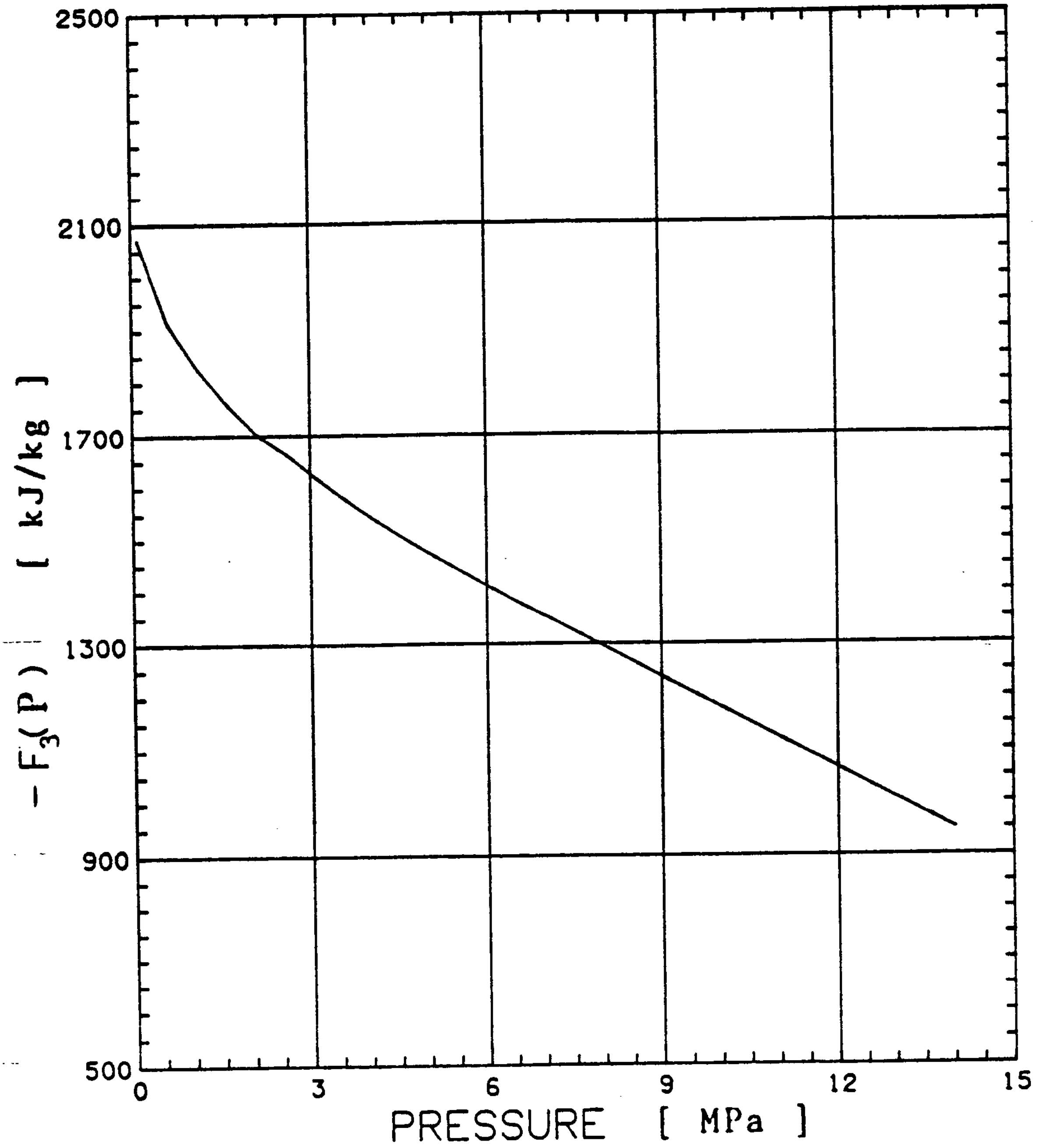

FIGURE 4 : Characteristic Of Thermodynamic Function $F_3(P)$

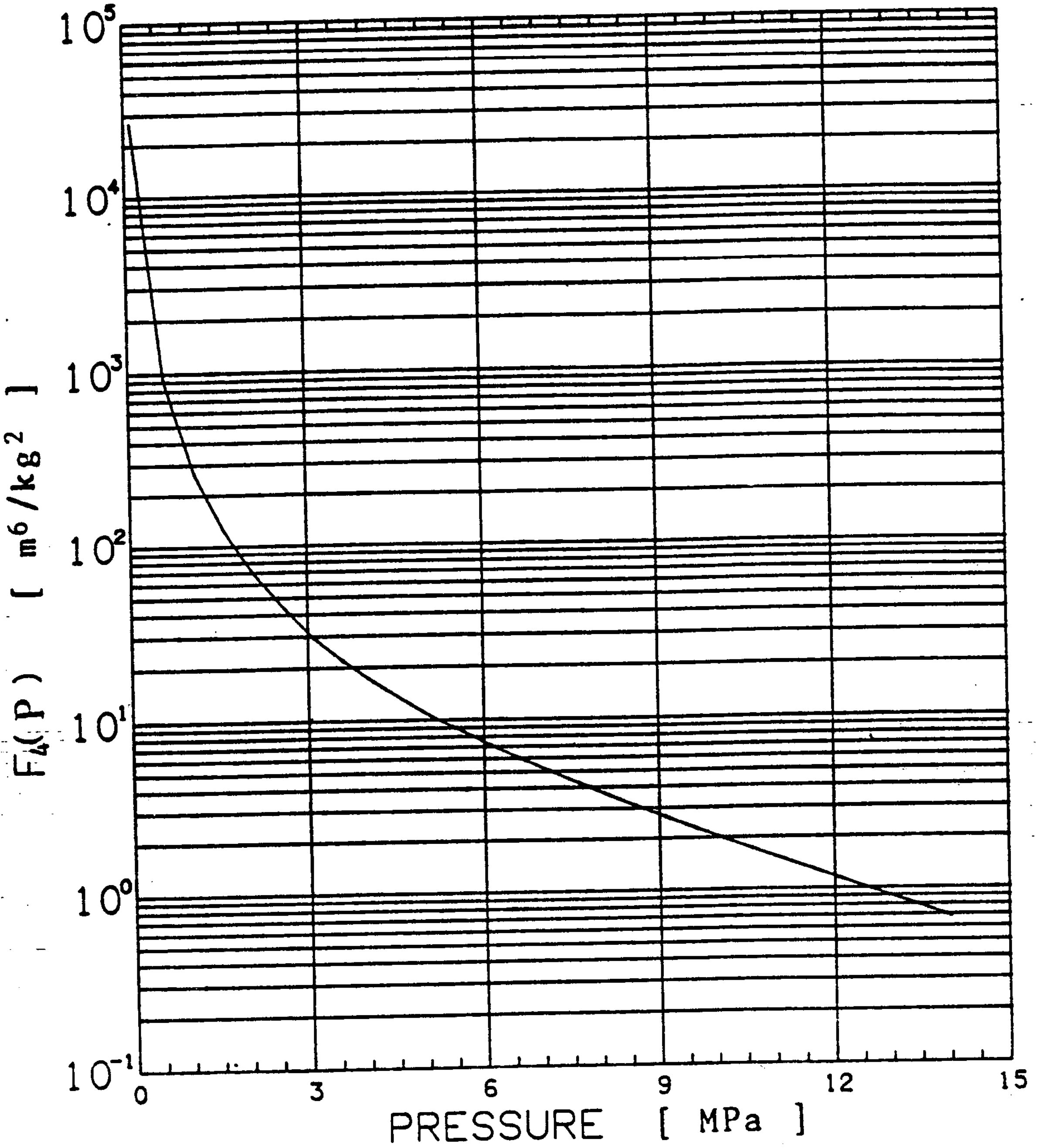

FIGURE 5 : Characteristic Of Thermodynamic Function $F_4(P)$

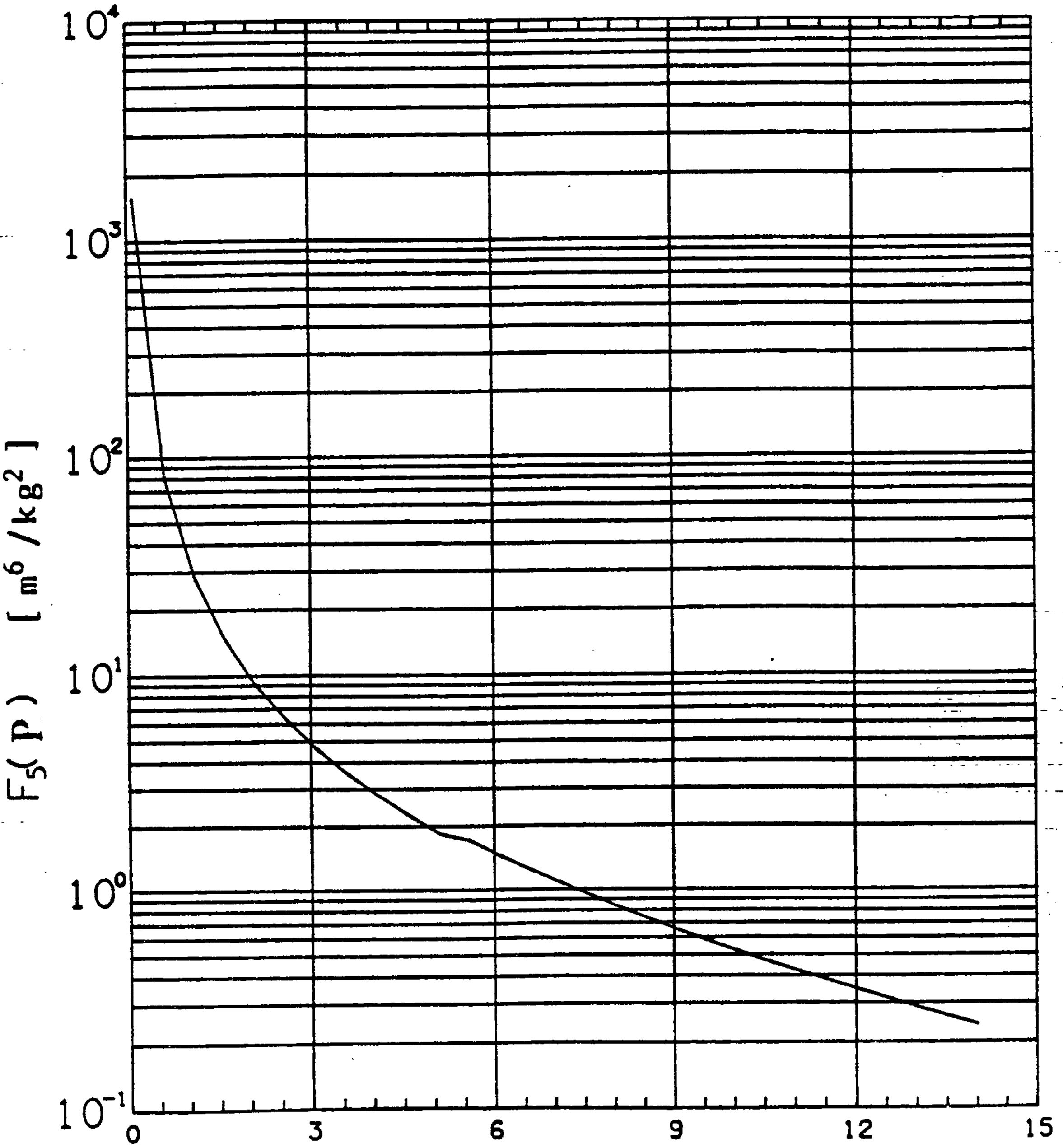

FIGURE 6 : Characteristic Of Thermodynamic Function $F_5(P)$

$$\frac{\partial P}{\partial t} = \frac{F_2(P)\frac{\partial h}{\partial t} + F_3(P)\frac{\partial v}{\partial t}}{xF_4(P) + (1-x)F_5(P)} \qquad (18)$$

To transfer eqn. (18) into the form of eqn. (6), it is noted that v = 1/P, where P is the average density of the fluid in the system, hence

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

$$= -[xv_g + (1-x)v_f]^2\frac{\partial \rho}{\partial t}$$

Eqn. (18) can therefore be written finally as

$$\frac{\partial P}{\partial t} = G_1(P,x)\frac{\partial \rho}{\partial t} + G_2(P,x)\frac{\partial h}{\partial t} \qquad (6)$$

where $G_1(P,x)$ and $G_2(P,x)$ are properties functions which only depend on pressure and quality:

$$G_1(P,x) = \frac{-F_3(P)[xv_g + (1-x)v_f]^2}{xF_4(P) + (1-x)F_5(P)}$$

$$= \frac{(h_g-h_f)[xv_g + (1-x)v_f]^2}{\left[x\frac{dh_g}{dP} + (1-x)\frac{dh_f}{dP}\right](v_g-v_f) - \left[x\frac{dv_g}{dP} + (1-x)\frac{dv_f}{dP}\right](h_g-h_f)}$$

$$G_2(P,x) = \frac{F_2(P)}{xF_4(P) + (1-x)F_5(P)}$$

$$= \frac{v_g - v_f}{\left[x\frac{dh_g}{dP} + (1-x)\frac{dh_f}{dP}\right](v_g-v_f) - \left[x\frac{dv_g}{dP} + (1-x)\frac{dv_f}{dP}\right](h_g-h_f)}$$

4.0 Application of The Non-iterative Equation of State In Various Two-Phase Flow Modelling

Two time derivative forms of non-iterative equation of state have been derived in the previous section:

$$\frac{\partial P}{\partial t} = \frac{F_1(P)\frac{\partial M}{\partial t} + F_2(P)\frac{\partial H}{\partial t} + F_3(P)\frac{\partial V}{\partial t}}{M_g F_4(P) + M_f F_5(P)} \qquad (5)$$

and

$$\frac{\partial P}{\partial t} = G_1(P,x)\frac{\partial \rho}{\partial t} + G_2(P,x)\frac{\partial h}{\partial t} \qquad (6)$$

It has been shown that eqn. (5) is derived for control volume, whose thermodynamic condition depends on values of M, H and V of the system. Hence eqn. (5) is suitable for two-phase flow models with nodal formulations, in which size (volume V) and fluid content (mass M) of the individual node contribute to the characteristic of the node's thermodynamic condition.

On the other hand, M and V do not appear explicitly in eqn. (6). Although eqn. (6) is derived from eqn. (5), no restriction of any kind are imposed on the nature and values of M and V in eqn. (5). Hence eqn. (6) is valid for any value of M and V. It is hereby an equation expressing a characteristic thermodynamic property of the fluid, locally at a point in the fluid and instantaneously at a particular time. Eqn. (6) can therefore be applied to almost any formulation of two-phase flow model, including those with governing equations written in area-averaged form or local instantaneous form [4]. It is noted that eqn. (5) can not be directly applied to the later two kinds of models.

A more serious limitation of the applicability of eqn. (5) and (6) is on a different aspect: the inter-phase equilibrium assumption.

This assumption therefore excludes the application of the eqn. (5) and eqn. (6) to the UVUT mixture model, for example. Nevertheless, they can be applied to UVET non-homogeneous saturation model such as that for steam generator or pressurizer simulations.

Moreover, eqn. (6) can probably be used under certain additional circumstances as well. For example in using the Drft-flux model, eqn. (6) can be used for determining pressure of the mixture (which mainly consists of the continuum phase). The pressure of the dispersed phase (bubbles or droplets) can be determined by other treatment such as by assuming the mixture pressure as its saturation pressure. Hence the dispersed phase pressure is equal to the sum of the mixture pressure and a correction term reflecting the pressure difference due to the bubble or droplet's surface tension.

In the case of modelling separated flow by a non-equilibrium two-fluid model, it is purposed to use two separate equations for the two-phase equation of state: one for the gas phase and one for the liquid phase. At any time step in the numerical calculation, the steam's equation of state is set-up by setting $M_f = 0$ and $M_g = M$ (if using eqn. (5) or by setting $x = 1$ (if using eqn. (6)); the liquid's equation of state is set-up by having $M_g = 0$ and $M_f = M$ or $x = 0$. At the end of the numerical calculation, any new quality calculated in the steam phase which is less than unity, and any new quality calculated in the liquid phase which is greater than zero provide some basis for the calculations of interfacial mass and energy transport in the next time step.

To summarize, due to vast number of two-phase flow models available, it is impossible to common on all the possible methods of applying eqn. (5) and eqn. (6) as the supplementing equation of state. The technique of application is basically an art by itself. The detail is up to the individual users. The only caution has to be taken is that the saturation assumption is deriving eqn. (5) has to be taken into consideration.

5.0 Numerical Aspects of the Application

As was mentioned in Section 2.0, that in two-phase flow modelling, the equation of state is used to supplement the governing equations. Conventionally, the solving of the equation of state is performed separately, while the governing equations are solved simultaneously or semi-simultaneously. In solving the governing equations, the pressure parameter P, which is one of the variables, is treated as a constant (or constants). The resulting new values of mass (or density) and enthalpy)or specific enthalpy) are fed into the equation of state, which is then solved to give a new value of P.

A new approach of solving all the governing equations as well as the equation of state simultaneously has been purposed recently [5]. Basically the governing equations and the equation of state are arranged in a matrix equation.

The following example illustrates the process. A set of governing equation written in the local instantaneous form is used in this example since they are mathematically simple and hence can better illustrate the process converting the equations into a matrix equation. A similar approach can be applied to other forms of governing equations, such as the volume-averaged form or the lumped (macroscopic) form, which are more widely used in engineering practice.

The local instantaneous conservation equations for mass momentum and energy can be written as:

mass:

$$\frac{\partial \rho_k}{\partial t} + \nabla\cdot(\rho_k \quad \mathbf{v}_k) = 0 \qquad k = 1,2 \qquad (19)$$

momentum:

$$\frac{\partial}{\partial t}(\rho_k \quad \mathbf{v}_k) + \nabla\cdot(\rho_k \ \mathbf{v}k \ \mathbf{v}_k) + \nabla P_k - \nabla\cdot\bar{\bar{\tau}}_k - \rho_k g = 0$$

$$k = 1,2 \qquad (20)$$

enthalpy:

$$\frac{\partial}{\partial t}(\rho_k \ h_k) + \nabla\cdot(\rho_k \ h_k \ V_k) + \nabla\cdot q_k - \nabla P_k \cdot \mathbf{v}_k + (\nabla\cdot \tau_k)\cdot \mathbf{v}_k = 0$$

$$k = 1,2 \qquad (21)$$

Eqn. (19) is rewritten by expanding the derivative in the second term:

$$\frac{\partial \rho_k}{\partial t} + \rho_k \ \nabla\cdot\mathbf{v}_k + \mathbf{v}_k \nabla \rho_k = 0 \qquad (22)$$

Eqn. (20) can also be rearranged by expanding the derivatives:

$$\rho_k \ \frac{\partial \mathbf{v}_k}{\partial t} + \rho_k \ \mathbf{v}_k \ \nabla\cdot \ \mathbf{v}_k + \nabla P_k - \nabla\cdot \bar{\bar{\tau}}_k - \rho_k g$$

$$+ \mathbf{v}_k \ [\frac{\partial \rho_k}{\partial t} + \nabla\cdot \ (\rho_k \ \mathbf{v}_k)] = 0$$

The last term is zero according to eqn. (19). Thus

$$\frac{\partial \mathbf{v}_k}{\partial t} + \mathbf{v}_k \ \nabla\cdot \ \mathbf{v}_k + \frac{1}{\rho_k} \nabla P_k = \frac{1}{\rho_k} \ \nabla\cdot \ \bar{\bar{\tau}}_k + g_k \qquad (23)$$

Similarly, eqn. (21) can also be rearranged to:

$$\rho_k \frac{\partial h_k}{\partial t} + \rho_k \ \mathbf{v}_k \cdot \nabla h_k - \mathbf{v}_k \nabla P_k - \mathbf{v}_k \nabla P_k + \nabla\cdot q_k + (\nabla\cdot \bar{\bar{\tau}}_k)\cdot \ \mathbf{v}_k$$

$$+ h_k [\frac{\partial \rho_k}{\partial t} + \nabla \ \rho_k \ \mathbf{v}_k] = 0$$

Substituting eqn. (19) into the above equation yields:

$$\frac{\partial h_k}{\partial t} + \mathbf{v}_k \nabla h_k - \frac{\mathbf{v}_k}{\rho_k} \nabla P_k = -\frac{1}{\rho_k} \nabla q_k - (\nabla \cdot \bar{\bar{\tau}}_k) \frac{\mathbf{v}_k}{\rho_k} \qquad (24)$$

Combining eqn. (6) with eqn. (22) and (24) gives:

$$\frac{\partial P_k}{\partial t} = G_1 (P_k, x_k) [-\rho_k \nabla \mathbf{v}_k - \mathbf{v}_k \nabla \rho_k] + G_2 (P_k, x_k) [- \mathbf{v}_k \nabla h_k + \frac{\mathbf{v}_k}{\rho_k} \nabla P_k$$
$$- \frac{1}{\rho_k} \nabla g_k - (\nabla \cdot \bar{\bar{\tau}}_k) \cdot \frac{\mathbf{v}_k}{\rho_k}]$$

rearranging yields:

$$\frac{\partial P_k}{\partial t} + G_2 \mathbf{v}_k \nabla h_k - G_2 \frac{\mathbf{v}_k}{\rho_k} \nabla P_k + G_1 \rho_k \nabla \mathbf{v}_k + G_1 \mathbf{v}_k \nabla \rho_k$$
$$= \frac{G_2}{\rho_k} \nabla \cdot q_k - (\nabla \cdot \bar{\bar{\tau}}_k) \frac{\mathbf{v}_k G_2}{\rho_k} \qquad (25)$$

Eqn. (22), (23), (24) and (25) are now grouped into a matrix form:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ \mathbf{v}_k \\ h_k \\ P_k \end{bmatrix} + \begin{bmatrix} \mathbf{v}_k & \rho_k & 0 & 0 \\ 0 & \mathbf{v}_k & 0 & \frac{1}{\rho_k} \\ 0 & 0 & \mathbf{v}_k & -\frac{\mathbf{v}_k}{\rho_k} \\ G_1 \mathbf{v}_k & G_1 \rho_k & G_2 \mathbf{v}_k & -G_2 \frac{\mathbf{v}_k}{\rho_k} \end{bmatrix} \nabla \cdot \begin{bmatrix} \rho_k \\ \mathbf{v}_k \\ h_k \\ P_k \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{\rho_k} \nabla \cdot \bar{\bar{\tau}}_k + g \\ \frac{-1}{\rho_k} \nabla q_k - (\nabla \cdot \bar{\bar{\tau}}_k \frac{\mathbf{v}_k}{\rho_k} \\ \frac{G_2}{\rho_k} \nabla q_k - \nabla \cdot \bar{\bar{\tau}}_k \frac{\mathbf{v}_k G_2}{\rho_k} \end{bmatrix}$$

The two phase flow problem now reduced to solving the above matrix equation. The possibility of reducing the two-phase flow problem into eigenvalue problem based on the above matrix equation has been suggested [5].

Another consideration is the possibility of utilizing eqn. (5) or eqn. (6) for variable-time-step control purpose. In the simulation of two-phase systems by computer code, certain numerical instabilities can be identified by the drastic increase of predicted value of pressure. If the instantaneous form of equation of state (eqn. (1)) is used in the code and when an instability occurs, it is sometimes necessary to repeat the simulation with smaller time-step. However, if time derivative form of equation of state such as eqn. (5) or eqn. (6) is used, it can provide a basis for an instability prevention mechanism. At any time during the simulation, by comparing the time rate of change of pressure with some predetermined criteria, a potential instability can be forecasted. The time-step is pre-programmed in such a way that it is automatically reduced when an instability is forecasted. Hence the instability can be prevented without having to repeat the simulation.

6.0 Future Developments

It is hoped that the development of the non-iterative equation of state presented in this paper will be a step toward finding the most efficient equation of state in two-phase flow modelling.

It is noted that eqn. (5) and (6) can be useful only because the properties function Fi (P), i=1 to 5, can be calculated directly by combining several thermodynamic properties, whose values are conveniently given by the correlations suggested by Firla [3]. However, errors are expected to be generated during this two-stage calculations. This error can be minimized if correlations of Fi(P) can be directly formulated from thermodynamic properties table. This is therefore an aspect that will receive attention in the future.

As pointed out in Section 4.0, the detailed applications of eqn. (5) and (6) into two-phase flow modelling depend on the nature of the model. Hopefully, the proposal presented in this paper can be carried out by other workers who are currently active in developing various two-phase flow models. Their findings and experience would be highly appreciated by the authors.

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