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A COMPARISON OF THE RATE FORM OF THE EQUATION OF STATE TO THE JACOBIAN FORM

by

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ABSTRACT

Porsching's solution algorithm for the simulation of thermalhydraulic systems is compared to a new method based on the rate form of the equation of state. Both algorithms are developed and discussed. A direct comparison is made for a simple 2 node-1 link case to illustrate and numerically test the ideas presented.

It is shown that the final algorithms of the two methods are identical and that the rate method is more intuitive, easy to implement and permits eigenvalue extraction. The modelling of the nonlinear damping term was found to be important when large time steps were taken.

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INTRODUCTION

One of the more successful algorithms for thermalhydraulic simulation is based on the work of Porsching (PO 69, 71). This algorithm, involving the Jacobi (or derivative of the system state matrix), is used originally in FLASH-4 (PO 69), and subsequently SOPHT (CH 77). The strength of Porsching's approach lies in the recognition of flow as the most important dependent parameter and, hence, its fully implicit treatment of flow. This leads to excellent numerically stability, consistency and converge. Further, the Jacobian permits a generalized approach to the linearization of nonlinear systems. This allows the development of a system state matrix which contains all the system dynamics in terms of the dependent parameters of mass, energy and flow. Back substitution finally gives a matrix rate equation in terms of the system flow (the unknown) and the system derivatives. While this approach is certainly a proven and successful one, it has some disadvantages. First, as will be shown later, the matrix rate equation to be solved is not in a characteristic or eigenvalue form. Hence, it is not directly possible to extract the system eigenvalues and thus determine the stability of a state without performing a costly time solution. Secondly, the matrix rate equation involving the Jacobi is as complicated as it is general. The resulting expressions are somewhat obtuse and it is difficult to obtain an intuitive feel for the system. This complexity also hinders implementation in a simulation code and makes error tracking a tedious process.

Recently (GA86a, GA86b, SO85), work has been presented on the use of the rate form of the equation of state. These works showed that by casting the equation of state in the form of a rate equation rather than the normal algebraic form, the system state matrix, can be more logically formed of the normal conservation rate equations for mass, energy and momentum plus the pressure rate equation. This forms the four cornerstone equations in thermalhydraulic systems analysis (Figure 1). It was found (GA86a) that the mass and energy equations did not contribute to the eigenvalues of the system for the simple cases studied. This agrees with the intuitive analogy of springs and masses. Further, numerical implementation prove to be very successful, leading to roughly a factor of 10 improvement

over the algebraic form of the equation of state, largely due to the iterative nature of the algebraic form. Incorporating the implicit pressure dependency in the numerical method also drastically improved the numerical stability.

Since Porsching's method also carried the pressure dependency implicitly (via the Jacobi), the question arises as to how the Rate Form compares to Porsching's method Specifically, is the pressure treatment of the two methods different? If so, what are the advantages and disadvantages of each? How do the two compare in terms of robustness, ease of implementation, clarity, stability, etc?

To investigate these questions, the following two sections are devoted to concise but explanatory derivations of Porsching's method and the Rate Form. Subsequently, a numerical test is performed on a simple system to illustrate the similarities and differences.

DERIVATION OF PORSCHING'S FORM

Following Porsching (PO71), the thermalhydraulic system equations can be written in node-link form (see Figure 2):

Momentum:

$$\dot{W}_k = f_k(t, P_i, P_j, W_k)\,; \tag{1}$$

Enthalpy:

$$\dot{H}_i = \sum_{\nu \in T_i} \frac{H_\nu}{M_\nu} W_\nu - \sum_{\nu \in I_i} \frac{H_\nu}{M_\nu} W_\nu + Q_i\,; \tag{2}$$

Mass:

$$\dot{M}_i = \sum_{\nu \in T_i} W_\nu - \sum_{\nu \in I_i} W_\nu\,; \tag{3}$$

where

W = mass flow rate;

P = pressure;

M = mass;

H = total enthalpy;

f = some function;

Q = heat source;

t = time;

T_i = terminating node for link k;

I_i = initiating node for link k;

subscripts;

i,j = node indices;

k = link index;

ν = summation index;

superscript

$\bullet = \partial/\partial t$

These equations can be written in matrix form:

$$\dot{\mathbf{y}} = \mathbf{F}(t,\mathbf{y}), \tag{4}$$

where y is the column vector:

$$\mathbf{y} = \begin{bmatrix} W_1 \\ \vdots \\ W_k \\ H_1 \\ \vdots \\ H_N \\ M_1 \\ \vdots \\ M_N \end{bmatrix} \tag{5}$$

for the case of K links and N nodes.

An implicit solution is sought for its stability advantages over explicit methods. First, we expand **F** via the Taylor series:

$$\mathbf{F}(t^{n+1}, y^{n+1}) = \mathbf{F}(t^n, y^n) + \Delta t \left[\left. \frac{\partial \mathbf{F}(t, y)}{\partial t} \right|_n + \left. \frac{\partial \mathbf{F}}{\partial y}(t, y) \right|_n \frac{\partial y}{\partial t} \right] + 0(\Delta t^2) \tag{6}$$

where the superscript, n, denotes some reference at iteration n and $n+1$ denotes the time of iteration $n+1$. The time difference Δt is simply $t^{n+1} - t^n$. It is assumed that **F** contains no explicit time dependence (i.e. terms such as at^2 or bt, where a and b are constants). Rather, the time dependency in **F** is through the implicit dependence of mass, energy and flow on time. That is:

$$\mathbf{F}(t,y) \Rightarrow \mathbf{F}(y(t)). \tag{7}$$

Thus, in equation 6,

$$\left. \frac{\partial \mathbf{F}}{\partial t}(t, y) \right|_n = 0$$

the implicit form for equation 4 is

$$\frac{y^{n+1} - y^n}{\Delta t} = \mathbf{F}(t^{n+1}, y^{n+1}). \tag{8}$$

Substituting in the expansion of equation 6:

$$\dot{y} = \mathbf{F}(t^n, y^n) + \Delta t \, \mathbf{J} \, \dot{y}, \tag{9}$$

where the Jacobi is:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & \cdots \\ \vdots & \vdots & \end{bmatrix}. \tag{10}$$

Rearranging equation 9:

$$\dot{y} = [\mathbf{I} - \Delta t \, \mathbf{J}]^{-1} \mathbf{F}(t^n, y^n) = \frac{y^{n+1} - y^n}{\Delta t} \tag{11}$$

or

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t[\mathbf{I} - \Delta t\,\mathbf{J}]^{-1}\,\mathbf{F}(t^n, \mathbf{y}^n) \tag{12}$$

or

$$\Delta \mathbf{y} \equiv \mathbf{y}^{n+1} - \mathbf{y}^n = \Delta t[\mathbf{I} - \Delta t\,\mathbf{J}]^{-1}\,\mathbf{F}(t^n, \mathbf{y}^n) \quad . \tag{13}$$

Equations 12 and 13 are the general forms for the implicit method. Note that the function, **F**, is general. It is only required that it be differentiable. In practice, it is required that **F** be smooth so that there are no discontinuities in **J**. Discontinuities tend to play havoc on the numerical stability of simulations. For this reason, the steam tables employed in the simulation must have continuous derivatives (see also GA 86c).

The Jacobi, **J**, is of size K + 2N by K + 2N. For practical simulations (50 or more nodes), this gives rather large matrices to invert. To reduce the cost of inversion, Porsching utilized the fact that flow is the major parameter and eliminated $\mathbf{M}^{n+1}$ and $\mathbf{H}^{n+1}$ from the matrix equation 12 (or 13) by backsubstituting, leaving a matrix equation implicit in **W**, but not in **M** and **H**. To illustrate, consider a two node, one link case (figure 3). The governing equations are:

Mass:

$$\frac{\partial M_1}{\partial t} = -W\,, \qquad \frac{\partial M_2}{\partial t} = W\,. \tag{14}$$

Energy:

$$\begin{aligned} \frac{\partial H_1}{\partial t} &= -(H_1/M_1)W\,, \qquad \frac{\partial H_2}{\partial t} = (H_1/M_1)W\,, \quad \text{for } W>0\,, \\ \frac{\partial H_1}{\partial t} &= -(H_2/M_2)W\,, \qquad \frac{\partial H_2}{\partial t} = (H_2/M_2)W\,, \quad \text{for } W<0\,. \end{aligned} \tag{15}$$

Momentum:

$$\frac{\partial W}{\partial t} = \frac{A}{L}(P_1 - P_2) - K|W|\,W\,. \tag{16}$$

State:

$$P_i = \pi(H_i, M_i, V_i)\,, \quad i = 1, 2. \tag{17}$$

where V = volume.

The Jacobi for this case is:

$$J = \begin{bmatrix} -2K|W| & \frac{A}{L}\frac{\partial P_1}{\partial H_1} & -\frac{A}{L}\frac{\partial P_2}{\partial H_2} & \frac{A}{L}\frac{\partial P_1}{\partial M_1} & -\frac{A}{L}\frac{\partial P_2}{\partial M_2} \\ -H_1/M_1 & -\frac{W}{M_1} & 0 & +\frac{H_1 W}{M_1^2} & 0 \\ +H_1/M_1 & +\frac{W}{M_1} & 0 & -\frac{H_1 W}{M_1^2} & 0 \\ -1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 \end{bmatrix} . \tag{18}$$

When flow reverses, the source node is 2 rather than 1, and the Jacobi becomes:

$$J = \begin{bmatrix} -2K|W| & \frac{A}{L}\frac{\partial P_1}{\partial H_1} & -\frac{A}{L}\frac{\partial P_2}{\partial H_2} & \frac{A}{L}\frac{\partial P_1}{\partial M_1} & -\frac{A}{L}\frac{\partial P_2}{\partial M_2} \\ -H_2/M_2 & 0 & -\frac{W}{M_2} & 0 & +\frac{H_2 W}{M_2^2} \\ +H_2/M_2 & 0 & \frac{W}{M_2} & 0 & -\frac{H_2 W}{M_2^2} \\ -1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 \end{bmatrix} . \tag{19}$$

Thus, the matrix equation to be solved is:

$$[I - \Delta t\, J]\ \Delta y = \Delta t\, F(t^n, y^n)\,, \tag{13}$$

where $[I - \Delta t\, J]$ is given by:

$$\begin{bmatrix} 1+2\Delta t K|W| & -\frac{A}{L}\frac{\partial P_1}{\partial H_1}\Delta t & \frac{A}{L}\frac{\partial P_2}{\partial H_2}\Delta t & -\frac{A}{L}\frac{\partial P_1}{\partial M_1}\Delta t & -\frac{A}{L}\frac{\partial P_2}{\partial M_2}\Delta t \\ H_1/M_1\,\Delta t & 1+\frac{W}{M_1}\Delta t & 0 & -\frac{H_1 W}{M_1^2}\Delta t & 0 \\ -H_1/M_1\,\Delta t & -\frac{W}{M_1}\Delta t & 1 & \frac{H_1 W}{M_1^2}\Delta t & 0 \\ (+1)\Delta t & 0 & 0 & 1 & 0 \\ (-1)\Delta t & 0 & 0 & 0 & 1 \end{bmatrix} \quad (20)$$

and F is:

$$\begin{bmatrix} \frac{A}{L}(P_1-P_2)-K|W|W \\ -H_1/M_1\,W \\ +H_1/M_1\,W \\ -W \\ +W \end{bmatrix} \quad (21)$$

for the case where $W>0$. Since the same arguments apply for the case where $W<0$, further discussion will confine itself to the case where $W>0$.

Multiply through in equation 13, using equations 20 and 21, noting that:

$$\Delta y = \begin{bmatrix} \Delta W_1 \\ \Delta H_1 \\ \Delta H_2 \\ \Delta M_1 \\ \Delta M_2 \end{bmatrix}, \quad (22)$$

we find:

$$(1+2\Delta t\,K|W|)\Delta W - \frac{A}{L}\frac{\partial P_1}{\partial H_1}\Delta t\,\Delta H_1 + \frac{A}{L}\frac{\partial P_2}{\partial H_2}\Delta t\,\Delta H_2 - \frac{A}{L}\frac{\partial P_1}{\partial M_1}\Delta t\,\Delta M_1$$

$$+ \frac{A}{L}\frac{\partial P_2}{\partial M_2}\Delta t\,\Delta M_2 = \Delta t\left[\frac{A}{L}(P_1 - P_2) - K|W|W\right], \tag{23a}$$

$$\frac{\Delta W H_1}{M_1}\Delta t + \left(1 + \frac{W}{M_1}\Delta t\right)\Delta H_1 - \frac{\Delta t H_1 W \Delta M_1}{M_1^2} = \Delta t\left(-\frac{H_1 W}{M_1}\right), \tag{23b}$$

$$-\frac{\Delta W H_1}{M_1}\Delta t - W\frac{\Delta H_1}{M_1}\Delta t + \Delta H_2 + \frac{\Delta t H_1 W \Delta M_1}{M_1^2} = \frac{\Delta t H_1 W}{M_1}, \tag{23c}$$

$$\Delta W\,\Delta t + \Delta M_1 = -W\Delta t, \tag{23d}$$

and

$$\Delta W\,\Delta t + \Delta M_2 = W\Delta t. \tag{23e}$$

Thus, from equations 23d and 23e:

$$\Delta M_1 = -(W + \Delta W)\Delta t \tag{24a}$$

$$\Delta M_2 = (W + \Delta W)\,\Delta t \tag{24b}$$

$$\Delta H_1 = -\frac{\Delta t\ H_1 W/M_1 - \Delta t\,\Delta W H_1/M_1 + \Delta t\ H_1 W\,\Delta M_1/\Delta M_2^2}{1 + W/M_1\,\Delta t}$$

$$= -\Delta t\frac{H_1}{M_1}(W + \Delta W) \quad \text{after simplification.} \tag{24c}$$

and

$$\Delta H_2 = \Delta t\frac{H_1}{M_1}(W + \Delta W). \tag{24d}$$

Note that mass and enthalpy are conserved.

We note also that the expressions for ΔM and ΔH are similar to what you would obtain by the straightforward application of implicit forward differencing of the orginal equations 14 and 15, i.e:

$$\frac{M_1^{n+1}-M_1^n}{\Delta t} = -W^{n+1}, \qquad \frac{M_2^{n+1}-M_2^n}{\Delta t} = +W^{n+1},$$

$$\frac{H_1^{n+1}-H_1^n}{\Delta t} = -\frac{H_1^{n+1}}{M_1^{n+1}} W^{n+1}, \qquad \frac{H_2^{n+1}-H_1^n}{\Delta t} = \frac{H_1^{n+1}}{M_1^{n+1}} W^{n+1}. \tag{25}$$

The only difference between equations 24 and 25 is the treatment of the H_1/M_1 factor. To arrive at 24c and d, the mass equations (24a and b) were used and indeed, implicit treatment of M and H was used. The result (24a to d) appears explicit in M and H when compared to equation 25. This does not mean that the Jacobi form leads to a semi-implicit method (implicit in flow, explicit in mass and enthalpy). It means that the implicit contributions cancel out. (Note, however, it can be shown that for the general case, Porsching's method is fully implicit in its treatment of the mass equation but not for the enthalpy equation.) Thus we conclude that there is little merit in carrying the mass and enthalpy equations in implicit form. This agrees with earlier observations (GA 86a) that the eigenvalues of a thermal-hydraulic system are associated with the flow and pressure equations, not with the mass and energy equations.

To finish off the derivation of Porsching's approach, we use equations 24a to d in equation 23a to give:

$$\left\{1+2\Delta t\, K|W| + \frac{A}{L}\Delta t^2\left[\frac{H_1}{M_1}\left(\frac{\partial P_1}{\partial H_1}+\frac{\partial P_2}{\partial H_2}\right)+\left(\frac{\partial P_1}{\partial M_1}+\frac{\partial P_2}{\partial M_2}\right)\right]\right\}\Delta W$$

$$= \Delta t\left\{\frac{A}{L}(P_1-P_2) - K|W|W - \Delta t\frac{A}{L}W\left[\frac{H_1}{M_1}\left(\frac{\partial P_1}{\partial H_1}+\frac{\partial P_2}{\partial H_2}\right)+\left(\frac{\partial P_1}{\partial M_1}+\frac{\partial P_2}{\partial M_2}\right)\right]\right\} \tag{26}$$

Setting:

$$C_1 = \frac{H_1}{M_1}\frac{\partial P_1}{\partial H_1} + \frac{\partial P_1}{\partial M_1} \tag{27}$$

and

$$C_2 = \frac{H_1}{M_1}\frac{\partial P_2}{\partial H_2} + \frac{\partial P_2}{\partial M_2} \tag{28}$$

we have

$$\left\{1+2\Delta t\,K|W|+\frac{A}{L}\Delta t^2(C_1+C_2)\right\}\Delta W$$

$$=\Delta t\left\{\frac{A}{L}(P_1-P_2)-K|W|W-\Delta t\frac{A}{L}W(C_1+C_2)\right\} \tag{29}$$

Of course, the general case of N nodes and K links would follow the same substitution route with greatly increased complexity (see PO71). It is not evident from Porsching's general expressions that the resulting flow equations (equation 26 for the simple case of 2 nodes and 1 link) are more dependent on pressure and its derivatives (with respect to mass and energy) than it is on the mass and the enthalpy themselves. This observation, once pointed out, is obvious and undeniable. Yet, no existing thermalhydraulic code for system simulation takes full advantage of this observation.

Does a formulation which contains the appropriate implicit treatment without the large overhead of the general perturbation approach of Porsching's method? A clue exists in equation 17:

$$P = \pi(M, H, V) \tag{17}$$

This can be rewritten:

$$dP = \frac{\partial P}{\partial M}\,dM + \frac{\partial P}{\partial H}\,dH + \frac{\partial P}{\partial V}\,dV. \tag{30}$$

The form of equation 30 suggests that equation (26) contains some version of the total pressure derivative. Indeed we shall see in the next section that the rate form of the equation of state yields the same expression as Porsching's method, without the large overhead.

DERIVATION OF THE RATE FORM OF THE EQUATION OF STATE (from GA86a)

The determination of pressure from known values of other thermodynamic properties is not direct since interpolation and iteration is required because the independent (known) parameters are temperature, T, and pressure, P. Unfortunately, T and P are rarely the independent parameters in system dynamics since the numerical solution of the conservation equations yield mass and energy as a function of time. Hence, from the point of view of the

equation of state, it is mass and energy which are the independent parameters. Consequently, system codes are hampered by the form of water property data.

Consider the algebraic form:

$$P = \pi(\rho,h) \tag{31}$$

Traditionally, an iterative scheme (such as Newton-Raphson, AG83) is used to solve Equation 31. The value of P is initially guessed. Iteration is then performed if P fails to satisfy a designated 'error' equation within a preset tolerance. At each iteration a new (and hopefully better) approximation of P is calculated by the Newton-Raphson formula.

The designated 'error' equation can be either an equation expressing the error in specific enthalpy:

$$\mathrm{erh}(P) = h - h_{\mathrm{ESTIMATED}}(P, x) = 0, \tag{32}$$

or one expressing the error in density:

$$\mathrm{erd}(P) = \rho - \rho_{\mathrm{ESTIMATED}}(P, x) = 0, \tag{33}$$

where x is the quality.

Hence the solving of the equation of state is reduced to the finding of the root of the 'error' equation.

Alternatively, a method has been developed to solve the equation of state by deriving a rate form of Equation 31. The case of two-phase equilibrium was previously discussed (GA86a). It will now be summarized in the following. Subsequently, the results are quoted for the extension to single phase and two-phase non-equilibrium fluid.

For a volume, V, of mass, M, and total energy H, we have:

$$M = M_g + M_f, \tag{34}$$

$$H = M_g h_g + M_f h_f, \tag{35}$$

and

$$V = M_g \nu_g + M_F \nu_f. \tag{36}$$

Differentiating Equation 35:

$$\frac{dH}{dt} = M_g \frac{dh_g}{dt} + h_g \frac{dM_g}{dt} + M_f \frac{dh_f}{dt} + h_f \frac{dM_f}{dt}$$

$$= M_g \frac{\partial h_g}{\partial P} \frac{dP}{dt} + h_g \frac{dM_g}{dt} + M_f \frac{\partial h_f}{\partial P} \frac{dP}{dt} + h_f \frac{dM_f}{dt} , \quad (37)$$

Differentiating and combining Equations 4 and 6, the following can be obtained:

$$\frac{dM_g}{dt} = \frac{\frac{dV}{dt} - v_f \frac{dM}{dt} - M \frac{dv_f}{dt}}{v_g - v_f} - \frac{(V - Mv_f)}{(v_g - v_f)^2} \left(\frac{dv_g}{dt} - \frac{dv_f}{dt} \right) . \quad (38)$$

and

$$\frac{dM_f}{dt} = \frac{\frac{dV}{dt} - v_g \frac{dM}{dt} - M \frac{dv_g}{dt}}{v_f - v_g} - \frac{(V - Mv_g)}{(v_f - v_g)^2} \left(\frac{dv_f}{dt} - \frac{dv_g}{dt} \right) . \quad (39)$$

Substituting Equations 38 and 39 into Equation 37, and solving for dP/dt we find:

$$\frac{dP}{dt} = \frac{(v_g - v_f) \frac{dH}{dt} + (h_g v_f - h_f v_g) \frac{dM}{dt} + (h_f - h_g) \frac{dV}{dt}}{\left[M_g (v_g - v_f) \frac{\partial h_g}{\partial P} - h_g M \frac{\partial v_f}{\partial P} - h_g M_g \left(\frac{\partial v_g}{\partial P} - \frac{\partial v_f}{\partial P} \right) - \right.$$

$$\left. M_f (v_f - v_g) \frac{\partial h_f}{\partial P} + h_f M \frac{\partial v_g}{\partial P} - h_f M_f \left(\frac{\partial v_g}{\partial P} - \frac{\partial v_f}{\partial P} \right) \right] \quad (40)$$

Simplifying and defining

$$F_1 = h_g v_f - h_f v_g ,$$

$$F_2 = v_g - v_f ,$$

$$F_3 = h_f - h_g ,$$

$$F_4 = \frac{\partial h_g}{\partial P} (v_g - v_f) - \frac{\partial v_g}{\partial P} (h_g - h_f) , \quad (41)$$

$$F_5 = \frac{\partial h_f}{\partial P} (v_g - v_f) - \frac{\partial v_f}{\partial P} (h_g - h_f) ,$$

we have:

$$\frac{dP}{dt} = \frac{F_1 \frac{dM}{dt} + F_2 \frac{dH}{dt} + F_3 \frac{dV}{dt}}{M_g F_4 + M_f F_5} , \tag{42}$$

where the F's are smooth, slowly varying functions of pressure (SO85) only. Note that $M_g = xM$ and $M_f = (1-x)M$, where x which can be calculated directly from $h = H/M = xh_g + (1-x)h_f$. This is the rate form of the Equation of State for two-phase equilibrium fluid in terms of the extensive properties (which are obtained from the continuity equations). This can be cast in the intensive form by substituting

$$H = Mh, V = M\nu, M_g = xM, M_F = (1-x)M$$

to give

$$\frac{dP}{dt} = \frac{[F_1(P) + F_2(P)h + F_3(P)\nu] \frac{\partial M}{\partial t} + F_2(P) \frac{\partial h}{\partial t} M + F_3(P) \frac{\partial \nu}{\partial t} M}{x M F_4(P) + (1-x) M F_5(P)} . \tag{43}$$

But since $F_1(P) + F_2(P)h + F_3(P)\nu$ is equal to zero by expansion, and since

$$\frac{\partial \nu}{\partial t} = \frac{-1}{\rho^2} \frac{\partial \rho}{\partial t} = -[x\nu_g + (1-x)\nu_f]^2 \frac{\partial \rho}{\partial t} .$$

Equation 43 can be written as

$$\frac{\partial P}{\partial t} = G_1(P,x) \frac{\partial \rho}{\partial t} + G_2(P,x) \frac{\partial h}{\partial t} \tag{44}$$

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

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

$$= \frac{(h_g - h_f)[x\nu_g + (1-x)\nu_f]^2}{\left[x \frac{dh_g}{dP} + (1-x) \frac{dh_f}{dP}\right](\nu_g - \nu_f) - \left[x \frac{d\nu_g}{dP} + (1-x) \frac{d\nu_f}{dP}\right](h_g - h_f)} \tag{45}$$

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

$$= \frac{v_g - v_f}{\left[x\frac{dh_g}{dP} + (1-x)\frac{dh_f}{dP}\right](v_g - v_f) - \left[x\frac{dv_g}{dP} + (1-x)\frac{dv_f}{dP}\right](h_g - h_f)} \quad (46)$$

The F functions are smooth, slowly varying functions of pressure provided good curve fits are used. The latest steam tables (HA84) were used to fit saturated properties to less than 1/4% accuracy using low order polynomials and exponentials (GA86c). 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.

In general, the equation of state can be written in rate form for all situations (GA86a). We adopt the general form:

$$\frac{dP}{dt} = \frac{F_1\frac{dM}{dt} + F_2\frac{dH}{dt} + F_3\frac{dV}{dt} + M_v F_6\frac{dT_v}{dt} + M_l F_7\frac{dT_l}{dt}}{M_v F_4 + M_l F_5}$$

$$= G_1\frac{d\rho}{dt} + G_2\frac{dh}{dt} + G_3\frac{dT_v}{dt} + G_4\frac{dT_l}{dt} \quad (47)$$

The expressions for the F and G functions are summarized as in GA86a. These expressions cover the full range from subcooled liquid to superheated steam.

Thus, in addition to the system conservation equations 14 to 16, we have two pressure rate equations:

$$\frac{\partial P_1}{\partial t} = \frac{F_{11}\frac{\partial M_1}{\partial t} + F_{12}\frac{\partial H_1}{\partial t}}{M_{1v}F_{14} + M_{1\ell}F_{15}} \equiv G'_{11}\frac{\partial M_1}{\partial t} + G'_{12}\frac{\partial H_1}{\partial t} \quad (48)$$

$$\frac{\partial P_2}{\partial t} = \frac{F_{21}\frac{\partial M_2}{\partial t} + F_{22}\frac{\partial H_2}{\partial t}}{M_{2v}F_{14} + M_{2\ell}F_{25}} \equiv G'_{21}\frac{\partial M_1}{\partial t} + G'_{22}\frac{\partial H_2}{\partial t} \quad (49)$$

Substituting in equations 48 and 49 for dM/dt and dH/dt we have:

$$\frac{\partial P_1}{\partial t} = -\left(G'_{1i} + G'_{1i}\frac{H_1}{M_1}\right)W \tag{50}$$

$$\frac{\partial P_2}{\partial t} = +\left(G'_{2i} + G'_{2i}\frac{H_1}{M_1}\right)W \tag{51}$$

But G_{11}' is simply $\partial P_1/\partial M_1$, G_{12}' is simply $\partial P_1/\partial H_1$, etc. Thus, we see that equations 50 and 51 can be rewritten as:

$$\frac{\partial P_1}{\partial t} = -C_1 W \tag{52}$$

$$\frac{\partial P_2}{\partial t} = +C_2 W \tag{53}$$

In matrix form, considering just the flow and pressure equations, we have:

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{A}(\mathbf{U}, t)\,\mathbf{U}(t) + \mathbf{B} \tag{54}$$

$$\mathbf{U} = \begin{bmatrix} W \\ P_1 \\ P_2 \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix},$$

$$\mathbf{A} \equiv \begin{bmatrix} -K|W| & \frac{A}{L} & -\frac{A}{L} \\ -C_1 & 0 & 0 \\ +C_2 & 0 & 0 \end{bmatrix}. \tag{55}$$

A typical implicit treatment would be:

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = \mathbf{A}(\mathbf{U}^{n+1}, t)\,\mathbf{U}^{n+1}. \tag{56}$$

Often, to simplify, **A** is treated explicitly, i.e $\mathbf{A} \rightarrow \mathbf{A}(\mathbf{U}^n, t)$. This yields:

$$(\mathbf{I} - \Delta t\mathbf{A})\,\mathbf{U}^{n+1} = \mathbf{U}^n \tag{57}$$

to be solved for $\mathbf{U}^{n+1}$ by matrix inversion.

In this case, since **A** contains a major nonlinearity in flow (the term K|W|), it is best to treat it more carefully.

Consider the fully implicit form of the flow equation of (54):

$$\frac{W^{n+1}-W^n}{\Delta t} \equiv \frac{\Delta W}{\Delta t} = -K|W^{n+1}|W^{n+1} + \frac{A}{L}(P_1^{n+1}-P_2^{n+1})$$

$$= -K|W^n+\Delta W|(W^n+\Delta W)+\frac{A}{L}(P_1^n-P_2^n)-\frac{A}{L}\Delta t(C_1+C_2)W^{n+1}$$

$$= -K|W^n|W^n-2K|W^n|\,\Delta W+0(\Delta W^2)+\frac{A}{L}(P_1^n-P_2^n)$$

$$-\frac{A}{L}\Delta t(C_1+C_2)W^n-\frac{A}{L}\Delta t(C_1+C_2)\Delta W\,. \tag{58}$$

Collecting terms:

$$\left\{1+2K|W^n|\Delta t+\frac{A}{L}\Delta t^2(C_1+C_2)\right\}\Delta W$$

$$= \Delta t\left\{\frac{A}{L}(P_1-P_2)-K|W|W-\Delta t\frac{A}{L}W(C_1+C_2)\right\}. \tag{59}$$

This is identical to equation 29 obtained from Porsching's method.

Thus, to answer the question posed in the beginning: Yes, a formulation, which contains the appropriate implicit treatment without the large overhead of Porsching's method, does exist. That formulation is obtained via the rate form of the equation of state. The solution algorithm is now straight forward. All the needed partial derivatives are contained in the coefficients, C_1 and C_2, and once coded, can be used for all thermodynamic phases, from single phase subcooled liquid through to superheated steam, and for all the thermal-hydraulic models, from the simple HEM through to the six-equation model. Case dependent system Jacobi's are not required. The system equations are of the simple form of 54 and the user is free to choose from the existing spectrum of numerical schemes, depending on the user's needs. The next section explores a few such schemes to test the importance of implicitly modelling the nonlinear damping term K|W|.

NUMERICAL TEST

Of course, the numerical treatment is not unique. Equally, for both the rate form and Porsching's form, equations 58 (or equivalently 26) could be solved for W^{n+1} to give:

$$\frac{W^{n+1}-W^n}{\Delta t} = -K|W^n|W^n - 2K|W^n|(W^{n+1}-W^n) + 0(\Delta W^2)$$

$$+\frac{A}{L}(P_1^n - P_2^n) - \frac{A}{L}\Delta t\,(C_1+C_2)W^{n+1} \tag{60}$$

and finally:

$$\left\{1+2K|W|\,\Delta t + \frac{A}{L}\Delta t^2(C_1+C_2)\right\}W^{n+1}$$

$$= W^n + \Delta t\left\{\frac{A}{L}(P_1-P_2) + K|W|W\right\} \tag{61}$$

If the nonlinear term, K|W| were treated explicitly, as per equation 57, this would lead to

$$\left\{1+\Delta t\,K|W| + \frac{A}{L}\Delta t^2(C_1+C_2)\right\}\Delta W^{n+1}$$

$$= W^n + \Delta t\frac{A}{L}(P_1-P_2) \tag{62}$$

For the sake of discussion, this method solving for W^{n+1} employing the explicit treatment of K|W| will be called Method 1. Method 2 is that of equation 59, i.e. solving for ΔW with fully implicit treatment for K|W|. Method 3 is that of equation 61, i.e. solving for W^{n+1} with fully implicit treatment for K|W|. Thus, a comparison of Methods 1 and 3 will show how sensitive the solution is to the treatment of the nonlinear term and a comparison of Methods 2 and 3 will show the difference in solving for ΔW (subsequently generating W^{n+1} from $W^{n+1} = W^n + \Delta W$) vs. solving directly for W^{n+1}.

As a base run, the 2 node-link case of Figure 4 was run with a maximum Δt of 0.02 sec and a tolerance requirement of 0.001 (i.e. the time step was restricted so that the maximum fractional change in any dependent variable was limited to 0.001 of the nominal value of that dependent variable. As shown in figure 4 (and figure 5, in expanded scale), all three methods gave identical results. To test stability of the three algorithms, the time step was preset in a series of runs. Time steps were set at 0.1, 0.5, 1 and 10 seconds, respectively. Figures 6

to 9, comparing methods 2 and 3 showed identical results. We conclude that it does not matter whether the algorithm solves for ΔW or for W^{n+1}. Figures 10 to 13, comparing methods 1 and 3 show that the treatment of the nonlinear term, K|W|, does affect the solution to some degree. The implicit treatment appears smoother in general. Both treatments are stable and converge to the steady state at roughly the same rate.

Previously (GA86b) it was noted that terms in the numerator of equations such as:

$$W^{n+1} = \frac{\{1 + \Delta t\, K|W|\}W^n + \Delta t \frac{A}{L}(P_1 - P_2)}{\left\{1 + 2K|W|\,\Delta t + \frac{A}{L}\Delta t^2(C_1 + C_2)\right\}} \tag{61}$$

or

$$W^{n+1} = \frac{W^n + \Delta t \frac{A}{L}(P_1 - P_2)}{\left\{1 + K|W|\,\Delta t + \frac{A}{L}\Delta t^2(C_1 + C_2)\right\}} \tag{62}$$

can cause numeric instabilities if the factors involving Δt can go negative. Negative factors for large Δt causes a flipping of sign for subsequent W's, i.e. $W^{n+1} < 0$, $W^{n+2} > 0$, etc. Since K|W| is always >0, there should be no difference in stability in equations 61 and 62 (methods 3 and 1 respectively). This was found to be true.

EIGENVALUE ANALYSIS

The eigenvalue analysis for the rate form has been presented previously (GA86a). The analysis is straightforward since the rate form naturally leads to the matrix system equation which, in general, has the form

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{A}\,\mathbf{U} + \mathbf{B} \tag{54}$$

with a solution for constant **A** and **B**:

$$\mathbf{U}(t) = \mathbf{U}(0) \sum_i e^{\lambda_i t} - \mathbf{A}^{-1}\,\mathbf{B}\,. \tag{63}$$

It is easily shown that the eigenvalues of $\mathbf{A} - \lambda\mathbf{I}$ are the eigenvalues of equation 54. Thus system codes that are formulated based on the rate form are already in a form that permits

the numeric calculation of eigenvalues using existing algorithms. Hence system stability is obtainable without effecting a time solution.

The same cannot be said of Porsching's method. The equation form for this method is

$$\frac{\partial \mathbf{y}}{\partial t} = (\mathbf{I} - \Delta t\, \mathbf{J})^{-1}\, \mathbf{F}(t, \mathbf{y}), \tag{11}$$

which is not of the form leading to eigenvalues of dimension $\sec^{-1}$.

CONCLUSIONS

The comparison between Porsching's Method and the Rate Method revealed, at least in the simple case, that the two methods are equivalent in that the resulting time advancement algorithms are identical. However, the comparison further revealed that the Rate Method is more straightforward to implement. The Rate Method also permits eigenvalue extraction whereas Porsching's Method does not. Both methods showed excellent numeric stability, consistency and convergence. Both methods also conserved mass and enthalpy.

An interesting byproduct of the comparison was the observation that there is no need to treat mass and enthalpy terms implicitly since the implicit contributions cancelled out. This was observed in the simple case and it is not true in general.

The modelling of the nonlinear damping term, $K|W|W$, does affect the smoothness of the solution of large time steps. Since no additional overhead is required, it is recommended that the term be cast as $K|W^{n+1}|W^{n+1}$ rather than $k|W^{n}|W^{n+1}$.

ACKNOWLEDGEMENTS

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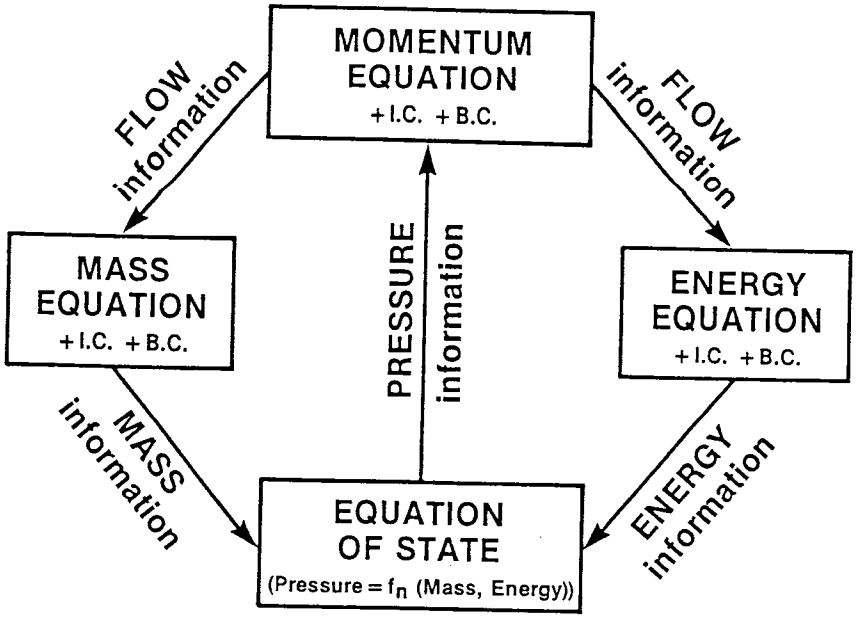

Figure 1. The four cornerstone equations for thermalhydraulic system simulation and the flow of information between them.

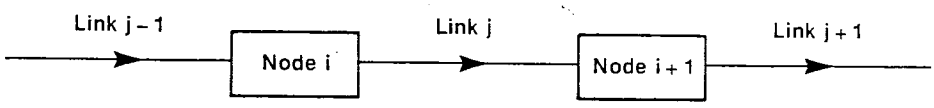

Figure 2. Node-link indice schema.

Parameter	Node 1	Node 2
Volume (m^3)	1.0	1.0
Pressure (MPa)	10.0	5.0
Mass (kg)	500.0	100.0

Link	
Diameter (m)	0.1
Length (m)	1.0
f	0.001
k	1.5

$$K = \frac{(A/L)(fL/D + k)}{2A^2p}$$

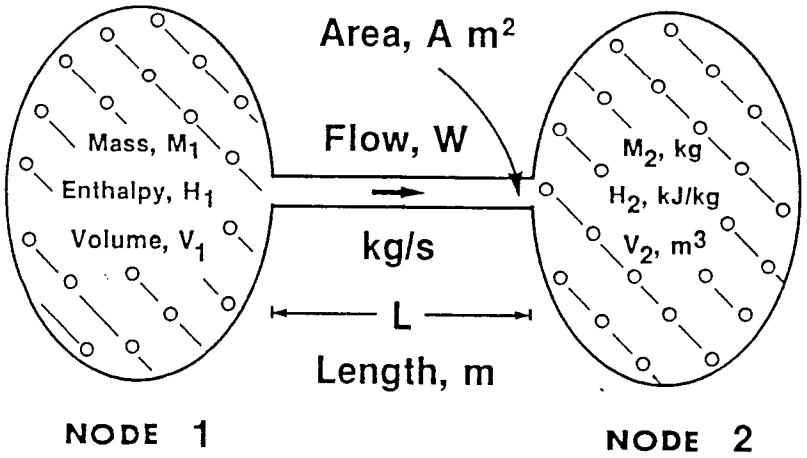

Figure 3. Simple 2 node, 1 link system.

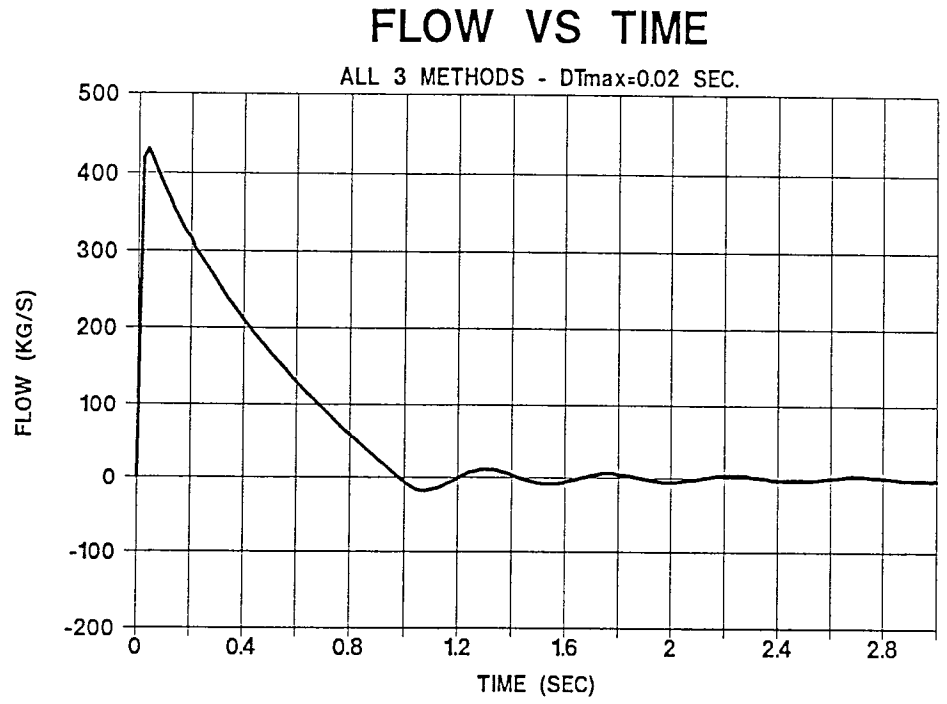

Figure 4. Link flow transient for the 2 node case: Converged solution for Methods 1, 2 & 3.

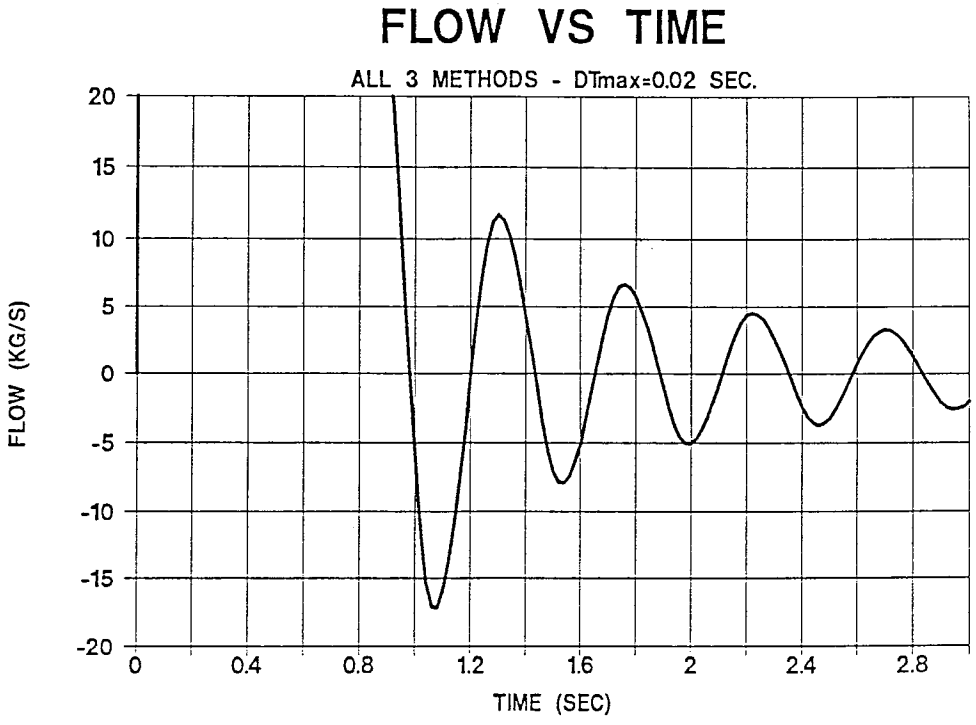

Figure 5. Link flow transient for the 2 node case: Converged solution for Methods 1, 2 & 3, expanded scale.

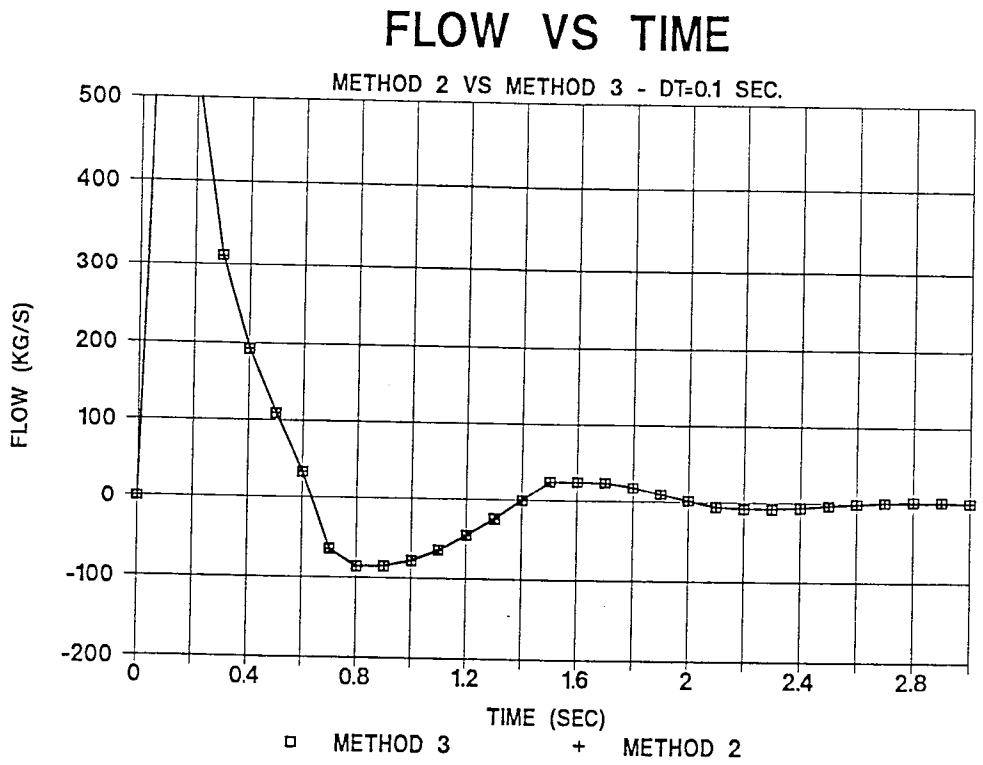

Figure 6. Method 2 vs. Method 3: Δt=0.1 sec.

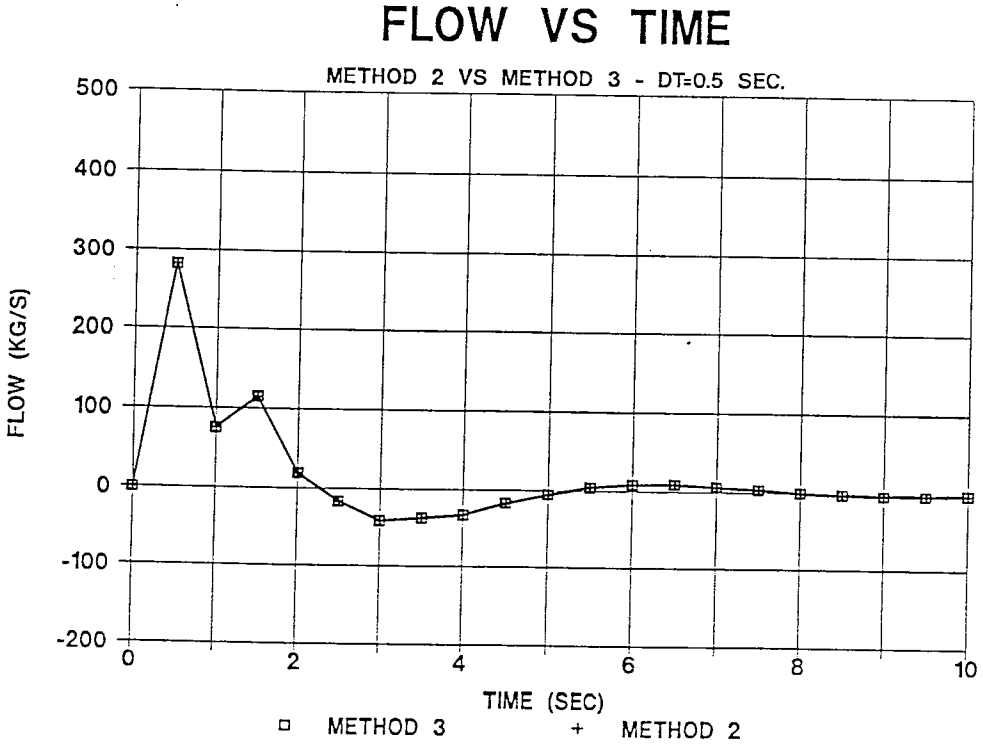

Figure 7. Method 2 vs. Method 3: Δt=0.5 sec.

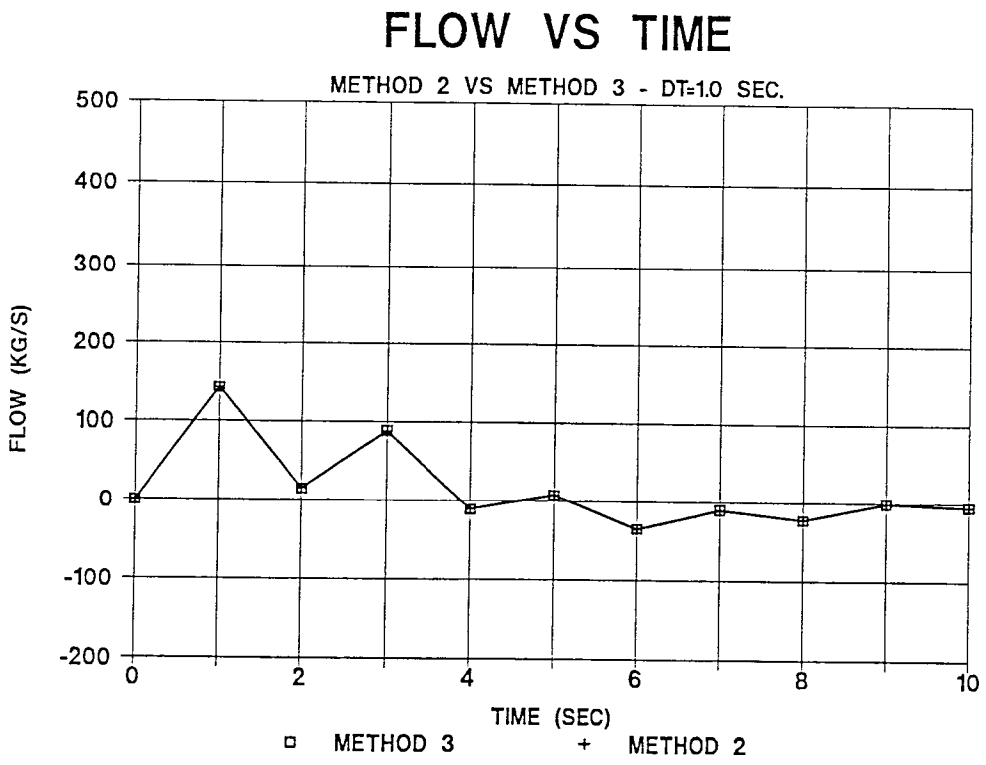

Figure 8. Method 2 vs. Method 3: Δt=1.0 sec.

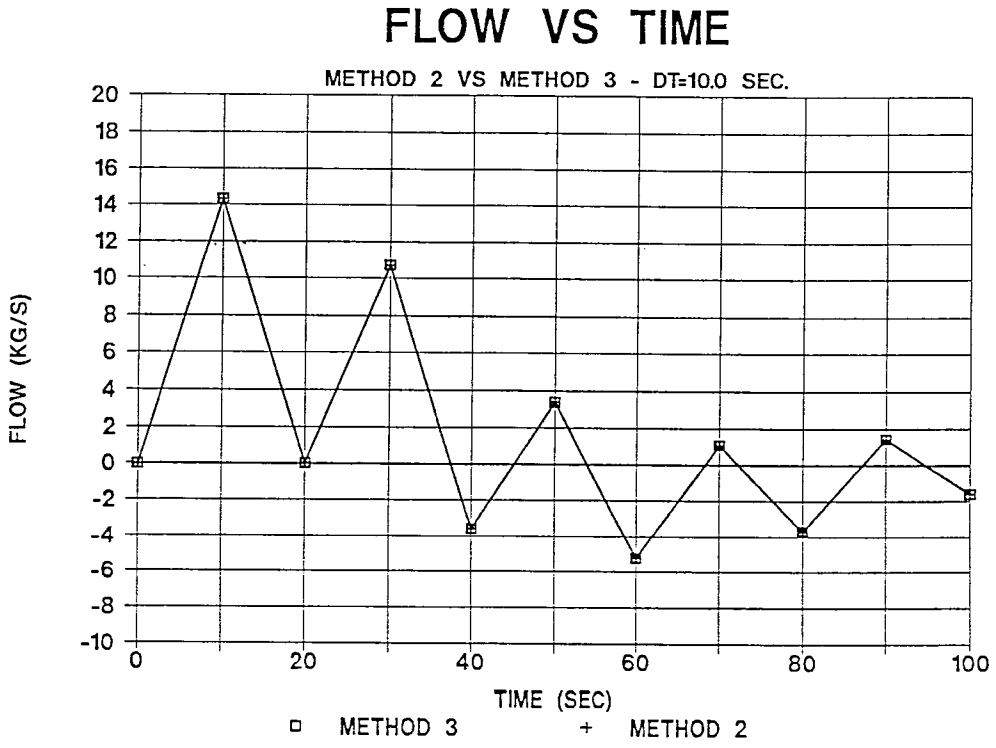

Figure 9. Method 2 vs. Method 3: Δt=10.0 sec.

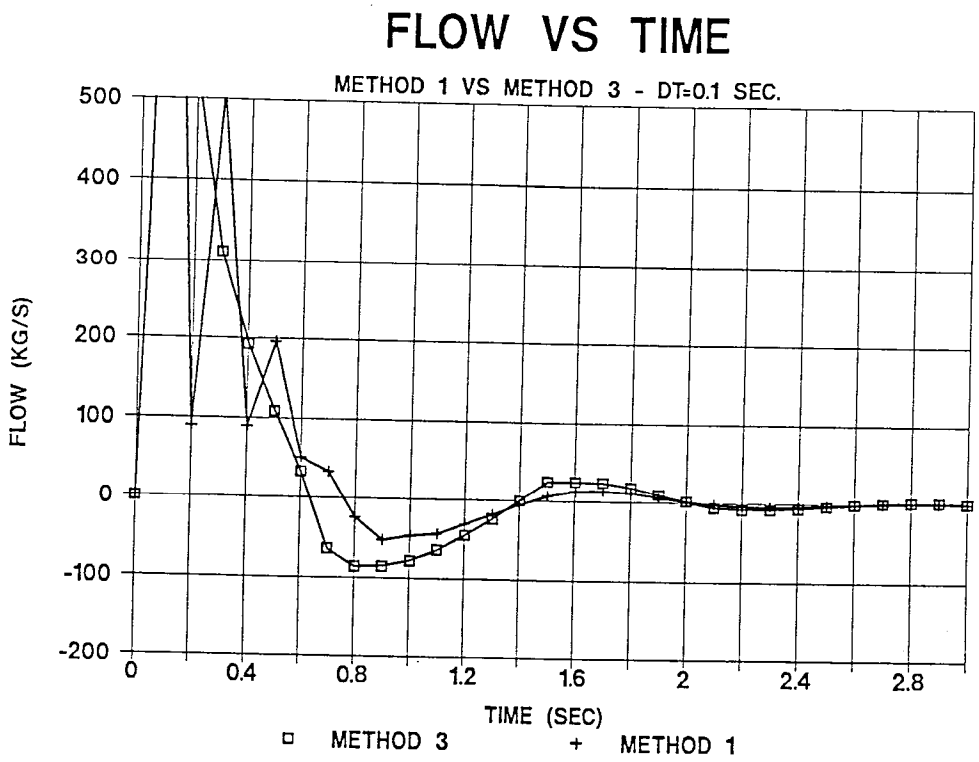

Figure 10. Method 1 vs. Method 3: Δt=0.1 sec.

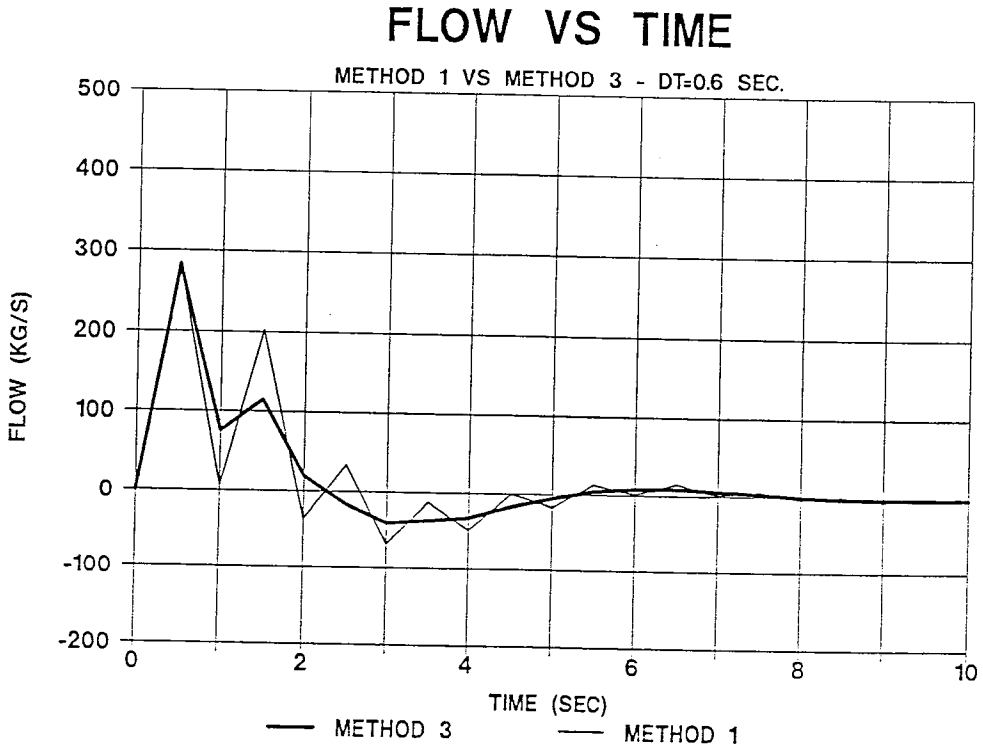

Figure 11. Method 1 vs. Method 3: Δt=0.5 sec.

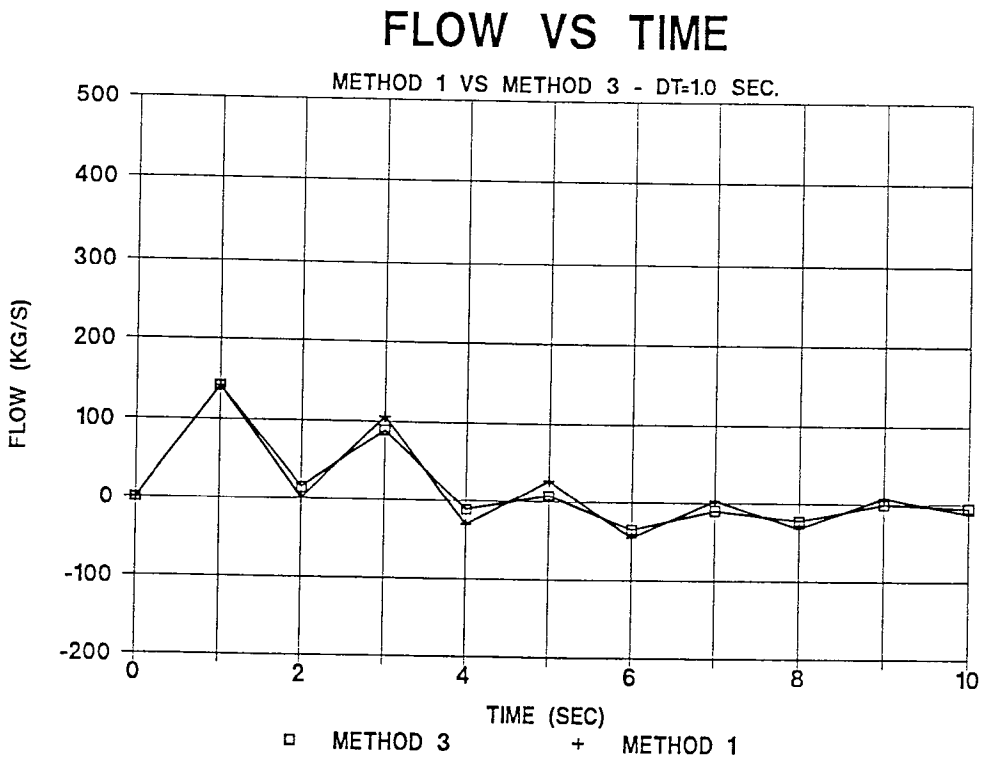

Figure 12. Method 1 vs. Method 3: Δt=1.0 sec.

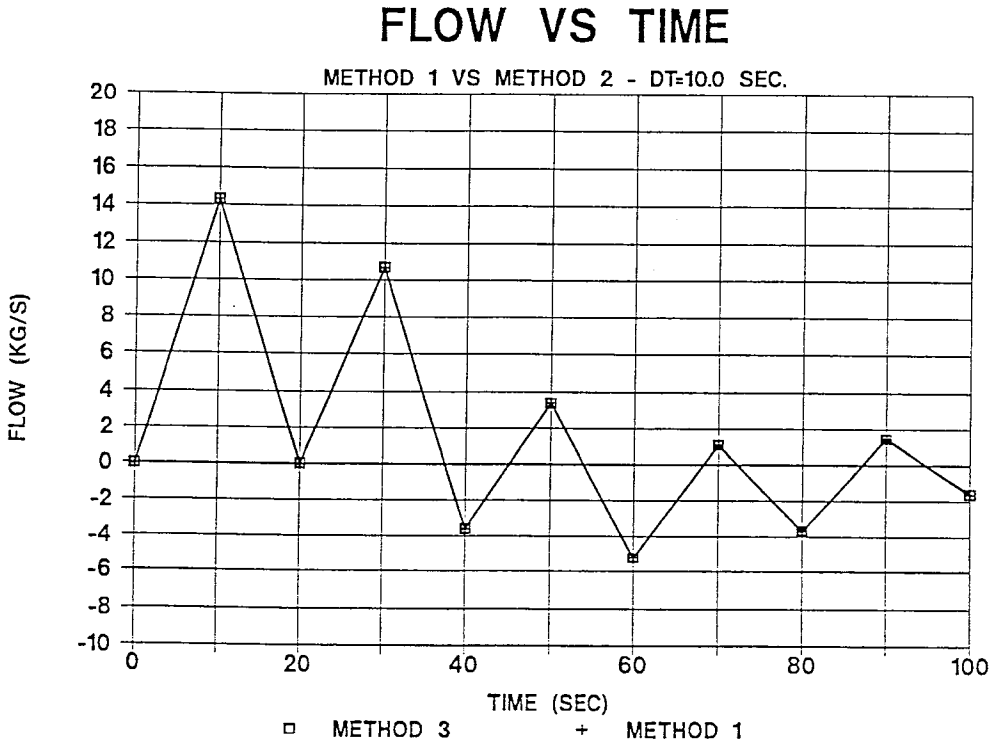

Figure 13. Method 1 vs. Method 3: Δt=10.0 sec.