

Implicit Function Theory Applications Part 0: Background and What We Can Do With It

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Introduction

I've developed a couple of analytical solutions for transient, compressible fluid flows that involve interactions with changes in the dimensions of the fluid container. The word pipe will almost always be used interchangeably with container in these notes.

Implicit function theory is the most critical aspect of getting the analytical solutions. In these notes I'll summarize the basis for implicit function theory and give some illustrative applications related to the analytical solutions.

Background

Let's say we have two functions that provide relationships between the quantities (Y_1, Y_2) as functions of (X_1, X_2) in the form

$$F(Y_1, Y_2; X_1, X_2) = 0 \tag{1.1}$$

and

$$G(Y_1, Y_2; X_1, X_2) = 0 \tag{1.2}$$

The notation is meant to convey the sense that both Y s are each a function of both X s.

The derivatives of Eqs. (1.1) and (1.2) with respect to X_1 , for example, are

$$\frac{\partial F}{\partial Y_1} \frac{\partial Y_1}{\partial X_1} + \frac{\partial F}{\partial Y_2} \frac{\partial Y_2}{\partial X_1} + \frac{\partial F}{\partial X_1} = 0$$

and (1.3)

$$\frac{\partial G}{\partial Y_1} \frac{\partial Y_1}{\partial X_1} + \frac{\partial G}{\partial Y_2} \frac{\partial Y_2}{\partial X_1} + \frac{\partial G}{\partial X_1} = 0$$

where each Y is taken to be a function of the X s. The derivatives with respect to X_2 are

$$\frac{\partial F}{\partial Y_1} \frac{\partial Y_1}{\partial X_2} + \frac{\partial F}{\partial Y_2} \frac{\partial Y_2}{\partial X_2} + \frac{\partial F}{\partial X_2} = 0$$

and

(1.4)

$$\frac{\partial G}{\partial Y_1} \frac{\partial Y_1}{\partial X_2} + \frac{\partial G}{\partial Y_2} \frac{\partial Y_2}{\partial X_2} + \frac{\partial G}{\partial X_2} = 0$$

Equations (1.3) are two equations for the two unknowns, $(\partial Y_1/\partial X_1)$ and $(\partial Y_2/\partial X_1)$ and likewise Eqs. (1.4) for $(\partial Y_1/\partial X_2)$ and $(\partial Y_2/\partial X_2)$.

The determinant of the coefficients to the unknowns

$$J = \begin{vmatrix} \frac{\partial F}{\partial Y_1} & \frac{\partial F}{\partial Y_2} \\ \frac{\partial G}{\partial Y_1} & \frac{\partial G}{\partial Y_2} \end{vmatrix}$$
(1.5)

That is, the Jacobian which is usually written

$$J = \frac{\partial(F, G)}{\partial(Y_1, Y_2)}$$
(1.6)

Applying the usual method for solving systems of linear equations, the solution for $(\partial Y_1/\partial X_1)$, for example, is

$$\left(\frac{\partial Y_1}{\partial X_1} \right)_{x_2} = -\frac{1}{J} \begin{vmatrix} \frac{\partial F}{\partial X_1} & \frac{\partial F}{\partial Y_2} \\ \frac{\partial G}{\partial X_1} & \frac{\partial G}{\partial Y_2} \end{vmatrix}$$
(1.7)

and the remaining three partial derivatives are solved by the same method. Recall that the RHS column is substituted for the column in the determinant for which the solution is sought.

As a general mnemonic device,

$$\left(\frac{\partial Y_i}{\partial X_j}\right)_{\dots} = -\frac{\frac{\partial(F_1, \dots, F_j, \dots)}{\partial(Y_1, \dots, X_j, \dots)}}{\frac{\partial(F_1, \dots, F_i, \dots)}{\partial(Y_1, \dots, X_i, \dots)}} \quad (1.8)$$

where the notation has been expanded to include any number of equations and unknowns, so long as these numbers are the same. The right-hand sides of Eqs. (1.3) and (1.4) are substituted into the column associated with the derivative of interest. The usual solution method for systems of algebraic equations.

Thermophysical Properties

The results in these notes can all be expressed in terms of some of the usual thermophysical material properties. These properties are derivatives of the thermodynamic state properties of the material, and thus they are second derivatives of the fundamental relation for the material. These properties are summarized in the following.

The *specific heat at constant volume* is

$$C_v = \left(\frac{\partial u}{\partial T}\right)_v \quad (1.9)$$

The *specific heat at constant pressure* is

$$C_p = \left(\frac{\partial h}{\partial T}\right)_p \quad (1.10)$$

The specific heats are related by

$$C_p = C_v + \frac{Tv\beta^2}{\kappa}$$

which is especially useful in the form (1.11)

$$\rho\kappa C_v = \rho\kappa C_p - T\beta^2$$

The *coefficient of isothermal compressibility* is

$$\kappa = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial P} \right)_T \quad (1.12)$$

The *coefficient of thermal expansion* is

$$\beta = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P \quad (1.13)$$

And the *coefficient of isentropic compressibility* is

$$\sigma_s = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial P} \right)_S \quad (1.14)$$

Finally, the *speed of sound* is

$$C_s^2 = \frac{C_p}{C_v \kappa \rho} \quad (1.15)$$

For an ideal gas the *specific internal energy* is

$$u = C_v T \quad (1.16)$$

the *enthalpy* is

$$h = C_p T \quad (1.17)$$

and

$$C_p = C_v + R_g \quad (1.18)$$

The ratio of specific heats is usually denoted

$$\gamma = \frac{C_p}{C_v} \quad (1.19)$$

Additionally, the above thermophysical properties are

$$\kappa = \frac{1}{P} \quad (1.20)$$

for the isothermal compressibility,

$$\beta = \frac{1}{T} \quad (1.21)$$

for the coefficient of thermal expansion,

$$\sigma_s = \gamma \frac{P}{\rho} \quad (1.22)$$

for the coefficient of isentropic compressibility, and the sound speed is

$$c_s^2 = \gamma R_g T \quad (1.23)$$

The Bridgman Method

P. W. Bridgman developed a simplified approach for expressing all derivatives of thermodynamic-state properties in terms of thermophysical properties of materials. In my opinion, the Wikipedia entry is correct and explains how Bridgman's very straightforward system works:

http://en.wikipedia.org/wiki/Bridgman's_thermodynamic_equations .

I have summarized results of his methodology in a nearby Table 1. Note that the entries above the diagonal are simply the negative of the corresponding entries below the diagonal; that is, $a_{ij} = -a_{ji}$. Additionally, one of these sets could be expressed in terms of the density, ρ , and the other in terms of the specific volume, v and reminding the user about the sign change. The Table is very handy when dealing with several aspect of equations of state.

I have uploaded the table as a PDF file and provided this URL link in my post:

<http://edaniel.files.wordpress.com/2011/01/testbridgmantable.pdf> . You'll have to copy-n-paste the link into your browser.

What can we do with it

So, now that we have the general idea, what can we do with it? One useful application is associated with solution methods for finite-difference approximations to partial differential equations as follows. For some solution methods, the FDEs for scalar properties, mass and energy, for examples, are based on solutions for the products of dependent variables and not an individual variable. This approach assists in preserving the conserved-property, property-flux characteristics of conservation equations.

As an example, a FDE approximation to an energy equation might be written so that the product ρe is the solution variable. For the case of two-phase flows, typical solution

methods might solve for the product $\alpha\rho$ from a continuity equation and $\alpha\rho e$ from an energy equation; α is the fraction of the control volume occupied by one of the phases or fluids. For more general mixtures, the product-variable approach expands to include several combinations of dependent variables; mixtures of gases and vapor along with liquid.

If then an iterative method is applied to solving the non-linear FDEs at a time level, and it is considered necessary that whenever possible analytical linearization of the EOS properties should be used in the Jacobian matrices, implicit function theory can be used to provide the EOS derivatives. The method provides also the various derivatives needed for iterative solution for non-linear EOS.

A very simple illustrative application is given in the following paragraphs. Consider the case in which the solution for the FDE approximations to the fundamental partial differential equations (PDEs) gives the products of the density and total internal energy content. That is

$$M = \rho V$$

and

$$E = Mu \tag{1.24}$$

The intensive microscopic density is not generally available as a function of the extensive macroscopic variables. That is, the density is generally available from an EOS like, for example

$$\rho = \hat{\rho}(P, T) \tag{1.25}$$

or

$$\rho = \hat{\rho}(P, h) \tag{1.26}$$

and not in the form

$$\rho = \hat{\rho}(M, E) \tag{1.27}$$

The specific example we consider here is for the pressure P and enthalpy h , with respect to the extensive macroscopic variables, M and E ; that is,

$$P = \hat{P}(M, E)$$

and

$$h = \hat{h}(M, E) \tag{1.28}$$

For this case, the latter can be written directly as

$$h = \frac{E}{M} + \frac{P}{\rho} \quad (1.29)$$

Setting two constraint functions, one for the mass and the other for the energy content

$$\begin{aligned} M - \hat{\rho}(P, h)V &= 0 \\ \text{and} & \\ E + PV - Mh &= 0 \end{aligned} \quad (1.30)$$

provides two implicit functions for the derivatives of the intensive microscopic EOS variables, P and h , with respect to the extensive macroscopic variables, M and E .

$$F_M(P, h; M, E) = 0 \quad (1.31)$$

and

$$F_E(P, h; M, E) = 0 \quad (1.32)$$

The Jacobian of Eq. (1.5) is

$$J = \begin{vmatrix} -\left(\frac{\kappa\rho C_v}{C_p} + \frac{\beta}{C_p}\right)V & \frac{\beta\rho}{C_p}V \\ V & -M \end{vmatrix} \quad (1.33)$$

which gives

$$J = MV \left(\frac{\kappa\rho C_v}{C_p} \right)$$

Continuing the procedure outlined previously above gives

$$\left(\frac{\partial P}{\partial M}\right)_E = \frac{1}{M} \frac{(C_p - \beta h)}{\kappa C_v}$$

$$\left(\frac{\partial P}{\partial E}\right)_M = \frac{1}{M} \frac{\beta}{\kappa C_v}$$
(1.34)

$$\left(\frac{\partial h}{\partial M}\right)_E = -\frac{h}{M} + \frac{1}{M} v \frac{(C_p - \beta h)}{\kappa C_v}$$

$$\left(\frac{\partial h}{\partial E}\right)_M = \frac{1}{M} + \frac{1}{M} v \frac{\beta}{\kappa C_v}$$

Note that the last two derivatives can be obtained directly from

$$h = \frac{E}{M} + \frac{1}{M} PV$$
(1.35)

and the first two of Eqs. (1.34). Finally, using the well-known inter-relationship

$$\frac{C_{sf}^2}{V} = \left(\frac{\partial P}{\partial M}\right)_E + h \left(\frac{\partial P}{\partial E}\right)_M$$
(1.36)

where C_{sf}^2 is the square of the fluid sound speed, gives

$$\frac{C_{sf}^2}{V} = \frac{1}{V} \frac{C_p}{\kappa \rho C_v}$$
(1.37)

All the above results are easily verified by taking the fluid to be an ideal gas with constant specific heats and the temperature, T in place of the enthalpy, h

$$h = C_p T$$

and

(1.38)

$$E = MC_v T$$

with

$$PV = MR_g T$$
(1.39)

The process above will give

$$\left(\frac{\partial P}{\partial M}\right)_E = 0$$

and

$$\left(\frac{\partial P}{\partial E}\right)_M = \frac{1}{V}(\gamma - 1) \tag{1.40}$$

Equations (1.40) can be obtained directly from the appropriate form of Eq. (1.39) while using Eq. (1.38). The fluid sound speed, Eq. (1.37) will be found to be

$$\frac{C_{sf}^2}{V} = \frac{1}{V} \gamma R_g T \tag{1.41}$$

Note that all aspects of the procedure are valid for the case of the volume of the fluid being a variable given by any function of any of the intensive or extensive fluid properties.

(As an aside, given the EOS of Eq. (1.39) and the thermal equation of state, Eq. (1.38) and allowing the volume, V , to be variable, and given no other additional information, what are the valid values that the volume can take on?)

The complete results for this case are summarized in the nearby Table 2.

With respect to		
With Derivative of	M	E
P	$\frac{C_{sf}^2}{V} \left(1 - \frac{h\beta}{C_p}\right)$	$\frac{C_{sf}^2}{V} \frac{\beta}{C_p}$
v	$-\frac{V}{M^2} = -\frac{v}{M}$	0
T	$\frac{1}{C_p}(\beta T - 1) \left(\frac{\partial P}{\partial M}\right)_E + \frac{1}{C_p} \left(\frac{\partial h}{\partial M}\right)_E$	$\frac{v}{C_p}(\beta T - 1) \left(\frac{\partial P}{\partial E}\right)_M + \frac{1}{C_p} \left(\frac{\partial h}{\partial E}\right)_M$
		$\frac{1}{MC_p} \left[1 + C_{sf}^2 \frac{T\beta^2}{C_p}\right]$
u	$-\frac{E}{M^2} = -\frac{u}{M}$	$\frac{1}{M}$

h	$-\frac{h}{M} + \frac{C_{sf}^2}{M}(1 - h\beta / C_p)$	$\frac{1}{M} + \frac{C_{sf}^2}{M} \frac{\beta}{C_p}$
s	$-\frac{v}{T} \left(\frac{\partial P}{\partial M} \right)_E + \frac{1}{T} \left(\frac{\partial h}{\partial M} \right)_E = -\frac{h}{MT}$	$-\frac{v}{T} \left(\frac{\partial P}{\partial E} \right)_M + \frac{1}{T} \left(\frac{\partial h}{\partial E} \right)_M = \frac{1}{MT}$
D	$\frac{M^2 v^2}{C_{sf}^2} = \frac{V^2}{C_{sf}^2}$	

Table 2. Derivatives of equation of state properties with respect to mass and energy content; rigid volume.

Note that there's a vacant cell in that Table. I have not yet been successful in arriving at a good reduction of the results in the cell above. Additionally, I have not reduced the entries for the entropy.

Another Example

Let's say we have a two-fluid model of a two-phase flow. Where two-fluid model means there are model equations for mass, momentum, and energy for each phase or fluid in the flow field. Basically, this allows each phase or fluid to have different flow speeds and temperature; there can be both mechanical (fluid velocity) and thermal (temperature differences) dis-equilibrium in the flow. An example would be the simultaneous flow of subcooled liquid water along with, say, air at a higher temperature. Let's also take the case that the saturation state of the liquid water might be attained, so we can't use the pressure, P , and temperature, T , as independent variables for the EOS. Instead, we'll use the pressure, P , and enthalpy, h , as independent variables in the EOS. Any other two thermodynamically independent properties could be used.

Typical solution variables for this case might be the products of the volume fraction and density, and the volume fraction and density and specific internal energy;

$$\overline{\alpha \rho} \tag{1.42}$$

and

$$\overline{\alpha \rho u} \tag{1.43}$$

for examples, where u is the specific internal energy, ρ is the density, and α is the fraction of the control volume occupied by, usually, the less dense phase or fluid.

Numerical solution methods frequently require linearization of fluid thermodynamic state properties in terms of the solution variables. For example, an approximation for a phase or fluid temperature at the new-time level might be needed. This temperature is not available as a function of the macroscopic properties above, but instead might be

available as a function of the pressure and enthalpy, or Implicit function theory can be used to get these derivatives as outlined in the following paragraphs.

The implicit dependency is

$$\mathfrak{F}_i(P, \alpha, h_g, h_l; M_g, M_l, E_g, E_l) = 0 \quad (i = 1, \dots, 4) \quad (1.44)$$

Other combinations of the mass and energy content can be used. The mass of the mixture and the energy of the mixture, for example, could be substituted for a phase or fluid equation.

The four functions that can be used to obtain the derivatives are

$$\begin{aligned} M_g \hat{v}_g(P, h_g) - \alpha V &= 0 \\ M_l \hat{v}_l(P, h_l) - (1 - \alpha)V &= 0 \\ E_g + \alpha PV - M_g h_g &= 0 \\ E_l + (1 - \alpha)PV - M_l h_l &= 0 \end{aligned} \quad (1.45)$$

where the functions have been multiplied through by the volume, V , as a small generalization. Note that I have used subscripts 'g' and 'l' which usually stand for gas, or vapor, and liquid, respectively. The void fraction, α , is associated with the phase or fluid represented by 'g'.

I get the determinant of the Jacobian

$$J = \frac{\partial(F_1, F_2, F_3, F_4)}{\partial(P, \alpha, h_g, h_l)} \quad (1.46)$$

to be

$$J = -\frac{C_{vg} K_g}{C_{pg}} M_g^2 M_l v_g V \left[1 - \frac{\beta_l P}{\rho_l C_{pl}} \right] - \frac{C_{vl} K_l}{C_{pl}} M_l^2 M_g v_l V \left[1 - \frac{\beta_g P}{\rho_g C_{pg}} \right] \quad (1.47)$$

which can be written in several other forms. An instructive form is

$$J = -M_g M_l V \left\{ M_g \frac{v_g^2}{C_{sg}^2} \left[1 - \frac{\beta_l P}{\rho_l C_{pl}} \right] + M_l \frac{v_l^2}{C_{sl}^2} \left[1 - \frac{\beta_g P}{\rho_g C_{pg}} \right] \right\} \quad (1.48)$$

[I have a career-long dis-function when signs are involved. Someone should verify this result. The process is straightforward algebra, but tedious to the extreme.]

The right-hand side of Eq. (1.48) can be viewed as an effective sound speed for the mixture

$$\frac{V}{C_{seff}^2} = M_g M_l V \left\{ M_g \frac{v_g^2}{C_{sg}^2} \left[1 - \frac{\beta_l P}{\rho_l C_{pl}} \right] + M_l \frac{v_l^2}{C_{sl}^2} \left[1 - \frac{\beta_g P}{\rho_g C_{pg}} \right] \right\} \quad (1.49)$$

and the equation can be written

$$J = -\frac{V}{C_{seff}^2} \quad (1.50)$$

The derivative of the pressure with respect to the mass content of phase or fluid M_g , as noted previously above, is

$$\left(\frac{\partial P}{\partial M_g} \right)_{\dots} = -\frac{1}{J} \frac{\partial (F_1, F_2, F_3, F_4)}{\partial (M_g, \alpha, h_g, h_l)} \quad (1.51)$$

and likewise for all the other partial derivatives.

The results from the procedure for the derivatives of the pressure and volume fraction are summarized in the nearby Table 3. Note that subscripts '1' and '2' are used in place of 'g' and 'l', respectively.

∂ of	with respect to	
	\mathbf{M}_1	\mathbf{E}_1
\mathbf{P}	$\frac{1}{D} \alpha M_2 V^2 \left(1 - \frac{\beta_1 h_1}{C_{p1}} \right) \left(1 - P \frac{\beta_2 v_2}{C_{p2}} \right)$	$\frac{1}{D} \alpha M_2 V^2 \frac{\beta_1}{C_{p1}} \left(1 - P \frac{\beta_2 v_2}{C_{p2}} \right)$
	\mathbf{M}_2	\mathbf{E}_2
	$\frac{1}{D} (1 - \alpha) M_1 V^2 \left(1 - \frac{\beta_2 h_2}{C_{p2}} \right) \left(1 - P \frac{\beta_1 v_1}{C_{p1}} \right)$	$\frac{1}{D} (1 - \alpha) M_1 V^2 \frac{\beta_2}{C_{p2}} \left(1 - P \frac{\beta_1 v_1}{C_{p1}} \right)$
α	\mathbf{M}_1	\mathbf{E}_1
	$\frac{1}{D} \frac{1}{C_{s2}^2} \frac{\alpha^2 (1 - \alpha)^2}{v_1} V^4 \left(1 - \frac{\beta_1 h_1}{C_{p1}} \right)$	$\frac{1}{D} \frac{1}{C_{s2}^2} M_1 (1 - \alpha)^2 V^2 \frac{\beta_1 v_1}{C_{p1}}$
	\mathbf{M}_2	\mathbf{E}_2

	$\frac{1}{D} \frac{1}{C_{s1}^2} \frac{\alpha^2 (1-\alpha)^2}{v_2} V^4 \left(1 - \frac{\beta_2 h_2}{C_{p2}} \right)$	$\frac{1}{D} \frac{1}{C_{s1}^2} M_2 \alpha^2 V^2 \frac{\beta_2 v_2}{C_{p2}}$
D	$-M_1 M_2 V \left[M_1 \frac{v_1^2}{C_{s1}^2} \left(1 - P \frac{\beta_2 v_2}{C_{p2}} \right) + M_2 \frac{v_2^2}{C_{s2}^2} \left(1 - P \frac{\beta_1 v_1}{C_{p1}} \right) \right]$	

Table 3. Derivatives of pressure and void fraction with respect to mass and energy content; two-region non-equilibrium case.

The partial derivatives of other intensive thermodynamic state properties can be obtained by application of the procedure, or as follows. The temperature of phase or fluid ‘g’ for example is

$$T_g = \hat{T}_g(P, h_g) \quad (1.52)$$

where

$$h_g = \frac{E_g}{M_g} + \alpha P V \quad (1.53)$$

For example, one of the derivatives of the temperature is

$$\left(\frac{\partial}{\partial M_g} T_g \right)_{\dots} = \left(\frac{\partial}{\partial P} \hat{T}_g \right)_{hg} \left(\frac{\partial P}{\partial M_g} \right)_{\dots} + \left(\frac{\partial}{\partial h_g} \hat{T}_g \right)_P \left(\frac{\partial}{\partial M_g} h_g \right)_{\dots} \quad (1.54)$$

where

$$\left(\frac{\partial}{\partial P} \hat{T}_g \right)_{hg} = -\frac{1}{\rho_g C_{pg}} (1 - \beta_g T_g) \quad (1.55)$$

and

$$\left(\frac{\partial}{\partial h_g} \hat{T}_g \right)_P = \frac{1}{C_{pg}}$$

and

$$\left(\frac{\partial}{\partial M_g} h_g \right)_{\dots} = -\frac{E_g}{M_g^2} + \alpha V \left(\frac{\partial P}{\partial M_g} \right)_{\dots} + PV \left(\frac{\partial \alpha}{\partial M_g} \right)_{\dots} \quad (1.56)$$

And, of course, all other derivative of the enthalpy can be obtained by the same way. As you can see, the number of terms in the equations can get to be frighteningly large.

And so it goes.

If the mass, M , and energy content, E , are the chosen dependent variables in the model equation system, and the thermodynamic state properties are available as function of the density, ρ , and specific internal energy, u , these can be directly determined from the solution variables by use of

$$\rho = \frac{M}{V} \quad (1.57)$$

and

$$u = \frac{E}{M} \quad (1.58)$$

The EOS for an ideal gas, as discussed previously above, is an example. And at the same time the simple form of the ideal gas EOS allows for writing the equation directly in terms of mass and energy content.

Single-Phase Fluid States

For the case of single-phase fluids, again with pressure and enthalpy as independent thermodynamic variables for the EOS, we write

$$M \hat{v}(P, h) - V = 0$$

and

$$E + PV - Mh = 0 \quad (1.59)$$

If anyone is interested in how to handle saturation states just let me know and I'll whip them out.

Independent variables pressure and temperature can also be used. The functions the are

$$\begin{aligned}
M\hat{v}(P,T) - V &= 0 \\
\text{and} \\
E - M\hat{u}(P,T) &= 0
\end{aligned}
\tag{1.60}$$

Application of the procedure to these is left as an exercise for the interested reader.

This ends the discussions about using implicit function theory to obtain partial derivatives of intensive thermodynamic state properties with respect to macroscopic extensive properties.

We could equally use the following formulation.

$$\begin{aligned}
\hat{v}(P,T) - \frac{V}{M} &= 0 \\
\text{and} \\
E + PV - M\hat{h}(P,T) &= 0
\end{aligned}
\tag{1.61}$$

The determinant is then

$$J = MC_v\kappa v \tag{1.62}$$

and

$$\begin{aligned}
\left(\frac{\partial P}{\partial M}\right)_E &= \frac{1}{MC_v\kappa}(C_p - h\beta) \\
\left(\frac{\partial P}{\partial E}\right)_M &= \frac{\beta}{MC_v\kappa} \\
\left(\frac{\partial T}{\partial M}\right)_E &= \frac{1}{MC_v\kappa}(v\beta T - h\kappa)
\end{aligned}
\tag{1.63}$$

and

$$\left(\frac{\partial T}{\partial E}\right)_M = \frac{1}{MC_v}$$

All other partial derivatives are easily obtained.

EOS Solution Methods

Another application of implicit function theory is to numerical solution methods for non-linear equation of state formulations; that includes almost all EOSs of interest. Let's say at the end of a time step the EOS has to be updated to get the new-time-level values for the thermodynamic-state properties. The iterative Newton-Raphson method is a typical numerical solution method for non-linear equations. To apply the method to an example already considered previously above, take the case of Eqs. (1.59) and now we need to find the pressure and enthalpy at the new-time level, (n+1). As a first step, we can get the first guess by use of, for the pressure

$$\tilde{P}^{n+1} = P^n + \left(\frac{\partial P}{\partial M} \right)_E^n (\Delta M)^{n+1} + \left(\frac{\partial P}{\partial E} \right)_M^n (\Delta E)^{n+1} \quad (1.64)$$

where the delta-mass and energy are the change in the mass and energy content over the just-finished time advancement. All the variables can be extrapolated this way. And can be applied to whatever the combination of fluid-flow model and EOS and solution variables.

Then, applying the usual linearization procedure to Eqs. (1.59) gives

$$M \left(\frac{\partial \hat{v}}{\partial P} \right)_T (\Delta P)^{k+1} + M \left(\frac{\partial \hat{v}}{\partial T} \right)_P (\Delta T)^{k+1} = -F_1^k(P, T)$$

and

$$-M \left(\frac{\partial \hat{u}}{\partial P} \right)_T (\Delta P)^{k+1} - M \left(\frac{\partial \hat{u}}{\partial T} \right)_P (\Delta T)^{k+1} = -F_2^k(P, T) \quad (1.65)$$

where the extrapolated values are used for the initial evaluation of the functions. The derivatives of the thermodynamic-state properties can be expressed in terms of the state and thermo-physical properties for the material.

Note that extrapolations like Eq. (1.64) can be used to approximate the change in solution variables expected to occur over a time step. In this way, for example, the effects of changes in the thermodynamic state of the fluid can be factored into the numerical solution method applied to the basic fluid-flow equations.

Implicit Coupling of Conduction and Convection Energy Exchange

An example of application of implicit function theory methodology to numerical solution methods is developed in the following paragraphs. Consider the lumped-parameter modeling of energy exchange between a solid material and a fluid. For the example, spatial variations will be neglected and only changes with time will be considered. An energy equation balance for the fluid is

$$\frac{d}{dt}E_f = h_c A_w (T_w - T_f) \quad (1.66)$$

and for the solid

$$M_m C_{pm} \frac{d}{dt}T_m = h_c A_w (T_f - T_m) \quad (1.67)$$

where we'll take the energy content of the fluid to be

$$E_f = \rho h \quad (1.68)$$

which will be the solution variable. The EOS for the fluid will be assumed to be available with the pressure and enthalpy as independent thermodynamic properties. But for this example the dependency on pressure will be neglected. Then we can write

$$T_f = \hat{T}_f(h) \quad (1.69)$$

Straightforward discrete approximations for Eqs. (1.66) and (1.67) are

$$(\Delta E_f)^{n+1} = (\Delta t) h_c A_w (T_m^{n+1} - T_f^{n+1})$$

and

$$(\Delta T_m)^{n+1} = (\Delta t) \frac{h_c A_w}{M_m C_{pm}} (T_f^{n+1} - T_m^{n+1}) \quad (1.70)$$

which can be written

$$(1 + \hat{H}_{cm})(\Delta T_m)^{n+1} - \hat{H}_{cm}(\Delta T_f)^{n+1} = -(\Delta t)(RHST_m)^n$$

Expanding the fluid temperature in a Taylor series gives

$$T_f^{n+1} = T_f^n + \left(\frac{\partial T_f}{\partial E_f} \right)^n (\Delta E_f)^{n+1} + \dots \quad (1.71)$$

and the first of Eqs. (1.70) becomes

$$\left[1 + (\Delta t) h_c A_w \left(\frac{\partial T_f}{\partial E_f} \right) \right] (\Delta E_f)^{n+1} - (\Delta t) h_c A_w (\Delta T_m)^{n+1} \quad (1.72)$$

$$= -(\Delta t) (RHSE_f)^n$$

where the derivative of the fluid temperature is obtained by use of implicit function theory as developed above in these notes.

Putting the fluid temperature expansion of Eq. (1.71) into the third of Eqs. (1.70) will give an equation for the change in the metal temperature in terms of the change in the fluid energy content. That equation is then put into Eq. (1.72) to get an equation for the change in the fluid energy. That is, the metal temperature has been eliminated from the fluid energy equation and the fluid-metal energy exchange is handled at the new-time level in both equations.

This approach can be generalized to various geometrical configurations of fluid energy equations and conduction heat transfer in solid materials. The parabolic nature of the heat conduction equation presents some interesting problems relative to treatment of boundary conditions; the existence of all boundaries is known to a given boundary all time.

Variable Fluid Control Volume

Let's next consider a case for which the volume is not constant but instead is a function of the pressure difference across the container walls. Again we'll use a straight constant-diameter pipe for convenience in word processing. At least two configurations are of interest; the first being a constant pressure condition outside the pipe and the second being a variable pressure on the outside.

The coupling between the fluid and the pipe wall is contained in the wall function

$$V(t) = V(0) + K_{wp} [P(t) - P(0)] \quad (1.73)$$

where K_{wp} represents the geometric details of the pipe wall and the pipe support method. For the case of pure radial deformation of the pipe wall with rigid constraints in the lateral direction, one form is

$$K_{wp} = \frac{\pi}{4} D^2 (\Delta z) \left(\frac{1 - \mu^2}{E} \right) \left(\frac{D}{t} \right) \quad (1.74)$$

D = pipe diameter

Δz = pipe length

μ = one of those strain ratios

E = modulus of elasticity for the pipe metal
 \bar{t} = pipe wall thickness.

If the pressure state on the other side of the pipe wall can change, the wall function becomes

$$V_k(t) = V_k(0) + K_{wp} \left\{ [P_k(t) - P_k(0)] - [P_z(t) - P_z(0)] \right\} \quad (1.75)$$

for volume 'k', and

$$V_z(t) = V_z(0) + K_{wp} \left\{ [P_z(t) - P_z(0)] - [P_k(t) - P_k(0)] \right\} \quad (1.76)$$

for volume 'z', where the subscripts 'k' and 'z' identify the two sides of the wall. We'll consider the first case in detail in the following paragraphs.

Because we have used pressure and enthalpy as independent variables for microscopic thermodynamic state properties, we'll use them again. The mass and energy functions to be used with implicit function theory, Eqs. (1.59), are repeated here

$$F_M(P, h; M, E) = M \hat{v}(P, h) - V(P) = 0$$

and

$$F_E(P, h; M, E) = E + PV(P) - Mh = 0 \quad (1.77)$$

where the volume is shown to be a function of the internal fluid pressure for the volume. The derivatives that go into the Jacobian are

$$\frac{\partial F_M}{\partial P} = M \left(\frac{\partial v}{\partial P} \right)_h - \frac{dV}{dP}$$

$$\frac{\partial F_M}{\partial h} = M \left(\frac{\partial v}{\partial h} \right)_P$$

$$\frac{\partial F_E}{\partial P} = V + P \frac{dV}{dP}$$

$$\frac{\partial F_E}{\partial h} = -M \quad (1.78)$$

and the determinant of the Jacobian is

$$D = \frac{V^2}{C_{sf}^2} + K_{wp} M \left(1 - P \frac{v\beta}{C_p} \right) \quad (1.79)$$

where K_{wp} is the change in the volume enclosed by the wall as the internal pressure changes as given by Eq. (1.74).

Equation (1.79) can be written

$$\frac{V^2}{C_{eff}^2} = \frac{V^2}{C_{sf}^2} + K_{wp}M \left(1 - P \frac{v\beta}{C_p} \right) \quad (1.80)$$

an effective pressure-wave propagation speed for the fluid-wall combination.

Proceeding as above for the single-phase fluid case, the remainder of the derivatives of the intensive thermodynamic properties with respect to the macro extensive properties are summarized in the nearby Table 4.

Derivative of	with respect to	
	M	E
P	$\frac{C_{eff}^2}{V} \left(1 - \frac{h\beta}{C_p} \right)$	$\frac{C_{eff}^2}{V} \frac{\beta}{C_p}$
v	$-\frac{V}{M^2} = -\frac{v}{M}$	0
T	$\frac{1}{C_p}(\beta T - 1) \left(\frac{\partial P}{\partial M} \right)_E + \frac{1}{C_p} \left(\frac{\partial h}{\partial M} \right)_E$	$\frac{v}{C_p}(\beta T - 1) \left(\frac{\partial P}{\partial E} \right)_M + \frac{1}{C_p} \left(\frac{\partial h}{\partial E} \right)_M$
		$\frac{1}{MC_p} \left[1 + C_{eff}^2 \frac{T\beta^2}{C_p} \right]$
u	$-\frac{E}{M^2} = -\frac{u}{M}$	$\frac{1}{M}$

h	$-\frac{h}{M} + \frac{C_{eff}^2}{M}(1 - h\beta / C_p)$	$\frac{1}{M} + \frac{C_{eff}^2}{M} \frac{\beta}{C_p}$
s	$-\frac{v}{T} \left(\frac{\partial P}{\partial M} \right)_E + \frac{1}{T} \left(\frac{\partial h}{\partial M} \right)_E = -\frac{h}{MT}$	$-\frac{v}{T} \left(\frac{\partial P}{\partial E} \right)_M + \frac{1}{T} \left(\frac{\partial h}{\partial E} \right)_M = \frac{1}{MT}$
D	$\frac{M^2 v^2}{C_{sf}^2} + MK_w \left(1 - P \frac{v\beta}{C_p} \right) = \left(\frac{V}{C_{eff}} \right)^2$	

Table 4. Derivatives of equation of state properties with respect to mass and energy content; flexible volume.

Note that there's a vacant cell in that Table. I have not yet been successful in arriving at a good reduction of the results in the cell above. Additionally, I have not reduced the entries for the entropy.

The analysis method can accommodate any description of the fluid flow. For the two-phase or -fluid, approach as given by Eqs. (1.44), the only change is that the volume is a function of the pressure. The additional equation required by the additional unknown, just as directly above, is the wall function.

Two-Sided Wall

If the pressure state on the other side of the pipe wall can change, the wall function is Eq. (1.75) and the volume occupied by the fluid is a function of the pressure on both sides of the wall. The fluid state in each volume is a function of the fluid state of both the volumes. The general form of the constraint functions is now

$$\mathfrak{S}_i(P_k, h_k, P_z, h_z; M_k, E_k, M_z, E_z) = 0 \quad (i = 1, \dots, 4) \quad (1.81)$$

The explicit form of these is easily obtained directly from Eqs. (1.77). An example is

$$F_{Mk}(P_k, h_k, P_z, h_z; M_k, E_k, M_z, E_z) = M_k \hat{v}_k(P_k, h_k) - V_k(P_k, P_z) = 0 \quad (1.82)$$

for mass content in volume 'k', and

$$F_{Ez}(P_k, h_k, P_z, h_z; M_k, E_k, M_z, E_z) = E_z + P_z V(P_k, P_z) - M_z h_z = 0 \quad (1.83)$$

for energy content for volume 'z'. And etc.

The wall function of Eq. (1.76) will give four derivatives of the volumes with respect to the pressure, noting that each volume is a function of both pressures. These derivatives are

$$V'_{kk} = \frac{\partial V_k}{\partial P_k}, \quad V'_{kz} = \frac{\partial V_k}{\partial P_z} \quad (1.84)$$

for volume K , and

$$V'_{zk} = \frac{\partial V_z}{\partial P_k}, \quad V'_{zz} = \frac{\partial V_z}{\partial P_z} \quad (1.85)$$

for volume Z .

Note that the derivatives satisfy the following conditions

$$\begin{aligned} \frac{\partial V_k}{\partial P_k} &= -\frac{\partial V_z}{\partial P_k} \\ \frac{\partial V_k}{\partial P_z} &= -\frac{\partial V_z}{\partial P_k} \end{aligned} \quad (1.86)$$

and that all these derivatives reduce to either $+K_{wp}$ or $-K_{wp}$.

By this point, everyone should know the drill for applying implicit function theory. I'll just note that we'll need 16 derivatives for each matrix and that that is lots o' algebra; straightforward but tedious algebra.

The results are summarized in a nearby Table 5 for a limited number of the derivatives.

∂ of	with respect to	
	\mathbf{M}_K	\mathbf{E}_K
\mathbf{P}_K	$\frac{1}{D} \left(1 - \frac{h_k \beta_k}{C_{pk}} \right) \left\{ \frac{V_z^2}{C_{sz}^2} v_z + K_w M_z V_k \left(1 - P_z \frac{v_z \beta_z}{C_{pz}} \right) \right\}$	$\frac{1}{D} \left[\left(M_k \frac{\beta_k v_k}{C_{pk}} \right) \frac{V_z^2}{C_{sz}^2} + K_w M_z \left(1 - P_z \frac{\beta_z v_z}{C_{pz}} \right) \right]$
	$\frac{1}{D} K_w M_k V_z \left(1 - \frac{\beta_z h_z}{C_{pz}} \right) \left(1 - P_k \frac{\beta_k v_k}{C_{pk}} \right)$	$\frac{1}{D} \left(K_w M_k M_z \frac{\beta_z v_z}{C_{pz}} \right) \left(1 - P_k \frac{\beta_k v_k}{C_{pk}} \right)$
\mathbf{P}_Z	\mathbf{M}_K	\mathbf{E}_K

	$\frac{1}{D} K_w M_z V_k \left(1 - \frac{\beta_k h_k}{C_{pk}}\right) \left(1 - P_z \frac{\beta_z v_z}{C_{pz}}\right)$	$\frac{1}{D} \left(K_w M_k M_z \frac{\beta_k v_k}{C_{pk}} \right) \left(1 - P_z \frac{\beta_z v_z}{C_{pz}}\right)$
	M_Z	E_Z
	$\frac{1}{D} \left(1 - \frac{h_z \beta_z}{C_{pz}}\right) \left[\frac{V_k^2}{C_{sk}^2} M_z + K_w M_k V_z \left(1 - P_k \frac{v_k \beta_k}{C_{pk}}\right) \right]$	$\frac{1}{D} \left[\left(M_z \frac{\beta_z v_z}{C_{pz}} \right) \frac{V_k^2}{C_{sk}^2} + K_w M_k \left(1 - P_k \frac{\beta_k v_k}{C_{pk}}\right) \right]$
D	$\frac{V_k^2 V_z^2}{C_{sk}^2 C_{sz}^2} + K_w \left[M_z \frac{V_k^2}{C_{sk}^2} \left(1 - P_z \frac{\beta_z v_z}{C_{pz}}\right) + M_k \frac{V_z^2}{C_{sz}^2} \left(1 - P_k \frac{\beta_k v_k}{C_{pk}}\right) \right]$	

Table 5. Derivatives of equation of state properties with respect to mass and energy content for two flexible wall case.

Maybe someday I'll get around to doing all the derivatives for all the models an all dependent variables for numerical solution methods and all the different forms of the constraint functions. By the latter I mean that the mass and energy functions can be written as

$$\begin{aligned}
F_{Mk} &= \hat{v}_k(P_k, h_k) - \frac{1}{M_k} V_k(P_k, P_z) \\
F_{Ek} &= M_k h_k - P_k V_k(P_k, P_z) - E_k \\
F_{Mz} &= v_z(P_z, h_z) - \frac{1}{M_z} V_z(P_k, P_z) \\
F_{Ez} &= M_z h_z - P_z V_z(P_k, P_z) - E_z
\end{aligned} \tag{1.87}$$

Finally, note in passing that a two-fluid formulation will require four functions for each coupled volumes and that leads to 64 entries in all matrices. Those are some bad matrices.

Conclusions

Implicit function theory is your friend.

