The matrix of coefficients on the right hand sides is to be inverted. The determinant of the matrix is the Jacobian of volume and internal energy with respect to pressure and temperature at constant composition. The elements of the inverse matrix may be found using properties of Jacobians.[26] Let J be the Jacobian

$$J = \frac{\partial(V,E)}{\partial(P,T)_x} \tag{4.44}$$

Then

$$\left(\frac{\partial P}{\partial V}\right)_{E,x} = \left(\frac{\partial E}{\partial T}\right)_{P,x} \Big/ J \tag{4.45}$$

$$\left(\frac{\partial P}{\partial E}\right)_{V,x} = -\left(\frac{\partial V}{\partial T}\right)_{P,x} \Big/ J \tag{4.46}$$

$$\left(\frac{\partial T}{\partial V}\right)_{E,x} = -\left(\frac{\partial E}{\partial P}\right)_{T,x} \Big/ J \tag{4.47}$$

$$\left(\frac{\partial T}{\partial E}\right)_{V,x} = \left(\frac{\partial V}{\partial P}\right)_{T,x} \Big/ J\ . \tag{4.48}$$

The solution for dP and dT is

$$dP = \left(\frac{\partial P}{\partial V}\right)_{E,x} dV_x + \left(\frac{\partial P}{\partial E}\right)_{V,x} dE_x \tag{4.49}$$

$$dT = \left(\frac{\partial T}{\partial V}\right)_{E,x} dV_x + \left(\frac{\partial T}{\partial E}\right)_{V,x} dE_x . \tag{4.50}$$

This solution for dP and dT is a subset of the solution of three simultaneous equations indicated by Eq. (4.39), if dx is determined from those equations. For arbitrary dx, Eqs. (4.49) and (4.50) give the solution satisfying the constraints of equal pressure and temperature in the two phases.

Given states of the individual phases, the matrix $\underline{\underline{A}}^{-1}$ may be determined by a sequence of explicit substitutions, starting from Eq. (4.24). This sequence of substitutions may form an algorithm for numerical calculations. For numerical calculation, differentials are to be replaced by finite differences and the matrix $\underline{\underline{A}}^{-1}$ is to be evaluated at the mid-point of the integration step,

$$(\underline{\underline{A}}^{-1})^h = \underline{\underline{A}}^{-1}(T^h, {V_1}^h, {V_2}^h, {E_1}^h, {E_2}^h, {S_1}^h, {S_2}^h) \ . \qquad (4.51)$$

In the finite difference analogue of Eq. (4.39) dV is to be replaced by ΔV, and dE by ΔE. If both the beginning and the end of the step are in the mixed phase region, then ${G_{21}}^n$ and ${G_{21}}^o$ are both zero and ΔG_{21} is zero. Both this case and the case in which the step goes from a single phase region into the mixed phase region are accounted for by the more general expression

$$\Delta G_{21} = -{G_{21}}^o . \qquad (4.52)$$

The case in which the step leaves the mixed phase region is accounted for by requiring that x be bounded by zero and one. The finite difference equations for ΔP, ΔT, and Δx are represented formally by