T and the $g_n(\tilde{v})$ are differentiable and also integrable in closed form, subject to the restriction that

$$p \to RT/\tilde{v} \text{ as } \tilde{v} \to \infty. \qquad (38)$$

All known analytic empirical thermal equations of state satisfy these conditions. From equation (37) one obtains

$$\left(\frac{\partial s}{\partial \tilde{v}}\right)_T = \left(\frac{\partial p}{\partial T}\right)_{\tilde{v}} = \sum_n f_n'(T) g_n(\tilde{v}), \qquad (39)$$

and

$$\left(\frac{\partial p}{\partial \tilde{v}}\right)_T = \sum_n f_n(T) g_n'(\tilde{v}). \qquad (40)$$

The caloric equation of state is obtained in terms of the zero pressure specific heat at constant volume $c_{\tilde{v}}^+(T)$, where $c_{\tilde{v}}^+(T)$ and $c_{\tilde{v}}^+(T)/T$ are both integrable in closed form. The caloric equation of state can then be written as

$$u = u^+(T) + \sum_n [Tf_n'(T) - f_n(T)] \int_\infty^v g_n(\tilde{v}) d\tilde{v}), \qquad (41)$$

where the zero pressure internal energy $u^+(T)$ is given by

$$u^+(T) = \int_0^T c_{\tilde{v}}^+(T) dT. \qquad (42)$$

The corresponding expression for $c_{\tilde{v}}$ is

$$c_{\tilde{v}} = c_{\tilde{v}}^+(T) + T \sum_n f_n''(T) \int_\infty^v g_n(\tilde{v}) d\tilde{v}. \qquad (43)$$

The speed of sound c can then be determined from

$$c^2 = -\tilde{v}^2 \left[\left(\frac{\partial p}{\partial \tilde{v}}\right)_T - \frac{T}{c_{\tilde{v}}} \left(\frac{\partial p}{\partial T}\right)_{\tilde{v}}^2 \right]. \qquad (44)$$

The specific heat at constant pressure c_p is most simply calculated from

$$c_p = -\frac{c_{\tilde{v}} c^2}{\tilde{v}^2 \left(\frac{\partial p}{\partial \tilde{v}}\right)_T}. \qquad (45)$$

The entropy can be obtained by integrating equation (38). It can be expressed as

$$s = s(T_0, \tilde{v}_0) + s^+(T) - s^+(T_0) + \sum_n \left[f_n'(T) \int_\infty^v g_n(\tilde{v}) d\tilde{v} - f_n'(T_0) \int_\infty^{v_0} g_n(\tilde{v}) d\tilde{v} \right], \qquad (46)$$

where $s^+(T)$ is given by the indefinite integral

$$s^+(T) = \int \frac{c_{\tilde{v}}^+(T)}{T} dT, \qquad (47)$$

and T_0, $\tilde{v}_0$ is some arbitrary reference state.

For isentropic flow from a reservoir with T_0 and p_0 given, the corresponding value of $\tilde{v}_0$ would in general be obtained from equations (37) and (40) using Newton's iteration. Instead of integrating

$$\left(\frac{\partial T}{\partial \tilde{v}}\right)_s = -\frac{T}{c_{\tilde{v}}} \left(\frac{\partial p}{\partial T}\right)_{\tilde{v}} \qquad (48)$$

to obtain $T(\tilde{v})$, as is done in the discussed paper, it is much simpler to solve for $T(\tilde{v})$ (or $\tilde{v}(T)$) using Newton's iteration from equation (46) by setting

$$s - s(T_0, \tilde{v}_0) = 0. \qquad (49)$$

The choice of $\tilde{v}$ or T as independent variable depends on the nature of equation (37) and the function $c_{\tilde{v}}^+(T)$. For the particular equations of Bober and Chow, the equation relating T and $\tilde{v}$ can be written as

$$s^+(T) - s^+(T_0) + R \ln\left(\frac{\tilde{v} - b}{\tilde{v}_0 - b}\right) + \frac{a}{2b} \left[T_0^{-3/2} \ln\left(1 + \frac{b}{\tilde{v}_0}\right) - T^{-3/2} \ln\left(1 + \frac{b}{\tilde{v}}\right) \right] = 0, \qquad (50)$$

where

$$s^+(T) = R\left[(A_0 - 1)\ln T + A_1 T + \frac{1}{2} A_2 T^2 + \frac{1}{3} A_3 T^3 + \frac{1}{4} A_4 T^4 \right]. \qquad (51)$$

For this case it would appear to be more efficient to choose T as the independent variable.

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Authors' Closure

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