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Note

Method of Local Approximations in Thermophysical Property Calculations: Estimation of Errors in Derived Thermodynamic Properties

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An algorithm for thermophysical property calculations based on the finite-element approximation in the thermodynamic plane has been suggested. As an example of using the algorithm, errors in obtaining the compressibility of ethane and its derivatives with respect to reduced density and temperature are discussed.

KEY WORDS: ethane; finite-element approximation; P, ρ, T data; thermodynamic plane.

1. INTRODUCTION

Estimation of the errors in obtaining thermodynamic functions is the weakest point of the procedure of computing thermophysical properties of liquids and gases from the experimental P, ρ, T data. Such a calculation presupposes determining of the thermodynamic surface $z(x, y)$, where $z = PV/RT$ stands for compressibility; $x = \rho/\rho_c$ is reduced density, and $T = T/T_c$ is reduced temperature. The computational formulas contain the values of the function z and its first- and second-order derivatives. The main difficulties in estimating the computational error arise in numerical determination of the partial derivatives of compressibility.

The error estimation effectiveness depends largely on the algorithm of calculating thermodynamic functions. If the basis of this algorithm is a mathematical evaluation of experimental data over a wide range of varia-

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tion of state variables, then final comparison with the experiment is the only way of proving validity of the calculation [1]. In this case, the local nature of the procedure of obtaining derivatives is partly concealed. In other words, the error of computing derivatives at (x_0, y_0) should be determined by a sufficient number of experimental data and their distribution in the thermodynamic plane.

In the present paper, as a basic step of the algorithm of calculation, we highlight determining the values of compressibility and its derivatives up to order two at a given point of the thermodynamic surface. Numerical realization of this step is based on finite-element approximation [2].

2. ALGORITHM OF DETERMINATION OF COMPRESSIBILITY AND ITS DERIVATIVES

Assuming that the experimental values of z are known at points (x_k, y_k), $k = 1, \ldots, K$. For determining the values of $z(x, y)$, $(\partial z/\partial x)$, and $(\partial z/\partial y)$ at a point (x_0, y_0), proceed as follows. Construct a triangulation in some neighborhood of this point in such a manner that (x_0, y_0) is the common vertex of all triangles (Fig. 1). Here, care must be taken that a sufficient number of experimental points falls within each triangle. The local approximation of a thermodynamic surface in the neighborhood of (x_0, y_0) is expressed as

$$z(x, y) = \sum_{i=1}^{N} \sum_{s=1}^{M_i} b_i^s \phi_i^s(x, y) \tag{1}$$

where N is the number of nodes of triangulation, M_i is the number of degrees of freedom in the ith node, $\phi_i^s(x, y)$ is the finite-element basic func-

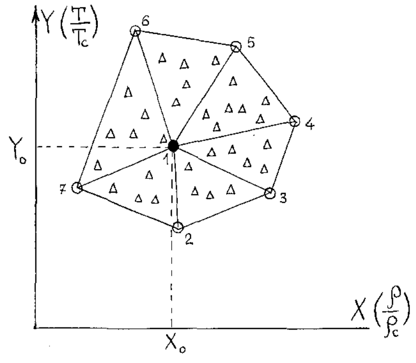

Fig. 1. Triangulation of the neighborhood of a calculated point in the thermodynamic plane. (●) Calculated point; (△) experimental data; (○) nodes of triangulation.

tion associated with the sth degree of freedom of the ith node, and b_i^s are unknown coefficients. The meaning of coefficients b_i^s is known to depend on the choice of the type of an element, i.e., its geometry and the degrees of freedom. As we are interested in knowing the values of the functions and its first derivatives at the point (x_0, y_0), it is natural to choose a Hermitian triangle of type 3′ (Zienkiewicz triangle) [3]. The coefficients b_i^s appearing in Eq. (1) are the values of the function and its first derivatives at the nodes of triangulation, i.e., at the vertexes of triangles. Thus, if we number the nodes as in Fig. 1, then the first three coefficients, b_1^1, b_1^2, and b_1^3, will yield, respectively, the unknown approximate values of $z(x, y)$, $(\partial z/\partial x)$, and $(\partial z/\partial y)$ at the point (x_0, y_0).

The basic functions on element for the Zienkiewicz triangle are determined by the following relationships [3]:

$$\begin{aligned}
&\psi_n^1 = -2\lambda_n^3 + 3\lambda_n^2 + 2\lambda_1\lambda_2\lambda_3 \\
&\psi_n^s = \sum_{\substack{j=1 \\ n \neq j}}^{3} [\lambda_n\lambda_j(2\lambda_n + \lambda_j - 1) + \tfrac{3}{2}\lambda_1\lambda_2\lambda_3]\, t_{jh}^s, \qquad s = 2, 3 \qquad (2) \\
&t_{jn}^2 = a_x^j - a_x^n, \qquad t_{jn}^3 = a_y^j - a_y^n, \qquad n = 1, 2, 3
\end{aligned}$$

where λ_1, λ_2, and λ_3 are the barycentric coordinates of the point (x, y), and a_x^n and a_y^n are the Cartesian coordinates of the nth vertex of the element. The $\phi_i^s(x, y)$ functions are related to the basic functions of the element by the following relationships:

$$\phi_i^s(x, y) = \psi_n^s(\lambda_1, \lambda_2, \lambda_3)$$

where n is the local number of the ith global node.

Thus, knowing z_n, $(\partial z/\partial x)_n$, and $(\partial z/\partial y)_n$, the values of the function and first derivatives at the nodes of triangulation (in the given case, at the vertexes of the triangle), we can write the following approximation for any interior point (x, y) of the element:

$$z(x, y) = \sum_{n=1}^{3} \left[z_n\psi_n^1 + \left(\frac{\partial z}{\partial x}\right)_n \psi_n^2 + \left(\frac{\partial z}{\partial y}\right)_n \psi_n^3 \right] \qquad (3)$$

The coefficients b are determined by minimizing the functional

$$S = \sum_{k=1}^{\mathscr{K}} W_k \left[\sum_{i=1}^{N} \sum_{s=1}^{M_i} b_i^s \phi_i^s(x_k, y_k) - Z_k \right]^2 \qquad (4)$$

where Z_k denotes the experimental value of compressibility at the kth point, and W_k stands for the weight characterizing the relative "value" of the kth experimental point [1]. The second derivatives can be determined in a similar way by minimizing the functionals

$$\begin{aligned} S_x &= \sum_{k=1}^{\mathcal{K}} \left[\sum_{i=1}^{N} \sum_{s=1}^{M_i} c_i^s \phi_i^s(x_k, y_k) - \left(\frac{\partial z}{\partial x}\right)_k \right]^2 \\ S_y &= \sum_{k=1}^{\mathcal{K}} \left[\sum_{i=1}^{N} \sum_{s=1}^{M_i} d_i^s \phi_i^s(x_k, y_k) - \left(\frac{\partial z}{\partial y}\right)_k \right]^2 \end{aligned} \qquad (5)$$

Here, $(\partial z/\partial x)_k$ and $(\partial z/\partial y)_k$ are the values of first derivatives of compressibility at the kth point; these values are obtained by differentiating (1). The corresponding values of second derivatives are

$$c_1^2 = \frac{\partial^2 z}{\partial x^2}, \qquad c_1^3 = \frac{\partial^2 z}{\partial y\, \partial x}, \qquad d_1^3 = \frac{\partial^2 z}{\partial y^2}, \qquad d_1^2 = \frac{\partial^2 z}{\partial x\, \partial y}$$

Thus, computation of first-order derivatives demands single construction of a local approximation (1). The determination of second-order derivaties presupposes (i) computation of values of first-order derivatives at the nodes of triangulation (Fig. 1), (ii) their interpolation at some interior points, and (iii) repeat construction of an approximation of type (1) after solving the least-squares problems (5).

3. RESULTS

For testing the above-described algorithm, seven domains were taken in the ρ–T plane as shown in Fig. 2. The values of the $z(x, y)$ function and

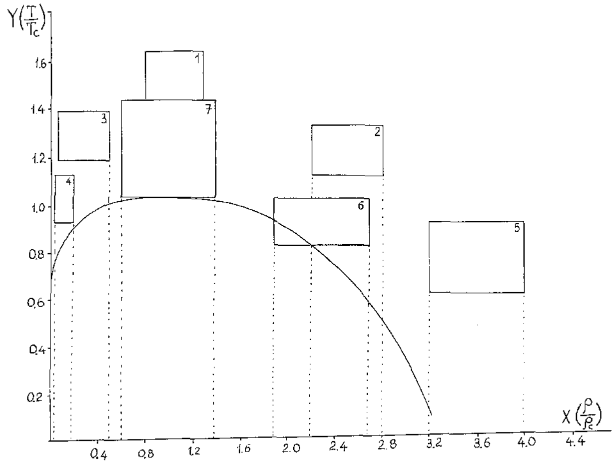

Fig. 2. Test domains for ethane. x, reduced density; y, reduced temperature.

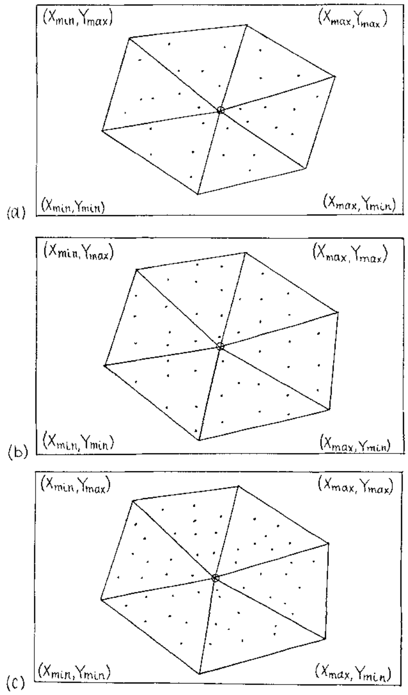

Fig. 3. Variants of triangulation and distribution of experimental points in the test domain: (a) $T06P030$; (b) $T06P43$; (c) $T06P051$. (⊙) Calculated point; (·) experimental data.

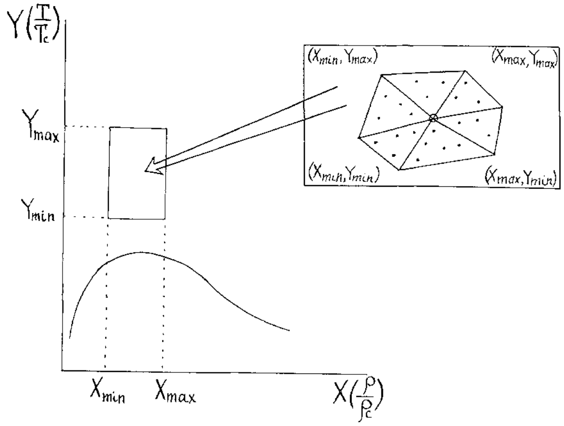

Fig. 4. Mapping of triangulation onto test domain. x, reduced density; y, reduced temperature.

Table I. Errors of Obtaining Compressibility of Ethane and First- and Second-Order Derivatives with Respect to Reduced Density and Temperature[a]

N	Triang	X_0	Y_0	dZ (%)	dZx (%)	dZy (%)	$dZxx$ (%)	$dZyy$ (%)	$dZyx$ (%)	$dZxy$ (%)	X_{min}	X_{max}	Y_{min}	Y_{max}
1	*t*06*p*030	1.05	1.50	0.00	0.03	0.33	0.00	6.32	−4.28	3.84	0.80	1.30	1.40	1.60
	*t*06*p*043			0.00	0.01	0.00	0.18	0.21	0.06	0.12				
	*t*06*p*051			0.00	0.12	0.01	0.74	−0.46	1.24	3.90				
2	*t*06*p*030	2.50	1.20	−0.01	−0.15	−0.15	3.83	18.30	6.62	7.94	2.20	2.80	1.10	1.30
	*t*06*p*043			0.00	−0.06	−0.22	3.54	−10.48	6.60	7.88				
	*t*06*p*051			−0.01	−0.08	−0.17	3.20	−7.21	6.34	8.61				
3	*t*06*p*030	0.28	1.25	0.00	−0.01	−0.18	−2.90	−4.68	28.78	−19.97	0.06	0.50	1.15	1.35
	*t*06*p*043			0.00	−0.01	0.02	0.31	0.40	−1.90	−0.90				
	*t*06*p*051			0.00	−0.07	−0.01	0.09	−1.27	3.40	5.70				
4	*t*06*p*030	0.11	1.00	0.00	−0.02	−0.13	−11.93	−6.11	60.99	−46.37	0.01	0.20	0.90	1.10
	*t*06*p*043			0.00	0.15	−0.03	4.03	−1.38	37.11	20.17				
	*t*06*p*051			0.00	0.03	−0.01	−2.58	−1.93	35.90	22.11				
5	*t*06*p*030	3.60	0.75	−0.11	−2.15	−0.80	12.62	8.61	8.54	4.08	3.20	4.00	0.60	0.90
	*t*06*p*043			−0.04	−1.44	−0.27	9.35	−1.63	1.87	5.92				
	*t*06*p*051			−0.08	−1.71	−0.31	6.72	1.17	2.84	4.66				
6	*t*06*p*030	2.30	0.90	−0.01	−0.10	−0.17	2.81	6.39	4.98	2.61	1.90	2.70	0.80	1.00
	*t*06*p*043			0.00	−0.07	−0.06	1.17	−1.88	1.91	3.94				
	*t*06*p*051			−0.01	−0.08	−0.08	0.87	1.44	2.23	3.59				
7	*t*06*p*030	1.00	1.20	0.00	0.21	0.13	3.44	1.99	−10.34	7.57	0.60	1.40	1.00	1.40
	*t*06*p*043			0.00	−0.15	−0.02	1.75	−0.85	1.45	1.95				
	*t*06*p*051			0.00	0.12	−0.02	1.56	−0.38	1.75	2.50				

[a] N—domain number (as in Fig. 2); Triang—variant of triangulation of test domain (see Fig. 3); X_{min}, X_{max}—minimum and maximum values of reduced density in domain; Y_{min}, Y_{min}—minimum and maximum values of reduced temperature in domain; X_0, Y_0—reduced density and temperature at the calculated point; dZ—relative error of obtaining compressibility (%); dZx, dZy—relative error of obtaining first derivatives of compressibility with respect to density and temperature, respectively (%); $dZxx$, $dZyy$—relative error of obtaining second-order derivatives of compressibility with respect to density and temperature, respectively (%); $dZxy$, $dZyx$—relative error of obtaining second-order mixed derivatives of compressibility (%).

its first- and second-order derivatives at the central point of each domain were determined for three variants of triangulation and distribution of experimental points, shown in Fig. 3. The rectangles shown in Fig. 3 were mapped onto any of the test domains to obtain images of corresponding triangulations and distributions directly in the thermodynamic plane. Here the corresponding vertexes of rectangles must coincide (Fig. 4).

Table I contains results of calculations for ethane. Exact values of compressibility and its derivatives were determined by the equation of state, given in Ref. 4. As seen from Table I, the relative errors of obtaining compressibility and its first derivatives with respect to reduced density and temperature, denoted by *dZ*, *dZx*, and *dZy*, are sufficiently small and do not exceed, on the average, tens of fractions of a percent. In typical cases, the errors of restoring second-order derivatives, denoted by *dZxx* and *dZyy*, do not exceed 5–10% for triangulations containing more then 30 experimental points. As the dimensions of test domains decrease and the number of experimental points increases, the restoration error decreases. The data listed in Table I illustrate also the dependence of error on the localization of the test domain in the thermodynamic plane, i.e., on the nature of variation of function $z(x, y)$.

4. CONCLUSION

In practice, estimation of the reliability of a calculation is of great importance. A great number of difficulties are faced in estimating the accuracy of determining derivatives. We believe that the use of finite-element approximations in the thermodynamic plane is sufficiently promising for overcoming these difficalties. Since a detailed discussion of this question is beyond the scope of the present paper, we restrict ourselves to the following remarks.

The accuracy of obtaining the values of a function and its derivatives is determined by the norm of the function, the method of constructing an approximation, and the characteristics of the experiment, such as errors in data and distribution of experimental points in the thermodynamic plane. The use of local approximations permits the statistical modeling methods to be utilized for establishing a relationship between the error of restoring the derivatives and the descriptors of these characteristics. The effect of the nature of distribution of experimental data is not sufficiently well studied; a more detailed study of this may provide answers to a number of practically important points.

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