AD/A-002 915

CREATING EQUATION OF STATE OF CONDENSED SYSTEMS FROM DYNAMIC EXPERIMENTS

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15 November 1974

UNCLASSIFIED
Security Classification

AD/A003 915

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Foreign Technology Division Air Force Systems Command U. S. Air Force	2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED 2b. GROUP

3. REPORT TITLE

CREATING EQUATION OF STATE FOR CONDENSED SYSTEMS FROM DYNAMIC EXPERIMENTS

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)
Translation

5. AUTHOR(S) (First name, middle initial, last name)

V. Ye. Fortov

6. REPORT DATE 1972	7a. TOTAL NO. OF PAGES ~~6~~ 12	7b. NO. OF REFS 12
8a. CONTRACT OR GRANT NO. b. PROJECT NO c. d.	9a. ORIGINATOR'S REPORT NUMBER(S) FTD-HT-23-1989-74 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Foreign Technology Division Wright-Patterson AFB, Ohio

13. ABSTRACT

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(18)

DD FORM 1 NOV 65 1473

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UNCLASSIFIED
Security Classification

FTD-HT-23-1989-74

FOREIGN TECHNOLOGY DIVISION

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EDITED TRANSLATION

FTD-HT-23-1989-74 15 November 1974

CSP 73193384

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By: V. Ye. Fortov

English pages: 6

Source: Goreniye i Vzryv, Izd vo Nauka,
Moscow, 1972, pp. 561-564

Country of Origin: USSR
Translated by: Marilyn Olaechea
Requester: FTD/PDTN
Approved for public release;
distribution unlimited.

PREPARED BY:

TRANSLATION DIVISION
FOREIGN TECHNOLOGY DIVISION
WP-AFB, OHIO.

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All figures, graphs, tables, equations, etc. merged into this translation were extracted from the best quality copy available.

U. S. BOARD ON GEOGRAPHIC NAMES TRANSLITERATION SYSTEM

Block	Italic	Transliteration	Block	Italic	Transliteration
А а	*А а*	A, a	Р р	*Р р*	R, r
Б б	*Б б*	B, b	С с	*С с*	S, s
В в	*В в*	V, v	Т т	*Т т*	T, t
Г г	*Г г*	G, g	У у	*У у*	U, u
Д д	*Д д*	D, d	Ф ф	*Ф ф*	F, f
Е е	*Е е*	Ye, ye; E, e*	Х х	*Х х*	Kh, kh
Ж ж	*Ж ж*	Zh, zh	Ц ц	*Ц ц*	Ts, ts
З з	*З з*	Z, z	Ч ч	*Ч ч*	Ch, ch
И и	*И и*	I, i	Ш ш	*Ш ш*	Sh, sh
Й й	*Й й*	Y, y	Щ щ	*Щ щ*	Shch, shch
К к	*К к*	K, k	Ъ ъ	*Ъ ъ*	"
Л л	*Л л*	L, l	Ы ы	*Ы ы*	Y, y
М м	*М м*	M, m	Ь ь	*Ь ь*	'
Н н	*Н н*	N, n	Э э	*Э э*	E, e
О о	*О о*	O, o	Ю ю	*Ю ю*	Yu, yu
П п	*П п*	P, p	Я я	*Я я*	Ya, ya

* ye initially, after vowels, and after ъ, ь; e elsewhere. When written as ё in Russian, transliterate as yё or ё. The use of diacritical marks is preferred, but such marks may be omitted when expediency dictates.

FOLLOWING ARE THE CORRESPONDING RUSSIAN AND ENGLISH DESIGNATIONS OF THE TRIGONOMETRIC FUNCTIONS

Russian	English
sin	sin
cos	cos
tg	tan
ctg	cot
sec	sec
cosec	csc
sh	sinh
ch	cosh
th	tanh
cth	coth
sch	sech
csch	csch
arc sin	$\sin^{-1}$
arc cos	$\cos^{-1}$
arc tg	$\tan^{-1}$
arc ctg	$\cot^{-1}$
arc sec	$\sec^{-1}$
arc cosec	$\csc^{-1}$
arc sh	$\sinh^{-1}$
arc ch	$\cosh^{-1}$
arc th	$\tanh^{-1}$
arc cth	$\coth^{-1}$
arc sch	sech^{-1}
arc csch	csch^{-1}

Russian	English
rot	curl
lg	log

GREEK ALPHABET

Alpha	Α	α	α		Nu	Ν	ν	
Beta	Β	β			Xi	Ξ	ξ	
Gamma	Γ	γ			Omicron	Ο	ο	
Delta	Δ	δ			Pi	Π	π	
Epsilon	Ε	ε	ε		Rho	Ρ	ρ	ρ
Zeta	Ζ	ζ			Sigma	Σ	σ	ς
Eta	Η	η			Tau	Τ	τ	
Theta	Θ	θ	ϑ		Upsilon	Τ	υ	
Iota	Ι	ι			Phi	Φ	φ	ϕ
Kappa	Κ	ϰ	κ	κ	Chi	Χ	χ	
Lambda	Λ	λ			Psi	Ψ	ψ	
Mu	Μ	μ			Omega	Ω	ω	

CREATING EQUATION OF STATE OF CONDENSED SYSTEMS FROM DYNAMIC EXPERIMENTS

V. Ye. Fortov
Moscow

Successive theoretical calculation of the thermodynamic properties of a substance in the condensed state involves the quantum mechanics problem of many bodies when there exists a strong interaction among them. At the present time this cannot be achieved in a general form. In this situation experimental, primarily dynamic, research methods based on obtaining the necessary state by compression and irreversible heating of the medium at the front of a strong shock wave [1] acquire particular significance.

The characteristic feature of dynamic experiments is direct registration of only the mechanical parameters of shock compression - pressure (p), specific volume (V), and internal energy (E). To construct the complete equation of state from these data we must introduce model representations of the properties of the studied substance. Here the data of the experiment were used to determine the constants and functions contained in the equation of state; for certain terms purely theoretical expressions are often used. The criterion of correctness for equations of state thus obtained is agreement between calculated and measured states of shock compression. Here a situation may arise in which various equations of state result in different values of the Grüneisen coefficient and temperature for the shock-compressed substance, even though the original experimental material was well described [2].

The thermodynamically complete equation of state, however, may be plotted from dynamic experiments without introducing limiting ideas concerning the properties and the nature of the studied medium [3, 4].

In dynamic experiments registration of the kinematic parameters of propagation of a shock discontinuity makes it possible, by using the general laws of conservation on the shock wave front, to determine the equation of state in a caloric form E=E(p, V) for the entire region of the pV plane accessible in the experiment [1]. The internal energy, however, does not represent thermodynamic potential with respect to the pV variable, and in order to plot the complete thermodynamics of the studied system we need the additional dependence T=T(p, V).

Proceeding from the first principle of thermodynamics and assuming that from the experiment the dependence E=E(p, V) is known, we can easily obtain [3]

$$\left[p + \left(\frac{\partial E}{\partial V}\right)_p\right] \cdot \frac{\partial T}{\partial p} - \left(\frac{\partial E}{\partial p}\right)_V \cdot \frac{\partial T}{\partial V} = T. \qquad (1)$$

The solution to this linear heterogeneous differential equation with variable coefficients is the dependence T=T(p, V) which interests us. Equation (1) has a corresponding system of characteristic differential equations:

$$\frac{dp}{dV} = -\frac{p + \left(\frac{\partial E}{\partial V}\right)_p}{\left(\frac{\partial E}{\partial p}\right)_V}; \qquad (2)$$

$$\frac{dT}{dV} = -\frac{T}{\left(\frac{\partial E}{\partial p}\right)_V}, \qquad (3)$$

the first of which determines pressure, the second - temperature on the isentrope. Equations (1) or (2) and (3) are completed by boundary conditions: temperature must be given in the region where it can be experimentally determined. In the present calculations the temperature was assigned as a function of specific volume on the isobar of atmospheric pressure; the experimental data of V=V(T) with respect to the thermal expansion of the substance were used.

The caloric equation of state E=E(p, V) was constructed from experimental points E_i, p_i, $V_i\}_{i=1}^{N}$ chaiotically arranged in the pV plane in the form of

$$E^q(p, V) = \sum_{k+l \leq q}\sum e_{kl} V^k p^l. \qquad (4)$$

In (4) the coefficients e_{ki} are found by the method of least squares [4]. In determining coefficients e_{kl} the weight inversely proportional to registration error of the shock compression states was assumed by each experimental point.

The degree of the polynomial q in (4) was selected by analyzing the residual sum of squares when the degree increased q→q+1. Here the statistical Fischer significance criterion [5] was used.

The equation of state in caloric form (4) can be used directly for hydrodynamic calculations of adiabatic flows.

The isentropes are determined by integrating differential equations (2) and (3); The shock adiabats are found by numerical solution to the Rankin-Hugonoit relationship:

$$\frac{1}{2}(p+p_0)(V_0-V)=E^q(p,V)-E_0(p_0,V_0), \qquad (5)$$

where $E^q(p, V)$ is taken in the form of (4).

The dependence between the accuracy of the obtained solution and error in the original data was determined by the Monte Carlo method by simulating the probability structure of the measuring process on the electronic computer [4]. The computer reassembled possible combinations of random factors resulting in experimental error and determined the effect of these factors on the solution to equations (2) and (3). The proposed method enabled a comprehensive estimate for the accuracy of the solution obtained for any given configuration of experimental points in the pV plane and the specific level of experimental errors.

As an example we introduce the results for the equation of state for nickel. For this we used experimental data for dynamic compression of solid [6, 7, 8] and porous specimens of a given element. In addition the internal energy (according to [10]) was assigned at two points on the atmospheric pressure isobar. As the original data for system (2), (3) we use the results of measuring the thermal expansion of nickel [11] at p=1 bar

Static analysis [4] showed that to describe the existing experimental data we must select the degree of the polynomial (4) q=3. Figure 1 shows the Hugonoit adiabats (Ni) plotted from the obtained equation of state. The difference between shock compression states calculated according to (4) and (5) and those which were measured lies within the limits of experimental error.

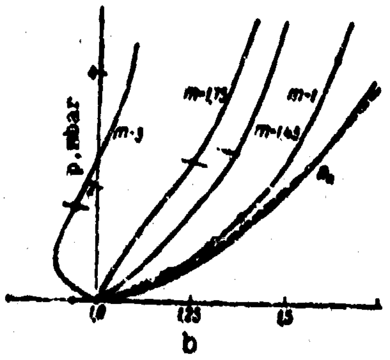

Figure 1. Hugonoit adiabats for nickel of different initial porosities $m=\frac{\rho_H}{\rho_0}$ (ρ_H- density of crystal, ρ_0- density of original specimen); p_x - zero isentrope for equations (2) and (4); dashed line - zero isentrope for [2]; O-[7]; ∇-[8]; Δ-[6]; ●-p=1 bar).

An important characteristic of the substance used in all model theories for the equation of state is the "cold" compression curve $p_x(V)$ - the dependence of pressure on specific volume at T=0°K. Existing methods for obtaining this curve from the results of the experiment involve introducing a large number of theoretical ideas about the properties of the studied substance. Assuming that the isotherm T=0°K coincides with the isentrope, the cold compression curve in this approach can be obtained by integrating equation (2) for T_0=0°K. The elastic pressure curve thus plotted is shown in Fig. 1, where it is compared with $p_x(V)$ from [2].

It should be mentioned that, in contrast to existing theories, there was no preliminary division of the thermodynamic factors into "thermal" and "cold" components in the method of constructing an equation of state which is discussed here.

Temperature was calculated by combined integration of equations (2) and (3). For the initial value of the specific volume temperature was determined by means of the thermal expansion curve introduced into the computer (p=1 bar). With these initial conditions system (2), (3) was integrated up to the intersection of the isentrope with the shock adiabat in the pV plane of the solid substance. Figure 2 shows the results of determining temperature; here we also see for comparison the results of calculating temperatures on shock adiabats for solid nickel according to the Mie-Grüneisen theory [6] and in the approximation of the theory of free volume [7].

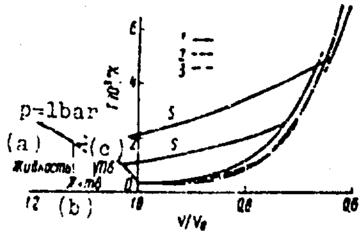

Figure 2. Calculation for temperature of nickel: 1 - from equations (2), (3), (4); 2 - study [6]; 3 - study [7]; s - isentropes.
Key: (a) Liquid; (b) Liquid+solid; (c) Solid.

The characteristic temperature "step" on the shock adiabat is the result of the melting of the substance at the front of the shock wave. The absence of detailed experimental data in the region of the melting curve resulted in a situation in which the melting curve coincided with the isentrope in this case; the real temperature "step" (according to [12]) is located somewhere above that which is shown in Fig. 2.

The statistical analysis made by Monte Carlo method showed that if accuracy in the nature of the arrangement of the experimental points in the pV plane are considered the error in determining temperature on the Hugonoit adiabat for solid nickel is on the order of 5-8%, which is independently confirmed by comparison to temperature calculations for model theories of the equation state

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