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**The Operational Equations of State, 3: Recovery of the EOS
for Hydrocode From the Measured Heat Capacity,
Isentrope, and Hugoniot Adiat**

by Michael Grinfeld

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The Operational Equations of State, 3: Recovery of the EOS for Hydrocode From the Measured Heat Capacity, Isentrope, and Hugoniot Adiabats

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14. ABSTRACT We present several novel explicit formulas for recovery of the complete EOS for hydrocode from experimental data. It is assumed that the substance in question possesses only two thermodynamic degrees of freedom – the specific volume V and the specific internal energy E . It is also assumed that the measurements of the heat capacity $C_V = C(V, E)$ at constant volume, of the isentrope $E_S = E_S^{\otimes\otimes}(V)$, passing through the state $(V^{\otimes}, E^{\otimes})$, and of the Hugoniot adiabat $E_H = E_H^{**}(V)$ with the initial state (V^*, E^*) , are presented in analytical form. No special explicit assumptions are made regarding those functions except their reasonable smoothness (which, however, excludes the possibility of phase transformations).					
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1. Introduction



“Yes, we have to divide up our time like that, between our politics and our equations. But to me our equations are far more important, for politics are only a matter of present concern. A mathematical equation stands forever.”

Attributed to Albert Einstein

This is a continuation of the previous reports in this series (1, 2), where the motivation is presented. In those reports, we gave several examples of generating complete thermodynamically consistent equations of state (EOS). The methodology used there was based on combining some ad-hoc generalizations of classical models with available experimental data. The EOS have been presented in analytical form as functions of the experimental data. Their numerical implementation has been discussed by Bilyk et al. (3).

We begin with the general analysis which does not rely on any particular assumptions but those of classical thermodynamics (like, for instance, the assumption of dealing with a two-parameter system). In this respect, our method reminds the remarkable short letters of Peek and Salsburg (4) and of Zel’dovich (5), although the differences between the two methods are quite significant and will be discussed elsewhere. Unfortunately, so far the Peek-Salburg-Zel’dovich approach did not find many followers neither in the former Soviet Union nor in the West. The only exception that this author is aware of is the paper of Fortov and Krasnikov (6).

In general, our approach leads to a pair of integro-differential equations which, probably, should be solved numerically. We then proceed with the special case of constant heat capacity. This special case is particularly important for applications and, fortunately, permits explicit solution.

2. Required Notions and Basic Formulas

In this report, we present a methodology which does not rely on any a priori guesses regarding the structure of the EOS. The only assumption made is that the substances under study can be treated as two-parameter thermodynamic systems with sufficiently smooth EOS.

According to our definition, for a medium with two thermodynamic parameters, the complete EOS for hydrocode is nothing but the specific entropy density S presented as a function of the specific volume V internal energy density E :

$$S = S(V, E) \quad (1)$$

In terms of this function, the pressure $P = P(V, E)$ and the absolute temperature can be presented in the following form:

$$P(V, E) \equiv \frac{\frac{\partial S(V, E)}{\partial V}}{\frac{\partial S(V, E)}{\partial E}}, T(V, E) \equiv \frac{1}{\frac{\partial S(V, E)}{\partial E}} \quad (2)$$

The isentrope in the (V, E) parametric space is a curve $E = E_s(V)$ along which entropy density remains constant. We use notation $E = E_s^{**}(V)$ for the isentrope passing through the state (V^*, E^*) . In figure 1, two isentropes, $E = E_s^{**}(V)$ and $E = E_s^{\otimes\otimes}(V)$, are presented in green: the former passing through the state (V^*, E^*) and the latter passing through the state $(V^{\otimes}, E^{\otimes})$.

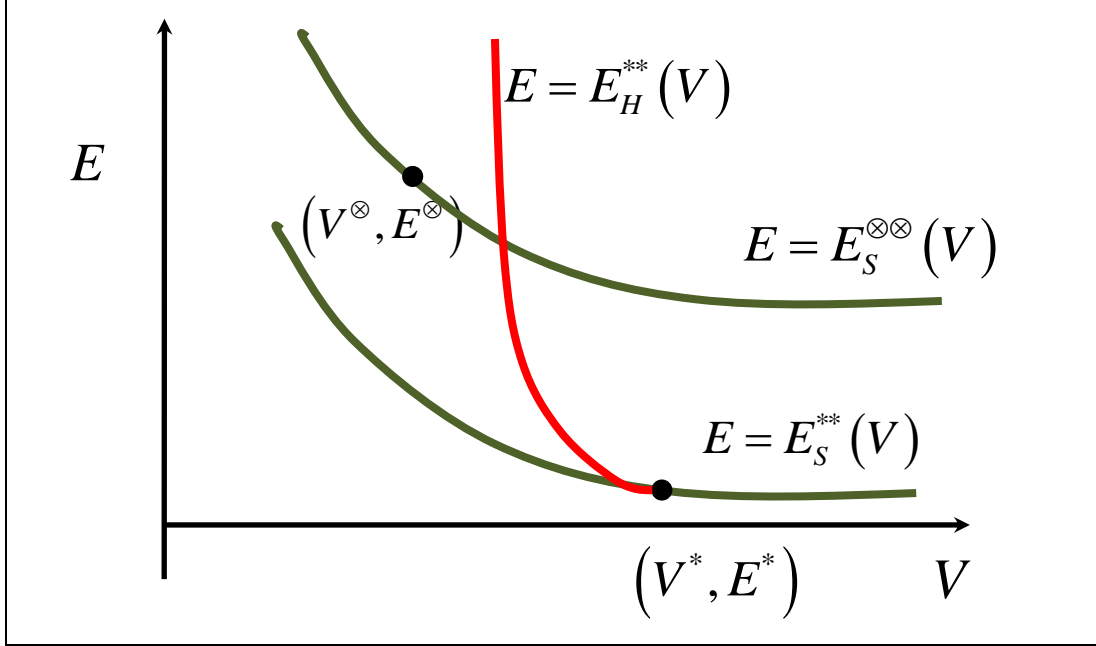


Figure 1. The isentropes (green) and the Hugoniot adiabat in the (V, E) plan.

Given the starting state (V^*, E^*) , the Hugoniot adiabat $E = E_H^{**}(V)$ is the curve presented all the states (V, E) , which can be reached from the starting state by means of the shock waves of different intensity. In the starting state (V^*, E^*) , the isentrope and the Hugoniot adiabat have common tangent lines. However, somewhat farther from that state, the Hugoniot adiabat has a bigger tangent line and, quite often, it even has a vertical asymptote at a finite value of the specific volume. There are two more principal distinctions between isentropes and Hugoniot adiabats. First, each isentrope can be extended from its pole $(V^{\otimes}, E^{\otimes})$ in both directions; the Hugoniot adiabat can be extended in a single direction only. Second, if a new point (V°, E°) on the Hugoniot adiabat $E = E_H^{**}(V)$ is chosen as a starting point, then the new Hugoniot adiabat $E = E_H^{\circ\circ}(V)$ does not coincide with $E = E_H^{**}(V)$. Further properties of the Hugoniot adiabat can be found in numerous textbooks, including the classical ones (7, 8).

Given the isentrope $E = E_S^{\otimes\otimes}(V)$, the pressure values $P = P_S^{\otimes\otimes}(V)$ on this very isentrope can be calculated by means of differentiation only as

$$P_S^{\otimes\otimes}(V) = -\frac{dE_S^{\otimes\otimes}(V)}{dV}. \quad (3)$$

The opposite is also true. Given the pressure values $P = P_S^{\otimes\otimes}(V)$, the equation of the isentrope can be calculated by means of straightforward integration:

$$E_S^{\otimes\otimes}(V) = \int_V^{V^{\otimes}} d\xi P_S^{\otimes\otimes}(\xi) . \quad (4)$$

Experimenters usually measure the pressure $P = P_S^{\otimes\otimes}(V)$ on isentropes, not the energy density $E = E_S^{\otimes\otimes}(V)$. When dealing with the Hugoniot adiabat, the situation is opposite (9, 10). The first things experimenters measure in typical experiments on shock waves are the velocities of the material particles in front of and behind the shock wave and the velocity of the shock front itself. Then, using those measurements and the conservation equations across the shock front, it is possible to calculate the specific energy density $E = E_H^{**}(V)$ and the pressure $P = P_H^{**}(V)$ behind the shock front. The functions $E = E_H^{**}(V)$ and $P = P_H^{**}(V)$ characterizing the Hugoniot adiabat are interrelated according to the classical Rankine-Hugoniot formula

$$P_H^{**}(V) = - \frac{2E_H^{**}(V) - 2E^* + P^*(V - V^*)}{V - V^*} . \quad (5)$$

Summarizing, having the experimentally determined data on $P = P_S^{\otimes\otimes}(V)$ and $E = E_H^{**}(V)$, we can automatically calculate two more functions: $E = E_S^{\otimes\otimes}(V)$ and $P = P_H^{**}(V)$.

If we have the experimentally determined specific heat capacity $C_V = C(V, E)$ at fixed volume, then the complete EOS for hydrocode can be presented in the following form:

$$S(V, E) = A(V) + \int_{E^*}^E \frac{d\varepsilon}{H(V, \varepsilon) + \Lambda(V)} , \quad (6)$$

where the function $H(V, E)$ is defined as

$$H(V, E) \equiv \int_{E^*}^E d\eta C_V^{-1}(V, \eta) , \quad (7)$$

whereas the functions $A(V)$ and $\Lambda(V)$ should be recovered from additional experimental data.

The value of the function $\Lambda(V)$ at $V = V^*$ is equal to the value of the absolute temperature T^* in the state (V^*, E^*) .

$$\Lambda(V^*) = T^* . \quad (8)$$

3. The EOS Recovery for a General Heat Capacity Function $C_V(V, E)$

The recovery of the EOS with non-constant heat capacity is important for application (see Segletes [11] and references therein). In order to recover the complete EOS (equation 6), we have to express the functions $A(V)$ and $\Lambda(V)$ in terms of experimental data. To find those functions from the isentrope $E = E_S^{\otimes\otimes}(V)$ and the Hugoniot adiabat $E = E_H^{**}(V)$ actually means to express the functions $A(V)$ and $\Lambda(V)$ in terms of the functions $C_V = C(V, E)$, $E = E_S^{\otimes\otimes}(V)$, and $E = E_H^{**}(V)$. From the previous discussion, it follows that we automatically get two additional functions, $P = P_S^{\otimes\otimes}(V)$ and $P = P_H^{**}(V)$, which can be calculated with the help of equations 3 and 5, respectively.

In fact, the functions $A(V)$ and $\Lambda(V)$ can be recovered with the help of the function $E = E_S^{\otimes\otimes}(V)$ and $E = E_H^{**}(V)$ by means of solving the following pair of the integro-differential equations:

$$A(V) + \int_{E^*}^{E_S^{\otimes\otimes}(V)} \frac{d\xi}{H(V, \xi) + \Lambda(V)} - S^{\otimes} = 0, \quad (9)$$

and

$$\frac{d}{dV} \int_{E_H^{**}(V)}^{E_S^{\otimes\otimes}(V)} \frac{d\xi}{H(V, \xi) + \Lambda(V)} + \frac{\frac{dE_H^{**}(V)}{dV} + P_H^{**}(V)}{H(V, E_H^{**}(V)) + \Lambda(V)} = 0, \quad (10)$$

that should be combined with the initial condition (equation 8).

In fact, the system (equations 9 and 10) can be solved sequentially. First, we solve equation 10 for the function $\Lambda(V)$, and then we calculate the function $A(V)$ with the help of equation 9.

The solutions should be then inserted into equation 6.

4. Explicit Recovery Formulas for the Case of Constant Heat Capacity

Solution of the general system (equations 9 and 10) requires computer-based methods. Fortunately, an explicit solution is possible in the case of constant heat capacity. This special case is important in many practical applications. In addition, when implementing computer-based methods, explicit solutions play a crucial role in validation and verification procedures.

In this case, the solution of equation 10 with the initial data (equation 8) for function $\Lambda(V)$ can be presented in the following explicit form:

$$\Lambda(V) = T^* [1 - \varepsilon(V, V^*)]. \quad (11)$$

Here, and in the following, we need two non-dimensional functions $\varepsilon(V, V^*)$ and $\tau(V, V^*)$ of two variables which can be presented in the form

$$\varepsilon(V, V^*) \equiv \frac{1}{V^*} \int_{V^*}^V d\theta \pi(\theta) \tau(V, \theta), \quad \tau(V, \theta) \equiv e^{-\int_{\theta}^V d\theta \varpi(\xi)}, \quad (12)$$

in which two non-dimensional functions $\varpi(V)$, $\tau(V)$ of one variable are expressed in terms of the measurable quantities only as

$$\varpi(V) = V^* \frac{P_H^{**}(V) - P_S^{\otimes\otimes}(V)}{E_H^{**}(V) - E_S^{\otimes\otimes}(V)}, \quad \pi(V) = \frac{V^*}{C_V T^*} \frac{P_H^{**}(V) E_S^{\otimes\otimes}(V) - P_S^{\otimes\otimes}(V) E_H^{**}(V)}{E_H^{**}(V) - E_S^{\otimes\otimes}(V)}. \quad (13)$$

In the case of constant heat capacity, the skeleton (6) reduces to the simpler form

$$S(V, E) - S^{\otimes} = C_V \ln \frac{E - E^* + C_V \Lambda(V)}{E_S^{\otimes\otimes}(V) - E^* + C_V \Lambda(V)}. \quad (14)$$

Inserting the solution (equation 11) in the formula (equation 14), we arrive at the following complete equation of state for hydrocode (where we made a special choice $E^* = CT^*$ for the arbitrary constant)

$$S(V, E) - S^{\otimes} = C_V \ln \frac{E - C_V T^* \varepsilon(V, V^*)}{E_S^{\otimes\otimes}(V) - C_V T^* \varepsilon(V, V^*)}. \quad (15)$$

Associated with equation 15, expressions of the absolute temperature and pressure are as follows:

$$T(V, E) = \frac{E - C_V T^* \varepsilon(V, V^*)}{C_V}, \quad (16)$$

and

$$P(V, E) = \frac{\varpi(V)}{V^*} E - \frac{E^*}{V^*} \pi(V) = \frac{P_H^{**} - P_S^{\otimes\otimes}}{E_H^{**} - E_S^{\otimes\otimes}} E - \frac{E_S^{\otimes\otimes} P_H^{**} - E_H^{**} P_S^{\otimes\otimes}}{E_H^{**} - E_S^{\otimes\otimes}}. \quad (17)$$

The formula of the pressure (equation 17) shows that $P(V, E)$ is a linear function of the internal energy density, as it should be in the case of constant heat capacity. In fact, the formula (17) is more general, and it does not require the assumption of constant heat capacity. It is valid when the heat capacity is arbitrary function of entropy. In many applications of the hydrocode in ballistics, only the incomplete EOS (equation 17) is required, not the complete EOS (equation 15).

5. Conclusion

We analyzed the important problem of thermodynamically consistent recovery of the complete EOS for hydrocode from experimental data. More specifically, we demonstrated how to accomplish the recovery based on the measurements of the heat capacity $C_V = C(V, E)$ at constant volume, of the isentrope $E_S = E_S^{\otimes\otimes}(V)$, passing through the state $(V^{\otimes}, E^{\otimes})$, and Hugoniot adiabat $E_H = E_H^{**}(V)$ with the initial state (V^*, E^*) .

We do not make any special *physical* hypothesis about the EOS to be recovered.

We assume that our media can be adequately described as a two-parameter model, that the generated EOS satisfy the thermodynamic stability conditions, and that phase transformations can be ignored (see Grinfeld [12] for further discussion).

It is demonstrated that the recovery basically reduces to solving a nonlinear integro-differential (equation 10). Generally speaking, this equation cannot be solved analytically. At the same time, it allows quite a straight-forward implementation into a computer-based numerical analysis.

In the practically important case of constant heat capacity, the integro-differential equation 10 allows explicit solution. The solution is given by the formulas in equations 11 and 12. The corresponding complete EOS for hydrocode is given by the explicit formula (equation 15). The

incomplete EOS for the absolute temperature and pressure are given by the formulas in equations 16 and 17, respectively.

The procedure of the recovery of the EOS from the measured constant heat capacity C at constant volume, measured pressure $P_S^{\otimes\otimes}(V)$ on the isentrope, and the internal energy density on the Hugoniot adiabat $E_H^{**}(V)$ is the following. First, using the functions $P_S^{\otimes\otimes}(V)$ and $E_H^{**}(V)$ and the relationships (equations 4 and 5), we calculated two additional functions $E_S^{\otimes\otimes}(V)$ and $P_H^{**}(V)$. Then, using the definitions (equation 13), we calculate the functions $\varpi(V)$ and $\pi(V)$. Afterwards, using the definitions (12), we calculate the functions $\varepsilon(V, V^*)$ and $\tau(V, V^*)$. At last, we substitute the function $\varepsilon(V, V^*)$ into the relationships (equations 15–17) in order to determine the complete EOS for the entropy potential $S(V, E)$ and two incomplete EOS for the absolute temperature $T(V, E)$ and pressure $P(V, E)$.

An important issue of tabulating the presented analytical forms for the EOS is discussed elsewhere (13, 14).

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