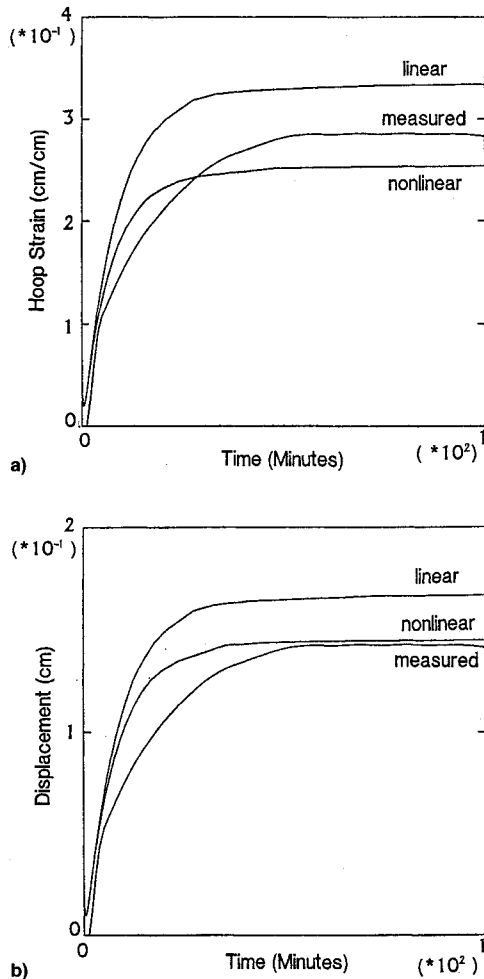


**Table 2** Data comparison between Eqs. (1) and (2)

Equation	$R^2$	$\beta$ , $1/^\circ\text{C}$	$\alpha$ , $1/^\circ\text{C}$	$T_s$ , $^\circ\text{C}$
(1)	0.89	1.90E-4	6.34E-5	85
(2)	0.99	2.74E-4	9.13E-5	71

**Fig. 3** Comparison between FEA and experiments in thermal shock condition: a) hoop strains and b) displacements.

be continuously developed. According to the above discussion, finite deformation could be a dominant effect for constructing thermomechanical nonlinear models.

### Conclusions

Our on-line system is workable to substitute x-ray and interferometer for measuring the i.d. of SEC.

A modified equation is derived for accurately assessing a stress-free temperature and thermal expansion coefficient of solid propellant grain.

For finite deformation, displacement is a proper parameter for comparing the SEC experiment and FEA.

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## Development of Equations of State for Compressible Liquids

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### Nomenclature

- $a$  = speed of sound
- $c_p$  = constant pressure specific heat
- $c_v$  = constant volume specific heat
- $e$  = internal energy
- $L$  = length
- $M$  = Mach number
- $\bar{P}$  = reference pressure
- $p$  = pressure
- $R$  = universal gas constant
- $s$  = entropy
- $T$  = temperature
- $\bar{T}$  = reference temperature
- $u$  = fluid velocity
- $\alpha$  = cubical expansion coefficient
- $\beta$  = isothermal bulk modulus
- $\kappa$  = reference density
- $v$  = volume
- $\rho$  = density

### I. Introduction

IN this Note two novel, general, caloric, and thermal equations of state (EOS) for liquids are derived from first principles. These equations are thermodynamically compatible. Moreover, an expression for entropy consistent with the new EOS is also developed. Curve-fitting techniques can be used to adjust physically significant equation parameters to fit the EOS to available thermodynamic data for particular liquids. The EOSs and the entropy expression are used in conjunction with the equations of motion to model liquid fluid flow. Specifically, they have been used in propulsion system dynamic modeling where the EOS have been successfully tailored to liquid hydrogen ( $\text{LH}_2$ ).<sup>1</sup> The derived model is compared to National Bureau of Standards (NBS) data with good results.

The basis for this work is rooted in the fact that the conservation equations of continuity, momentum, and energy (CME) are employed to describe the dynamic behavior of a fluid. In order to link the kinetic behavior of the medium with its thermodynamic behavior, the EOS are used. Together with the EOS, the CME equations hold kinetic and thermodynamic information to describe fluid system dynamics. The interest lies in finding suitable thermal and caloric EOS as density and internal energy appear in the CME equations. The EOS, cast in usual fluid dynamic variables of pressure and temperature, prove useful in the derivation of the entropy expression. The CME system can then be reformulated in terms of pressure, velocity, and entropy. Such a configuration readily provides insight when considering certain processes, e.g., isentropic. The CME equations for an ideal gas system have already been formulated in terms of entropy, pressure, and velocity.<sup>2</sup>

Traditionally in fluid dynamic problems, a liquid is considered to be incompressible. This approximation affords significant simplification to the governing CME equations and it

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eliminates the need for the EOS. While for many applications the incompressible assumption poses no real threat to fidelity to the real system, certain conditions arise where this assumption loses its validity. One such case is liquid subject to a large pressure surge, e.g., water hammer or oil hammer.<sup>3</sup> It was first shown<sup>4</sup> that compressibility effects should not be neglected when considering actual liquid rocket engine pumps and feed lines. In other words, the incompressible assumption may lead to poor model to actual plant fidelity. In fact, for the case of the Space Shuttle Main Engine (SSME) high-pressure turbo-pumps (HPT), the authors have shown<sup>1,5</sup> that the density of LH<sub>2</sub> changes by more than 40% from inlet to outlet of the HPT. Clearly, the incompressible assumption is not appropriate for LH<sub>2</sub> flow through the pump.

The complexity of the mathematical model increases significantly in the case of a liquid medium because the ideal gas law no longer applies. Unfortunately, no EOS relating density to pressure and volume of an arbitrary liquid exists.<sup>6</sup> All such equations come about using empirical methods. Many of the equations are useful only in limited ranges of the pressure, density, and temperature surface of a fluid. For example, a two-parameter equation of state developed in Ref. 7 was verified for liquid hydrocarbons, but not for LH<sub>2</sub>; and the Van der Waals equation reviewed in Ref. 8 works for gaseous hydrogen, but is not recommended for the liquid region. Moreover, many equations are complex involving several terms and coefficients, making them untoward in a system of equations. The Redlich-Kwong equation, although shown<sup>8</sup> to apply fairly well for several substances in the liquid range, uses experimentally fit parameters that have little apparent physical significance. The EOS used in conjunction with the CME developed in Ref. 1 should rely on experimental data in a physically meaningful way.

The basic methodology presented here for the derivations of EOSs applies to an arbitrary liquid. We turn to the SSME HPT as an example to illustrate the complete derivation of EOS for LH<sub>2</sub>. The HPT experiences large pressure and temperature variations from inlet to outlet. At 109% rated power level (RPL), the inlet pressure and temperature are about 350 psi and 26 K, while the output pressure and temperature of the HPT are about 6870 psi and 56 K, respectively. With such large pressure and temperature variations, one would not expect any one equation to cover the entire range. Indeed, as evidenced by Fig. 1, the equation given in Ref. 9 for LH<sub>2</sub> does not fit the available thermodynamic data very well in the normal operating levels of the SSME HPT.

In the next two sections, general thermal EOS and caloric EOS for liquids are derived and then tailored specifically to LH<sub>2</sub> and compared to an existing EOS. Section IV develops an expression for entropy using results from the previous two sections. Conclusions are given in Sec. V.

## II. Thermal EOS

First principles facilitate the first part of the derivation of the EOS used here. The EOS takes the form  $\rho = f(p, T)$ . The total differential of density can be written<sup>10</sup> as

$$d\rho = \left. \frac{\partial \rho}{\partial T} \right|_p dT + \left. \frac{\partial \rho}{\partial p} \right|_T dp \quad (1)$$

This equation can be simplified by noting that  $\beta$  and  $\alpha$  are defined, respectively, as<sup>10</sup>

$$\beta := \rho \left. \frac{\partial \rho}{\partial p} \right|_T, \quad \alpha := -\frac{1}{\rho} \left. \frac{\partial \rho}{\partial T} \right|_p$$

Substituting these definitions into Eq. (1) and integrating from  $(\bar{p}, \bar{p}, \bar{T})$  to  $(\rho, p, T)$  yields

$$\ell n(\rho/\bar{\rho}) = (1/\beta)(p - \bar{p}) - \alpha(T - \bar{T})$$

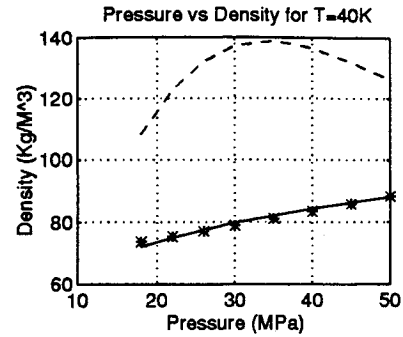


Fig. 1 Comparison of CRC EOS and the new EOS to data. —, CRC data; ---, CRC equations; and \*\*\*, new EOS.

where  $\bar{\rho}$ ,  $\bar{p}$ , and  $\bar{T}$  are reference values. Isolating density in this expression yields

$$\rho = \kappa \exp[(p/\beta) - \alpha T] \quad (2)$$

where the reference values have been collected into the constant term  $\kappa = \exp[-(\bar{p}/\beta) + \alpha \bar{T}]$ .

Constant bulk modulus and cubic expansion coefficients have been assumed in the integration step. In general, these properties are functions of pressure and temperature. If appropriately sized operating ranges are used, then constant bulk modulus and cubic expansion coefficients can safely be assumed. The better fit to the data of the new EOS over the CRC equation (shown in Fig. 1), demonstrates the validity of this assumption. Empirical data and normalized gradient optimization methods<sup>11</sup> are used to identify the various parameters and reference values.

## III. Caloric EOS

Recall that for a perfect gas the caloric EOS is the well-known thermodynamic equation relating the internal energy and temperature. This equation is thermodynamically consistent with the ideal gas law, meaning that the two equations satisfy the reciprocity condition.<sup>10</sup> As Eq. (2) can easily be shown to be inconsistent with the calorically perfect EOS, a new caloric EOS is now derived using the reciprocity condition in conjunction with Eq. (2) and CRC table data<sup>9</sup> to curve fit a function of integration specifically for LH<sub>2</sub>. Applying the reciprocity condition

$$\left. \frac{\partial e}{\partial p} \right|_T = \frac{p}{\rho^2} - \frac{T}{\rho^2} \left. \frac{\partial p}{\partial T} \right|_\rho$$

to Eq. (2) gives

$$\left. \frac{\partial e}{\partial p} \right|_T = \frac{1}{\rho^2} \beta \ell n \frac{\rho}{\kappa}$$

Integration yields

$$e = -(\beta/p)[\ell n(\rho/\kappa) + 1] + f(T) \quad (3)$$

where  $f(T)$  is a function of integration to be determined. Observing that

$$f(T) = e + (\beta/p)[\ell n(\rho/\kappa) + 1]$$

$f(T)$  can be found by plotting the left-hand side using CRC table data for  $e$  and Eq. (2) in the pressure and temperature ranges of interest and then finding a functional relation to fit the curve. As can be seen in Fig. 2a, the resulting family of curves consisting of isobars of  $f(T)$  plotted against temperature reveal that the function of integration appears essentially exponential in  $T$  and fairly constant, especially towards the higher pressures. However, rather than assume a particular

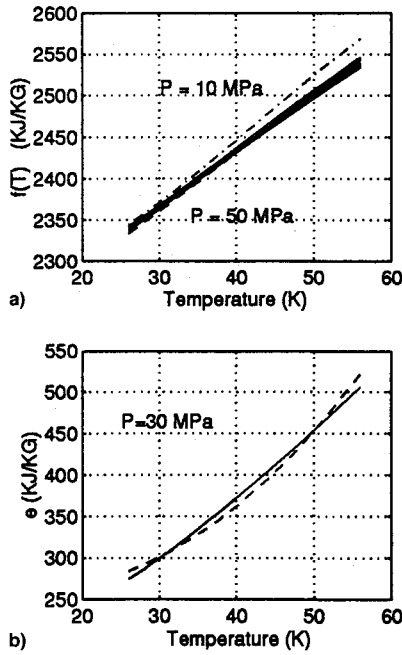


Fig. 2 a) Function of integration  $f(T)$  for various pressures; dashed lines represent upper and lower isobars and b) comparison of caloric EOS (---) and CRC data (—).

function for  $f(T)$  and attempt to fit it to the available data,  $f(T)$  is left as is for now. Realizing that the caloric EOS figures in the derivation of entropy, it is beneficial to carry  $f(T)$  through in the hope that a form congruous for both caloric and entropy EOSs can be specified in the end.

#### IV. Entropy Equation

An expression for entropy can now be derived using the thermal and caloric EOS. Starting with the first law of thermodynamics in terms of state variables

$$T ds = de + p d\nu \quad (4)$$

the idea is to then obtain expressions for  $de$  and  $d\nu$  in terms of  $p$  and  $T$ . First differentiating the thermal EOS gives

$$d\nu = \left. \frac{\partial \nu}{\partial p} \right|_T dp + \left. \frac{\partial \nu}{\partial T} \right|_p dT \quad (5)$$

where  $\nu = 1/\rho = 1/\kappa \exp[-(p/\beta) + \alpha T]$ , from where the partial derivatives of  $\nu$  are given by

$$\begin{aligned} \left. \frac{\partial \nu}{\partial p} \right|_T &= -\frac{1}{\beta\kappa} \exp\left(-\frac{p}{\beta} + \alpha T\right) \\ \left. \frac{\partial \nu}{\partial T} \right|_p &= \frac{\alpha}{\kappa} \exp\left(-\frac{p}{\beta} + \alpha T\right) \end{aligned} \quad (6)$$

Inserting Eqs. (6) into Eq. (5)

$$d\nu = \frac{1}{\kappa} \exp\left(-\frac{p}{\beta} + \alpha T\right) \left(-\frac{dp}{\beta} + \alpha dT\right) \quad (7)$$

gives an expression for  $d\nu$  in terms of  $T$  and  $p$ , as desired. Similarly, the caloric EOS is differentiated with respect to  $p$  and  $T$  and the resulting expressions are substituted in for  $de$  to yield

$$\begin{aligned} de &= (1/\kappa) \exp[-(p/\beta) + \alpha T] [(p/\beta) - \alpha T] dp \\ &+ \{(1/\kappa) \exp[-(p/\beta) + \alpha T] (-\alpha p + \beta \alpha^2 T) + f'(T)\} dT \end{aligned} \quad (8)$$

Now, substituting Eqs. (8) and (7) in the first law equation [Eq. (4)] and simplifying yields the following expression for  $ds$ :

$$\begin{aligned} ds &= -(\alpha/\kappa) \exp[-(p/\beta) + \alpha T] dp \\ &+ \{(\beta \alpha^2/\kappa) \exp[-(p/\beta) + \alpha T] + [f'(T)/T]\} dT \end{aligned} \quad (9)$$

Since  $s$  is a state variable, its derivative can be written as a function of  $T$  and  $p$  as was done with density in Sec. II:

$$ds = \left. \frac{\partial s}{\partial p} \right|_T dp + \left. \frac{\partial s}{\partial T} \right|_p dT \quad (10)$$

Equations (9) and (10) imply

$$\begin{aligned} \left. \frac{\partial s}{\partial p} \right|_T &= -\frac{\alpha}{\kappa} \exp[-(p/\beta) + \alpha T] \\ \left. \frac{\partial s}{\partial T} \right|_p &= \frac{\beta \alpha^2}{\kappa} \exp[-(p/\beta) + \alpha T] + \frac{f'(T)}{T} \end{aligned} \quad (11)$$

Integrating the two partials in Eqs. (11) over  $p$  and  $T$ , respectively, one obtains

$$s = (\alpha\beta/\kappa) \exp[-(p/\beta) + \alpha T] + g(T) \quad (12)$$

$$s = \frac{\alpha\beta}{\kappa} \exp[-(p/\beta) + \alpha T] + \int \frac{f'(T)}{T} dT + h(p)$$

Matching the functions of integration,  $g(T)$  and  $h(p)$ , in Eqs. (12) yields the following equation for entropy:

$$s = \frac{\alpha\beta}{\kappa} \exp[-(p/\beta) + \alpha T] + \int \frac{f'(T)}{T} dT \quad (13)$$

The integral expression on the right-hand side (RHS) of Eq. (13) remains the last hurdle to clear. The ability to express, in closed form, the other state variables, pressure and temperature, as functions of entropy is desired. Pressure can be isolated regardless of the choice of  $f(T)$ . Care must be taken, however, when considering temperature. Recall that Fig. 2a depicted  $f(T)$  as exponential in form. Note also that  $\alpha T$  appears in the exponent of the first term of the RHS of Eq. (13). A similar  $\alpha T$  term should appear as a factor in the integral term to be able to isolate  $T$ . To that end, let

$$f(T) = \gamma_1 e^{\alpha T} [T - (1/\alpha)] + \gamma_2 \quad (14)$$

where  $\gamma_1$  and  $\gamma_2$  afford two degrees of freedom. After taking the derivative of Eq. (14), dividing by  $T$ , and integrating and inserting the result into the second term of Eq. (13), the final form for entropy becomes

$$s = (\alpha\beta/\kappa) \exp[-(p/\beta) + \alpha T] + \gamma_1 e^{\alpha T} \quad (15)$$

Now that the function of integration needed for the caloric EOS has a definite form given by Eq. (14), it may be substituted into Eq. (3) to yield the complete form for the caloric EOS

$$e = -(\beta/\rho) [\ell n(\rho/\kappa) + 1] + \gamma_1 e^{\alpha T} [T - (1/\alpha)] + \gamma_2 \quad (16)$$

As with  $\alpha$ ,  $\beta$ , and  $\kappa$ , the  $\gamma$  parameters are fitted to NBS LH<sub>2</sub> data. Figure 2b compares the caloric EOS to the CRC data.

#### V. Conclusions

Novel thermal and caloric EOS are derived using a first principles approach. The equations are quite general in that no

assumptions regarding the type of liquid are made initially. Of particular importance is the fact that the EOS are thermodynamically significant in the sense that they satisfy the condition of reciprocity. Moreover, an expression for entropy is developed using the first law of thermodynamics in conjunction with the two EOS.

First principle considerations equip the new EOSs with physically significant parameters. Curve-fitting techniques then identify the parameters to fit the EOSs to available thermodynamic data. The parameters in the EOS were fitted to NBS  $\text{LH}_2$  data in the range of interest with good results.

The EOS lend themselves quite well to a set of CME equations as they provide the necessary thermodynamic information to complete the system of equations. Particularly, the thermal, caloric, and entropy EOS for  $\text{LH}_2$  figure in the CME equations used for rocket system propulsion modeling in other work done by the authors.<sup>1,5</sup>

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