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Calculation of propellant gas pressure by simple extended corresponding state principle

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Abstract

The virial equation can well describe gas state at high temperature and pressure, but the difficulties in virial coefficient calculation limit the use of virial equation. Simple extended corresponding state principle (SE-CSP) is introduced in virial equation. Based on a corresponding state equation, including three characteristic parameters, an extended parameter is introduced to describe the second virial coefficient expressions of main products of propellant gas. The modified SE-CSP second virial coefficient expression was extrapolated based on the virial coefficients experimental temperature, and the second virial coefficients obtained are in good agreement with the experimental data at a low temperature and the theoretical values at high temperature. The maximum pressure in the closed bomb test was calculated with modified SE-CSP virial coefficient expressions with the calculated error of less than 2%, and the error was smaller than the result calculated with the reported values under the same calculation conditions. The modified SE-CSP virial coefficient expression provides a convenient and efficient method for practical virial coefficient calculation without resorting to complicated molecular model design and integral calculation.

Keywords: Virial coefficient; Simple extended corresponding state principle; High temperature; Pressure; Propellant gas

1. Introduction

The equation of state is a basic equation of interior ballistics, and the accuracy of the equation has an effect on the veracity of ballistic calculation results [1]. The Nobel–Abel equation, truncated virial equation and Haar–Shenker equation have been applied successively to describe the propellant gas at high temperature and pressure [2–4]. Among those equations, the virial equation is more satisfactory in describing the state of propellant gas at high temperature and pressure. But the difficulty in acquiring the virial coefficient value greatly restrains the application of the virial equation. Various methods have been used to calculate the virial coefficients to obtain the empirical or semi-empirical equations of state, such as statistic mechanics and molecular model, intermolecular interaction, equation of state for elementary gas, reciprocal space computation, neural network prediction, and other ways [4–11], whereas the difficulty in calculating the virial coefficients still exists especially in integration.

Corresponding state principle (CSP) is widely used in engineering design and fluid characteristics prediction. Different pure gases have a common feature, which is that their compressibility factors are nearly the same when they reach their critical points. For this common feature, when the critical pressure and the critical temperature of a gas are known, the *P-V-T* characteristics of this pure gas could be calculated approximately without the complex integral calculation of virial coefficient. But the error due to the approximate calculation will accumulate with the increase in temperature and pressure. The accumulated error should not be neglected in predicting the virial coefficients of gas at high temperature and pressure. Therefore, the virial coefficients calculated by the approximation way could not be used in calculating the propellant gas at high temperature and pressure directly. Based on CSP, the main work of this paper is to introduce an extended corresponding state amendment to the virial coefficient expressions of the main components in propellant gas, which makes simple extended corresponding state principle (SE-CSP) available to describe the state of propellant gas at high temperature and pressure.

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2. Calculation principle of virial coefficients

2.1. Virial equation

The virial equation was proposed by Kammerlingh-Onnes in 1901, which could be described by the reciprocal of volume power as

$$Z = 1 + B/V_m + C/V_m^2 + \dots \tag{1}$$

where Z is compressive factor; B and C are the second and the third virial coefficients, respectively, which only depend on temperature.

Generally, the accuracy of Z calculation with the first three terms in Eq. (1) is sufficient [12].

The propellant gas is a mixture of several elementary gases. The second and the third virial coefficients of the elementary main component gases computed by using the Kay rule meet the requirement of engineering calculation accuracy.

$$B = \sum_{i=1}^{n} n_i B_i \tag{2}$$

$$C = \sum_{i=1}^{n} n_i C_i \tag{3}$$

2.2. Simple extended corresponding state principle (SE-CSP)

In CSP, if different substances have the same relative pressure P_r (the ratio of pressure P and critical pressure P_c) and the same relative temperature T_r (the ratio of temperature T and critical temperature T_c), they are in a corresponding state, and their physical properties have the simple corresponding relationships.

Since this relationship with two parameters is only appropriate for simple molecules, Pitzer et al. [13] and Xiang [14] introduced acentric factor ω and empirical parameter θ successively to amend the critical comparison factor Z_c, with $\theta = (Z_c - 0.291)^2$. The amendments make CSP fit for describing various properties of all kinds of molecule [13,14].

After introducing parameters ω and θ, CSP becomes SE-CSP, which could be expressed as

$$\begin{aligned} B_r &= BP_c / RT_c \\ &= B_r^{(0)}(T_r) + \omega B_r^{(1)}(T_r) + \theta B_r^{(2)}(T_r) \\ C_r &= CP_c^2 / (RT_c)^2 \\ &= C_r^{(0)}(T_r) + \omega C_r^{(1)}(T_r) + \theta C_r^{(2)}(T_r) \end{aligned} \tag{4}$$

2.3. Calculation of virial coefficients for propellant gas

The modified expressions for $B_r^{(0)}(T_r)$ and $Br^{(1)}(T_r)$ in Eq. (4) are shown in Ref. [15]

$$\begin{aligned} B_r^{(0)}(T_r) &= 0.13356 - 0.30252/T_r - 0.15668/T_r^{2.0} \\ &\quad - 0.00724/T_r^{3.0} - 0.00022/T_r^{8.0} \\ B_r^{(1)}(T_r) &= 0.17404 - 0.15581/T_r + 0.38183/T_r^{2.0} \\ &\quad - 0.44044/T_r^{3.0} - 0.00541/T_r^{8.0} \end{aligned} \tag{5}$$

Some studies have shown that the estimate accuracy of B in Eq. (4) is satisfactory for $T_r < 0.75$, whereas the estimate accuracy becomes more and more weak with the increase in T_r. The temperature range of propellant gas greatly exceeds $T_r = 0.75$. Therefore, SE-CSP like Eq. (4) should be revised before it is used to calculate the virial coefficients of propellant gas.

The main components of propellant gas are N_2, H_2, CO, H_2O and CO_2. Due to the good agreement between experimental data [16] and the calculated data by the second virial coefficient equation of CO_2 proposed in Ref. [17] and the precise second virial coefficient equation of H_2O proposed in Ref. [18], only the amended expressions for CO, H_2 and N_2 are required by fitting their experimental data [16]. The expressions obtained are

$$\begin{aligned} B_r^{(2)}(T_r) &= -30\theta T_r^{1.2} \\ B_r^{(2)}(T_r) &= -3\theta T_r^{0.78} \\ B_r^{(2)}(T_r) &= -708\theta T_r^{1.03} \end{aligned} \tag{6}$$

3. Applied results and analysis

The second virial coefficients of CO, H_2 and N_2 calculated by the revised SE-CSP expression were compared with their experimental data and other calculated values from different theories. The comparative results are shown in Figs. 1–3, respectively. It can be seen obviously that the values calculated by the revised SE-CSP expression have satisfactory accuracy and are in good agreement with the experimental data [16] at low temperature, and also agree well with the calculated values in Ref. [5,6] at high temperature.

When the virial coefficients of propellant gas at high temperature and pressure are calculated, the second virial coefficients of CO, H_2 and N_2 can be obtained by Eqs. (4) ~ (6); the second virial coefficients of H_2O and CO_2 can be obtained by Eq. (7) [17] and Eq. (8) [18]; the third virial coefficients of the five elementary gases can be obtained by Eqs. (9) ~ (10) and Table 1 [19].

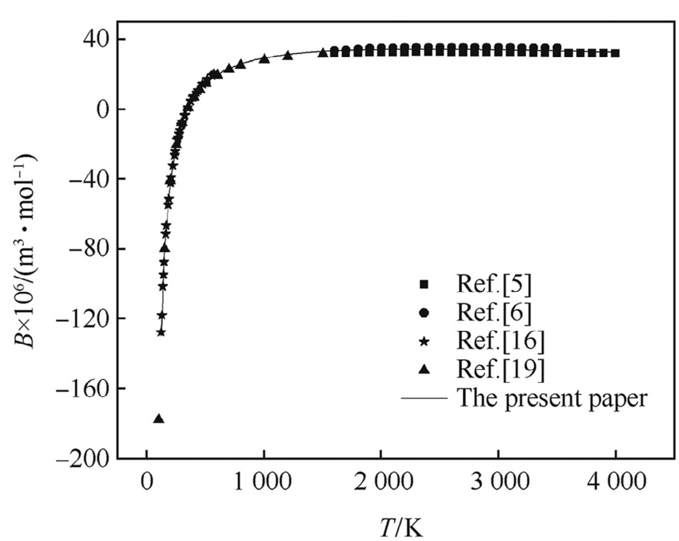

Fig. 1. The second virial coefficients of CO.