

A SIMPLE MODEL OF A THERMALLY PERFECT, CALORICALLY IMPERFECT DIATOMIC GAS. COMPARISON WITH REAL GASES

1. NOTATION AND UNITS

		SI	British
c_p	specific heat capacity at constant pressure	J/kg K	ft lbf/slug K
$(c_p)_0$	value of c_p for calorically perfect diatomic gas, equal to $3.5R$	J/kg K	ft lbf/slug K
i	specific enthalpy	J/kg	ft lbf/slug
i_0	value of i for calorically perfect diatomic gas	J/kg	ft lbf/slug
R	gas constant	J/kg K	ft lbf/slug K
T	temperature	K	K
γ	ratio of specific heat capacity at constant pressure to specific heat capacity at constant volume		
γ_0	value of γ for calorically perfect diatomic gas, equal to 1.4		
θ	characteristic vibrational temperature	K	K

2. NOTES

This Item presents charts giving values of γ , c_p/R and i/R calculated from a simplified model of the diatomic molecule and compares these with experimental data from Derivation 2 for undissociated nitrogen, oxygen and carbon monoxide and for air in dissociation equilibrium.

The assumption that the diatomic molecule behaves like a simple harmonic vibrator¹ yields the following analytical expressions:

$$\gamma = 1 + \frac{\gamma_0 - 1}{1 + (\gamma_0 - 1) \left(\frac{\theta}{T} \right)^2 \frac{e^{\theta/T}}{(e^{\theta/T} - 1)^2}}, \quad (2.1)$$

$$c_p = (c_p)_0 \left\{ 1 + \frac{\gamma_0 - 1}{\gamma_0} \left(\frac{\theta}{T} \right)^2 \frac{e^{\theta/T}}{(e^{\theta/T} - 1)^2} \right\} \quad (2.2)$$

$$\text{and} \quad \frac{i}{R} = \int_0^T c_p dT = T \left\{ \frac{(c_p)_0}{R} + \left(\frac{\theta}{T} \right) \frac{1}{(e^{\theta/T} - 1)} \right\}. \quad (2.3)$$

These expressions are plotted in Figures 1 to 3; the experimental data are shown by broken lines. The effect of varying the pressure is shown in detail for air in Figures 1 and 2 over the pressure range 0.01 to 1 atmosphere.

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The pressure relating to the curves shown for the other gases is 1 atmosphere. However, for these gases decreasing the pressure to 0.01 atmosphere results in insignificant changes in the properties presented. The effect of pressure variation over the range 0.01 to 1 atmosphere on the experimental value of i/R is negligible for the gases shown in Figure 3.

It can be seen that the analytical expressions are a good representation of the influence of caloric imperfections of diatomic gases over quite a wide temperature range. This range is bounded at lower temperatures by the approach of liquefaction and at higher temperatures by regions where anharmonicity effects become important or when dissociation is approached.

The values of θ and R for each gas are shown in Table 2.1. The values of θ are approximate and over small temperature ranges it is possible to choose a more appropriate value.

TABLE 2.1

Gas	θ K	R J/kg K	R ft lbf/slug K
Air	3050	287.1	3090
Nitrogen	3250	296.8	3194
Oxygen	2150	259.9	2797
Carbon Monoxide	3050	296.9	3195

3. DERIVATION

- EGGERS, A.J. One-dimensional flows of an imperfect diatomic gas. NACA Rep. 959, 1948.
- HISSENATH, J. *et al.* *Tables of thermodynamic and transport properties.* Pergamon Press, 1960. (Originally published as National Bureau of Standards Circular 564, 1955.).