

# Influence of Pressure Derivative of Partition Function on the Isentropic Coefficient and Sound Speed for NLTE Hydrogen Plasma

Gurpreet Singh

Department of Physics, DAV College Bathinda.  
e-mail: gurpreet.dav@gmail.com

**Abstract**—There has been a continued interest in computation of thermodynamic properties of plasmas, where the contribution of partition function and electronic excitation is of great significance. The computation of isentropic coefficient and sound speed with the help of a computer program has been performed using non- local thermodynamic equilibrium (NLTE) hydrogen thermal plasma for different values of pressure and non-equilibrium parameter  $\theta (= T_e / T_h)$  in the temperature range from 6000 K to 60000 K. In order to estimate the influence of pressure derivative of partition function on Isentropic Coefficient ( $\gamma_{isen}$ ) and Sound Speed ( $C_s$ ), two cases have been considered: (a) in which pressure derivative of partition function is taken into account in the expressions with symbol  $A$  and (b) without pressure derivative of partition function in their expressions. The isentropic coefficient with and without the inclusion of pressure derivative of partition function as a function of degree of ionization shows that its values decrease with an increase of  $\theta$  with  $\gamma_{isen}(A=0) > \gamma_{isen}(A)$ . It is also found that with an increase of  $\theta$ , sound speed  $C_s(A=0) > C_s(A)$ .

**Keywords**— Thermal Plasmas, non-equilibrium parameter, local thermodynamic equilibrium, partition function, degree of ionization

## I. INTRODUCTION

The design of heat shield and entry and re-entry of space vehicle, shock waves require accurate thermodynamic properties of high temperature high pressure [1-6]. The variations of partition function of constituent species with temperature and pressure [7-13] on the thermodynamic properties of thermal plasmas has been studied extensively

and are already available in literature. These properties are influenced by taking into account only the temperature derivative of partition function. Moreover, the expressions in analytic form for thermodynamic properties for thermal plasmas in the local thermodynamic equilibrium (LTE) conditions and in non-local thermodynamic equilibrium (NLTE) conditions have been developed by Capitelli and co-workers and Cardona et al by including temperature derivative of partition function.. Burm et al[12-13] have studied the effect of non-equilibrium parameter  $\theta (= T_e / T_h, T_e$  and  $T_h$  being electron and heavy particle temperatures respectively) and pressure for singly ionized plasmas with ground state partition functions whereas Capitelli and co-workers[14] have studied the role of electronically excited states (EES) in thermodynamic properties of hydrogen plasma with partition function depending upon temperature and pressure. Their expressions involve only temperature derivative of partition function (PF). Cardona et al[15] have studied the various thermodynamic properties by developing analytic expressions for LTE thermal plasma by considering ground state partition functions and have further emphasized the need of including both the temperature and pressure derivatives of PF in the appendix. This is because isentropic coefficient generates large deviation in expansion dynamics. Here, an attempt has been made to evaluate the thermodynamic properties with both temperature and pressure derivative of partition function by modifying the already available expressions and by developing a computer program. The computation of isentropic coefficient and sound speed has been performed

using non- local thermodynamic equilibrium (NLTE) hydrogen thermal plasma for different values of pressure and non-equilibrium parameter  $\theta (= T_e / T_h)$  in the temperature range from 6000 K to 60000 K. Two cases have been considered where expressions for thermodynamic properties

include (a)  $A = \frac{P}{f_H} \left( \frac{\partial f_H}{\partial P} \right)_T$ , the term containing pressure derivative of partition function  $f_H$  and (b)  $A = 0$ , when the expressions are without the pressure derivative of PF. The expressions for case (b) are already available in the literature for LTE plasmas.

## II. EEXPRESSIONS

The thermodynamic properties are evaluated by modified expressions developed[16-18] by authors and in the present work, plasma composition is obtained for species viz. electron, H,  $H^+$  by using modified Saha ionization equation of van de Sanden et al[19]. For both the LTE and NLTE thermal plasmas, the number density of each species in the mixture can be computed as a function of electron temperature  $T_e$  and non-equilibrium parameter  $\theta = T_e / T_h$  by solving the following set of equations

$$\frac{n_{H^+} n_e}{n_H} = \left( \frac{2\pi m_e k T_e}{h^2} \right)^{3/2} \frac{2}{f_H} \exp\left(-\frac{I_H}{k T_e}\right) \quad (1)$$

$$n_{H^+} = n_e \quad (2)$$

$$p = n_e k T_e + n_N k T_h \quad (3)$$

where  $n_e$ ,  $n_H$  and  $n_{H^+}$  are the number densities of electrons, H atoms and protons respectively,  $I_H$  is the ionization energy of atomic hydrogen and  $f_H$  is the electronic partition of atomic hydrogen defined by

$$f_H = \sum_{n=1}^{n_{\max}} 2n^2 e^{-\frac{E_n}{kT}}, \quad \text{where } E_n = I_H \left( 1 - \frac{1}{n^2} \right).$$

The derivative of ionization degree  $\alpha$  with temperature at constant pressure is

$$T \left( \frac{d\alpha}{dT} \right)_P = \frac{\alpha(1-\alpha)(1+\alpha\theta)}{[2+(\theta-1)\alpha]} \left( \frac{5}{2} + \frac{I_H}{kT} - \frac{T}{f_H} \frac{\partial f_H}{\partial T} \right)$$

and at constant volume is

$$T \left( \frac{d\alpha}{dT} \right)_V = \frac{\alpha(1-\alpha)(1+\alpha\theta)(1+A)^{-1}}{[2+(\theta-1)\alpha+\theta\alpha(1-\alpha)]} \left( \frac{3}{2} + \frac{I_H}{kT} - \frac{T}{f_H} \frac{\partial f_H}{\partial T} - \frac{P}{f_H} \frac{\partial f_H}{\partial P} \right)$$

$$A = \frac{P}{f_H} \left( \frac{\partial f_H}{\partial P} \right)_T = \left( \frac{\partial \ln f_H}{\partial \ln P} \right)_T$$

where

Using the analytic expression of  $\left( \frac{\partial f_H}{\partial P} \right)_T$  given by Cardona et al[20-21], the term  $A$  is given by

$$A = -\frac{1}{9f_H} \exp\left(-\frac{E_{n_{\max}}}{kT}\right) n_{\max} \left[ 3n_{\max}^2 - 2(n_{\max}^3 - 8) \frac{I_H}{n_{\max}^3 kT} \right]$$

The isentropic coefficient  $\gamma_{isen}$  for the plasma becomes

$$\gamma_{isen} = \gamma_a Z_\gamma \quad (4)$$

with compressibility coefficient  $Z_\gamma$  given by

$$Z_\gamma = \frac{\rho}{P} \left( \frac{\partial \rho}{\partial P} \right)_T^{-1} = \frac{2 + \alpha(\theta - 1)}{2 + \alpha(\theta - 1) + \alpha\theta(1 - \alpha)(1 + A)}$$

and  $\gamma_a$  is the adiabatic coefficient defined as ratio of the specific heat at constant pressure to the specific heat at constant volume.

Speed of sound  $c_s$  is given by [22]

$$c_s = \sqrt{\gamma_{isen} R(T_h + \alpha T_e)} \quad (5)$$

## III. INFLUENCE OF PRESSURE DERIVATIVE OF PARTITION FUNCTION

It is observed that  $Z_\gamma$  is a function of degree of ionization  $\alpha$ , non-equilibrium parameter  $\theta$  and the term  $A$ . As the partition function  $f_H$  decreases with increase of pressure, its pressure

derivative is negative. The equilibrium composition has been obtained by the subroutine as

```
almd (t,natm,ah,ahe,a0,a1,a2,b0,b1,c,p,rho,theta)
real t,natm,ne,ni,ih,ihe,ihep
al=1.44e-09
patm=natm*1.0139616e+06
avgdn=6.023e+23
pi=3.1415927
qe=4.8e-10
lh=13.6 and by taking concentration of electron c=.001
ass=(akk1*t/p1)**(1./3)
ns=sqrt(ass/a0)
nx0=sqrt(1*ass/a0)
nx1=sqrt(2*ass/a0)
fh=0.0
do in=1,ns
ein=13.6*(1-1./(in*in))
fh=fh+2*in*in*exp(-ein*11600/t)
enddo
```

From Figure 1, it is clear that, there is marginal change in value of  $\gamma_{isen}$  with the inclusion of pressure derivative of partition function in their expressions for NLTE hydrogen plasma. The maximum values of relative error  $RE_{TH} (TH = c_s)$  increase with  $\theta$  and occur at increasing temperatures and maximum is about 0.8% for isentropic coefficient  $\gamma_{isen}$  and about 0.4% for speed of sound  $c_s$  (Figure 2) and is almost independent of value of  $\theta$ . From the calculations, it is found that although there are significant deviations in  $Z_\gamma$ ,  $c_v$  and  $\gamma_a$  but has a little effect on  $\gamma_{isen}$  as well as  $RE_{TH}$  even at high pressures and high  $\theta$  with the inclusion of pressure derivative of partition function. This is due to the fact that both the values of  $Z_\gamma$  and  $c_v$  change almost equally and thus compensation occurs for  $\gamma_{isen}$  as well as  $c_s$ .

Here, the influence of pressure derivative of partition function is to make  $\gamma_{isen}(A)$  and  $c_s(A)$  slightly less than corresponding values for  $A=0$ .

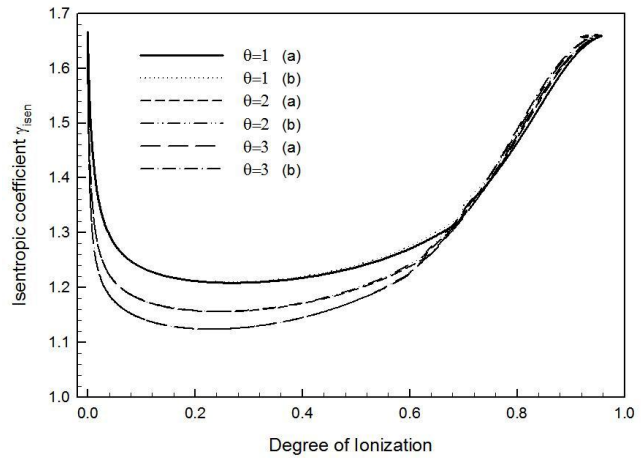


FIG 1: Variation of isentropic coefficient  $\gamma_{isen}$  with degree of ionization  $\alpha$  at atmospheric pressure for different values of the non-equilibrium

parameter  $\theta$  for (a)  $A = f_H \left( \frac{\partial f_H}{\partial P} \right)_T$  and (b)  $A=0$  in NLTE hydrogen plasma.

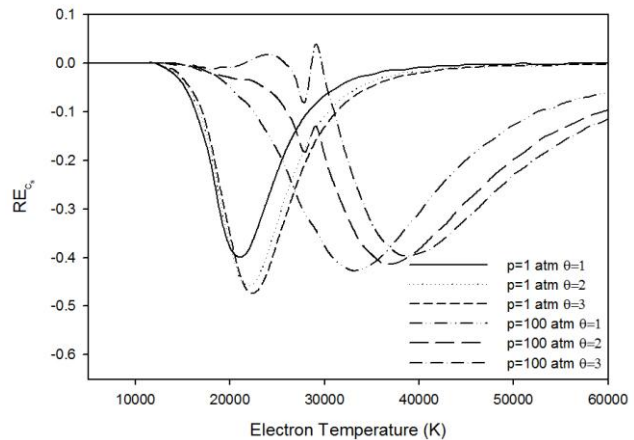


Fig 2: Variation of  $RE_T = [T(A) - T(A = 0)] \times 100 / T(A = 0)$  with electron temperature at different pressures for different values of the non-equilibrium parameter  $\theta$  in NLTE hydrogen plasma, where  $T$  is sound speed  $c_s$ .

## IV. RESULTS AND DISCUSSION

The computation of isentropic coefficient and sound speed with the help of a computer program has been performed using non- local thermodynamic equilibrium (NLTE) hydrogen thermal plasma for different values of pressure and non-equilibrium parameter  $\theta (= T_e / T_h)$  in the temperature range from 6000 K to 60000 K. The isentropic coefficient with and without the inclusion of pressure dependent partition function as a function of degree of ionization is illustrated such that its values decrease with an increase of  $\theta$  with  $\gamma_{isen}(A=0) > \gamma_{isen}(A)$ . This shows that the term  $A$  has marginal influence on  $\gamma_{isen}$  and  $c_s$ , at all pressures which may be attributed to fact that compensation takes place for  $\gamma_{isen}$  as  $Z_\gamma$  in the numerator and  $C_v$  in the denominator of equation(4) are affected similarly in going from the case (b) to the case(a). Thus, both the values of  $Z_\gamma$  and  $c_v$  change correspondingly and compensate each other for  $\gamma_{isen}$  as well as  $C_s$ .

## REFERENCES

- [1] D. G. Fletcher, Lecture Series on Critical Technologies for Hypersonic Vehicle Development, RTO-EN-AVT-116 (2004).
- [2] M. Capitelli, D. Bruno, G. Colonna, G. D'Ammando, A. D'Angola, D. Giordano, C. Gorse, A. Laricchiuta, S. Longo, Thermodynamic properties of gases behind shock waves. *Shock Wave Science and Technology bvReference Library* Vol 7, 11-58 (2012).
- [3] M. Capitelli, G. Colonna, D. Giordano and L. Marraffa, A. Casavola, P. Minelli, D. Pagano, L. Pietanza, and F. Taccogna, *J. Spacecraft and Rockets* **42**, 980 (2005).
- [4] J. D. Anderson, *Hypersonic and High Temperature Gas Dynamics* (AIAA, 2000).
- [5] A. B. Murphy and E. Tam, *J. Phys. D: Appl. Phys.* **47**, 295202 (2014).
- [6] J. P. Trelles, C. Chazelas, A. Vardelle and J. V. R. Heberlein, *J. Thermal Spray Technology* **18**, 728 (2009).
- [7] M. Capitelli, D. Bruno and G. Colonna, C. Catalfamo and A. Laricchiuta, *J. Phys. D: Appl. Phys.* **42**, 194005 (2009).
- [8] D. Pagano, A. Casavola, L.D.Pietanza, M. Capitelli, G. Colonna, D. Giordano, L. Marraffa, ESA Scientific Technical Review, vol. **257** (2009).
- [9] F De Palma, A R Casavola and M. Capitelli, *J. Thermophys. Heat Transfer* **20**, 921 (2006).
- [10] K. C. Meher, N. Tiwari and S. Ghorui, *Plasma Chem. Plasma Process.* **35**, 605(2015).
- [11] M. Capitelli, G. Colonna, and A. D'Angola, *Fundamental Aspects of Plasma Chemical Physics: Thermodynamics* (Springer, New York, 2012), Vol. **66**.
- [12] K. T. A. L. Burm, W.J. Goedheer and D.C. Schram, *J. Appl. Phys.* **90**, 2162 (2001).
- [13] K. T. A. L. Burm, W.J. Goedheer and D.C. Schram, *Phys. Lett. A* **294**, 47(2002).
- [14] F De Palma, A R Casavola and M. Capitelli, *J. Thermophys. Heat Transfer* **20**, 921 (2006).
- [15] O. Cardona, E. Simonneau, and L. Crivellari, *Astrophys. J.* **695**, 855 (2009).
- [16] R. Sharma, G. Singh, and K. Singh, *Phys. Plasmas* **18**, 083510 (2011).
- [17] Singh, G., Sharma, R., and Singh, K. (2008). Effect of excited states on higher-order contributions to electron transport in hydrogen thermal plasmas. *J. Phys. D: Appl. Phys.* **41**: 225203-7.
- [18] Singh, G., Sharma, R., and Singh, K. (2015) Influence of pressure derivative of partition function on thermodynamic properties of non-local thermodynamic equilibrium thermal plasma, *Phys Plasmas* **22**, 093516.
- [19] M. C. M. van de Sanden, P. P. J. M. Schram, A. G. Peeters, J. A. M. van de Mullen, and G. M. W. Kroesen, *Phys. Rev. A* **40**, 5273 (1989).
- [20] O. Cardona, E. Simonneau, and L. Crivellari, *Rev. Mex. Fis.* **51**, 476 (2005).
- [21] O. Cardona, M. Mart'inez-Arroyo, and M. A. L'opez-Castillo, *Astrophys. J.* **711**, 239(2010).
- [22] K. T. A. L. Burm, W.J. Goedheer and D.C. Schram, *Phys. Plasmas* **6**, 2628 (1999).