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A Study on the Prediction of Hydrogen Vehicle by the Thermodynamic Properties

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Abstract

Hydrogen has long been recognized as a fuel having some unique and highly desirable properties, for application as a fuel in engines. Hydrogen has some remarkably high values of the key properties for transport processes, such as kinematic viscosity, thermal conductivity and diffusion coefficient, in comparison to those of the other fuels. Such differences together with its extremely low density and low luminosity help to give hydrogen its unique diffusive and heat transfer characteristics. The thermodynamic and heat transfer characteristics of hydrogen tend to produce high compression temperatures that contribute to improvements in engine efficiency and lean mixture operation.

Key words : Hydrogen, thermodynamic properties, unburned mixture, relative air-fuel ratio, specific heat at constant pressure, specific heat at constant volume

1. Introduction

Hydrogen gas has been in wide use as a fuel for quite a long time. Additionally, enormous quantities of hydrogen are used increasingly as a raw material in a wide range of applications in the chemical industry, particularly in the upgrading of conventional fuel resources [1,2].

Hydrogen as a renewable fuel resource can be produced through the expenditure of energy to replace increasingly the depleting sources of conventional fossil fuels. Accordingly, research into all aspects of hydrogen technology, especially in recent years has been truly massive and diversified. A concise statement and discussion of the positive features of hydrogen as a fuel and the associated limitations that are impeding its wide application as an engine fuel are both necessary and needed [3,4].

Hydrogen is the only fuel that can be produced entirely from the plentiful renewable resource through the expenditure of relatively much energy. Its combustion in oxygen produces uniquely only water but in air it also produces some oxides of nitrogen. These features make hydrogen an excellent fuel to potentially meet the ever increasingly stringent environmental controls of exhaust emissions from combustion devices, including the reduction of green house gas emissions [5-7].

The viability of hydrogen as a fuel in general and in engine applications in particular, is critically dependent on the effective, economic and satisfactory solution of a number of remaining key limiting problems.

Hydrogen has some remarkably high values of the key properties for transport processes, such as kinematic viscosity, thermal conductivity and diffusion coefficient, in comparison to those of the other two fuels. Such differences together with its extremely

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low density and low luminosity help to give hydrogen its unique diffusive and heat transfer characteristics. The thermodynamic and heat transfer characteristics of hydrogen tend to produce high compression temperatures that contribute to improvements in engine efficiency and lean mixture operation.

2. Thermodynamic properties

Some of the key overall properties of hydrogen that are relevant to its employment as an engine fuel are listed in Table 1.

Hydrogen has some remarkably high values of the key properties for transport processes, such as kinematic viscosity, thermal conductivity and diffusion coefficient. The chemical kinetics of the combustion of hydrogen in air are well understood at present and its oxidation reaction rates and the associated temporal variation of the concentrations of the reactive species can be predicted well. Mainly relatively fast and nearly thermally neutral branching chain reactions are involved. Hydrocarbon fuels oxidation on the other hand, involves normally thermally significant chain reactions that contain relatively slower endothermic reaction steps that are associated with fuel breakdown. These differences together with those in the thermodynamic and transport properties of hydrogen, contribute in a big way to the substantially different combustion characteristics of hydrogen from those of other common fuels.

The use of hydrogen as an engine fuel has been attempted on very limited basis with varying degrees of success by numerous investigators over many decades, and much information about their findings is available in the open literature. However, these reported performance data do not necessarily display consistent agreement between various investigators.

There is also a tendency to focus on results obtained in specific engines and over narrowly changed operating conditions.

3. Hydrogen fueled engine applications

Moreover, the increasingly greater emphasis being placed on the nature of emissions and efficiency considerations often renders much of the very early work fragmentary and mainly of historical value.

For a thermodynamics cycle such as this, the thermal efficiency is

$$\eta = \frac{W_{out}}{Q_{in}} = 1 - \frac{Q_{out}}{Q_{in}} = 1 - \frac{1}{\gamma^{k-1}}$$

Table 1. Thermodynamic properties of gaseous hydrogen versus dry air at 0℃ and 1 atm [1].

Property	Unit	Hydrogen	Dry air
Molecular weight	kg/kmol	2.016	28.964
Gas constant	kJ/kgK	4.125	0.287
Diffusion coefficient in air	cm2/s	0.611	-
Density	kg/m3	0.083	1.293
Specific heat at con. pressure	kJ/kgK	14.420	1.004
Specific heat at con. volume	kJ/kgK	10.234	0.716
Specific heat ratio	-	1.409	1.4000
Viscosity	Pa s	8.34	17.11
Boiling point	℃	-252.8	99.2
Thermal conductivity	W/mK	0.175	0.024

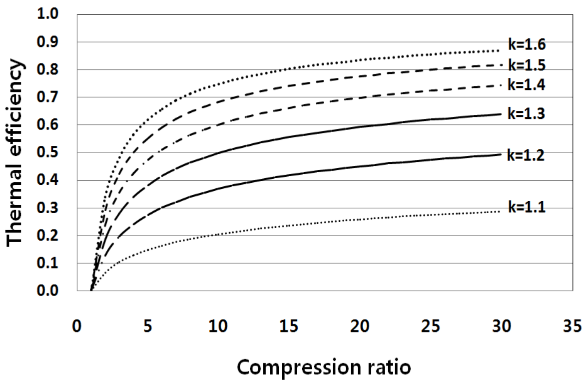

Fig. 1. Thermal efficiency vs. compression ratio with various specific heat ratios.

where

Q_{out}= heat rejection

Q_{in} = heat addition

W_{out}= work rejection

γ = compression ratio

k = ratio of specific heats

The efficiency of the Otto cycle depends on the specific heat ratio and on the compression ratio. A plot of efficiency over the same range of compression ratios found in ideal engines is shown in Fig. 1. The value of the thermal efficiency of the Otto cycle depends on the compression ratio and not the temperature in the cycle. To make a comparison with a real engine, only the compression ratio needs to be specified. And we need to select the bigger ratio of specific heats to increase the thermal efficiency.

4. Thermodynamic properties for mixtures

When a chemical reaction occurs, the bonds within molecules of the reactants are broken, and atoms and electrons rearrange to form products. In combustion reactions, rapid oxidation of combustible elements of the fuel results in energy release as combustion products are formed.

The balanced chemical reaction equation is

$$H_2 + 0.5\,(1+\alpha)\,O_2 + 3.76 \times 0.5\,(1+\alpha)\,N_2$$

where α is excess air factor, $(1 + \alpha) = \lambda$, and λ is relative air/fuel ratio.

In the following expression for the unburned specific heat at constant pressure is

$$C_{pu} = \sum_{i=1}^{j} f_i\, C_{pi}$$

where

f_i = mole fraction of component i

C_{pi}= specific heat at constant pressure of component i

The specific heat ratio is estimated using NASA interpolations of specific heats at constant pressure. The interpolating polynomials are given on a form

$$\frac{C_p}{R} = \alpha + \beta T^{-1} + \gamma T^{-2} + \delta T^{-3} + \epsilon T^{-4}$$

The specific heat ratio of unburned hydrogen-air mixture can then be calculated [8-11].

$$k_u = \frac{C_{pu}}{C_{pu} - R} = \frac{C_{pu}}{C_{vu}}$$

The unburned specific heat at constant volume is

$$C_{vu} = \sum_{i=1}^{j} f_i\, C_{vi}$$

where

C_{vi}= specific heat at constant volume of component i

Figure 2 shows specific heat at constant pressure of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio. The relative air-fuel ratio range (lambda, λ) is between 0.6 to 1.8. The results show that the specific heat at constant pressure decrease with increasing relative air-fuel ratio (lambda, λ)

Figure 3 shows specific heat at constant volume of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio. The lambda, λ range is between 0.6 to 1.8. The results show that the specific heat at constant volume decrease with increasing lambda, λ.

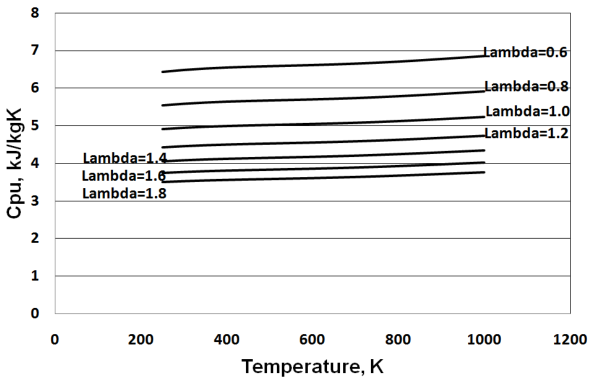

Fig. 2. Specific heat at constant pressure of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio.

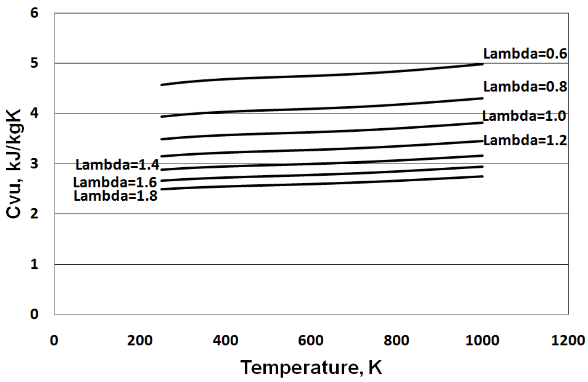

Fig. 3. Specific heat at constant volume of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio.

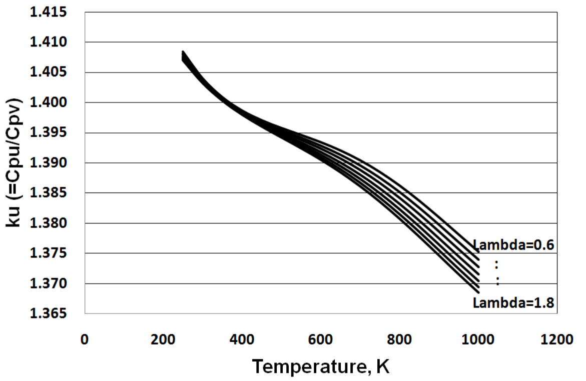

Fig. 4. Ratio of specific heat of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio.

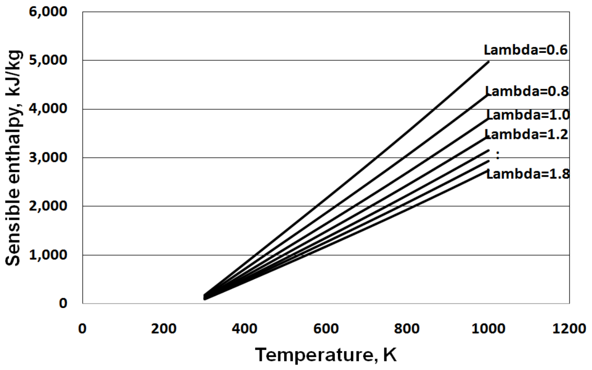

Fig. 5. Sensible enthalpy of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio.

Figure 4 shows ratio of specific heat of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio. The lambda, λ range is between 0.6 to 1.8. The results show that the ratio of specific heat decrease with increasing lambda, λ.

Then the differential changes in the sensible internal energy and sensible enthalpy of hydrogen-air mixtures can be expressed as

$$du = c_v\, dT$$

and

$$dh = c_p\, dT$$

The change in internal energy or enthalpy for an ideal gas during a process from state 1 to state 2 is determined by integrating these equations:

$$\triangle u = u_2 - u_1 = \int_1^2 c_v\, dT$$

and

$$\triangle h = h_2 - h_1 = \int_1^2 c_p\, dT$$

To carry out these integrations, we need to have relations for c_v and c_p as functions of temperature. Therefore the sensible enthalpy h_u is

$$h_u = c_{pu}\,(T - T_o)$$

and the sensible internal energy u_u is

$$u_u = c_{vu}\,(T - T_o)$$

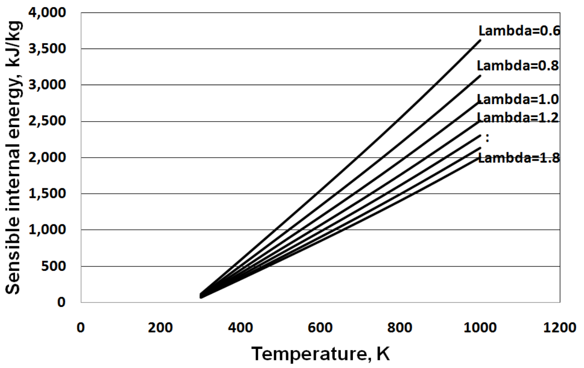

Fig. 6. Sensible internal energy of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio.

Figure 5 shows that sensible enthalpy of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio. The results show that sensible enthalpy of unburned hydrogen-air mixtures decrease with increasing lambda, λ.

Figure 6 shows that sensible internal energy of unburned hydrogen-air mixtures as a function of temperature and relative air-fuel ratio. The results show that sensible internal energy of unburned hydrogen-air mixtures decrease with increasing lambda, λ.

5. Conclusion

The value of the thermal efficiency of the Otto cycle depends on the compression ratio and not the temperature in the cycle. To make a comparison with a real engine, only the compression ratio needs to be specified. And we need to select the bigger ratio of specific heats to increase the thermal efficiency.

According to the lambda, λ range is between 0.6 to 1.8. The specific heat at constant volume and at constant pressure decrease with increasing lambda, λ and the results show that the ratio of specific heat decrease with increasing lambda, λ

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